Full wwPDB X-ray Structure Validation Report (i)

Apr 24, 2023 – 12:27 PM EDT

PDB ID	:	3GHG
Title	:	Crystal Structure of Human Fibrinogen
Authors	:	Doolittle, R.F.; Kollman, J.M.; Sawaya, M.R.; Pandi, L.; Riley, M.
Deposited on	:	2009-03-03
Resolution	:	2.90 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 (1)) were used in the production of this report:

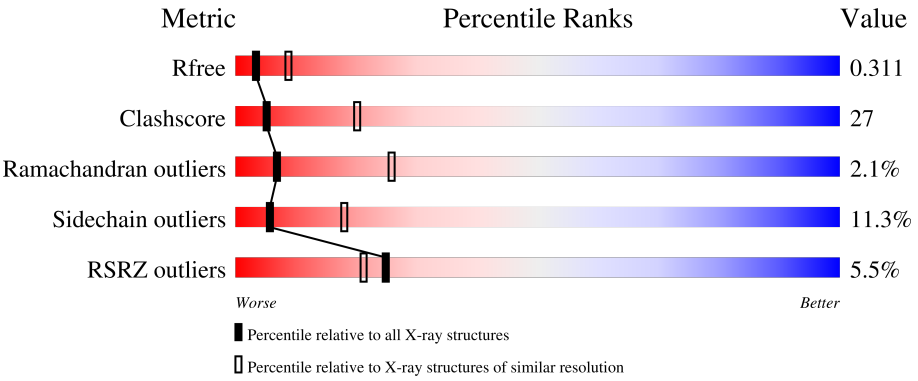
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	562	18% 12% 69%
1	D	562	6% 18% 12% 69%
1	G	562	2% 20% 10% 69%
1	J	562	4% 16% 15% 67%
2	B	461	46% 34% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	461	8% 46% 35% 6% 13%
2	H	461	3% 52% 31% 13%
2	K	461	% 50% 29% 8% 13%
3	C	411	4% 44% 43% 6% 7%
3	F	411	6% 53% 35% 5% 7%
3	I	411	5% 53% 37% 5%
3	L	411	5% 47% 41% 7% 5%
4	M	4	25% 50% 25%
4	N	4	75% 25%
4	Q	4	75% 25%
4	R	4	50% 50%
5	O	4	25% 75%
5	P	4	50% 50%
5	S	4	25% 75%
5	T	4	50% 50%
6	U	11	27% 73%
6	V	11	9% 91%
6	X	11	9% 91%
7	W	5	20% 20% 60%
8	Y	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	U	1	-	-	X	-
6	GAL	U	10	-	-	-	X
6	SIA	U	11	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	U	2	X	-	-	-
6	MAN	U	4	-	-	-	X
6	NAG	U	5	X	-	-	X
6	GAL	U	6	X	-	-	-
6	SIA	U	7	-	-	-	X
6	MAN	U	8	-	-	-	X
6	NAG	U	9	X	-	-	X
6	NAG	V	1	X	-	-	-
6	GAL	V	10	-	-	-	X
6	SIA	V	11	-	-	-	X
6	NAG	V	2	X	-	-	-
6	MAN	V	4	-	-	-	X
6	NAG	V	5	X	-	-	X
6	GAL	V	6	X	-	-	X
6	MAN	V	8	-	-	-	X
6	NAG	V	9	X	-	-	X
6	NAG	X	1	-	-	X	-
6	GAL	X	10	-	-	-	X
6	SIA	X	11	-	-	-	X
6	NAG	X	2	X	-	X	X
6	BMA	X	3	-	-	-	X
6	MAN	X	4	-	-	-	X
6	NAG	X	5	X	-	-	X
6	GAL	X	6	X	-	-	X
6	SIA	X	7	-	-	-	X
6	NAG	X	9	X	-	-	X
7	NAG	W	1	X	-	-	-
7	NAG	W	2	X	-	-	-
7	MAN	W	4	-	-	-	X
7	MAN	W	5	-	-	-	X
8	NAG	Y	1	-	-	X	X
8	NAG	Y	2	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 31833 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	D	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	G	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	J	186	Total	C	N	O	S	0	0	0
			1527	941	284	292	10			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	E	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	H	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	K	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	381	Total	C	N	O	S	0	0	0
			3050	1931	510	593	16			
3	F	382	Total	C	N	O	S	0	0	0
			3054	1933	511	594	16			
3	I	394	Total	C	N	O	S	0	0	0
			3145	1986	527	614	18			
3	L	391	Total	C	N	O	S	0	0	0
			3126	1974	524	610	18			

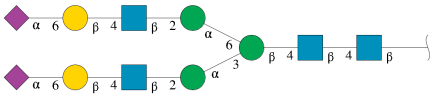
- Molecule 4 is a protein called A knob.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	M	4	Total C N O 30 18 7 5	0	0	0
4	N	4	Total C N O 30 18 7 5	0	0	0
4	Q	4	Total C N O 30 18 7 5	0	0	0
4	R	4	Total C N O 30 18 7 5	0	0	0

- Molecule 5 is a protein called B knob.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	O	4	Total C N O 33 19 9 5	0	0	0
5	P	4	Total C N O 33 19 9 5	0	0	0
5	S	4	Total C N O 33 19 9 5	0	0	0
5	T	4	Total C N O 33 19 9 5	0	0	0

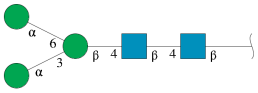
- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	U	11	Total C N O 151 84 6 61	0	0	0
6	V	11	Total C N O 151 84 6 61	0	0	0
6	X	11	Total C N O 151 84 6 61	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 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
8	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

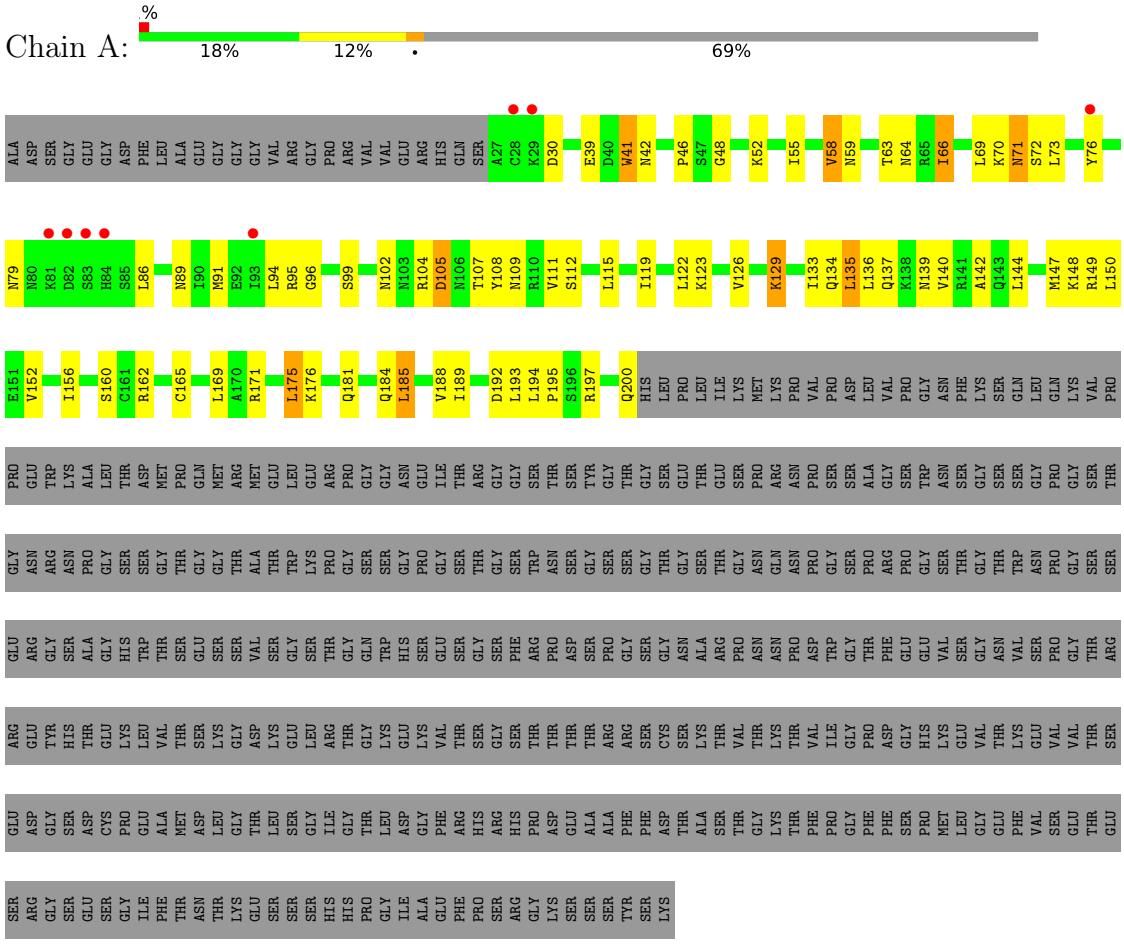
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		
9	E	1	Total	Ca	0	0
			1	1		
9	F	1	Total	Ca	0	0
			1	1		
9	H	1	Total	Ca	0	0
			1	1		
9	I	1	Total	Ca	0	0
			1	1		
9	K	1	Total	Ca	0	0
			1	1		
9	L	1	Total	Ca	0	0
			1	1		

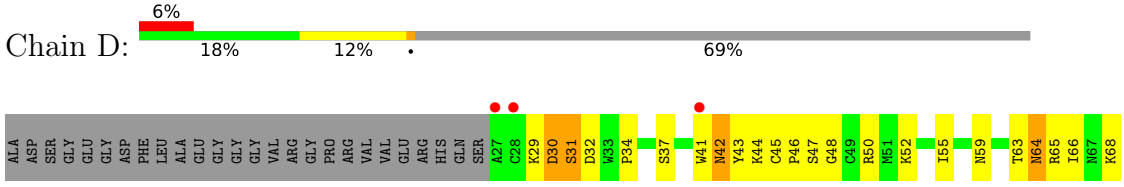
3 Residue-property plots (i)

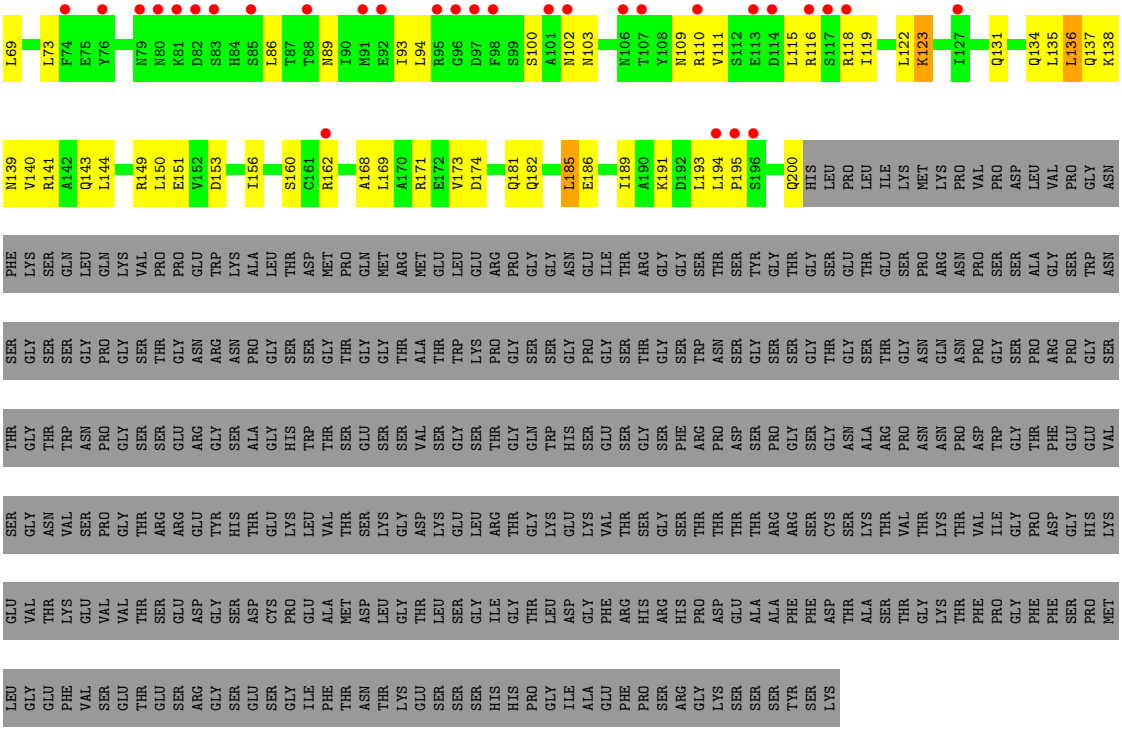
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



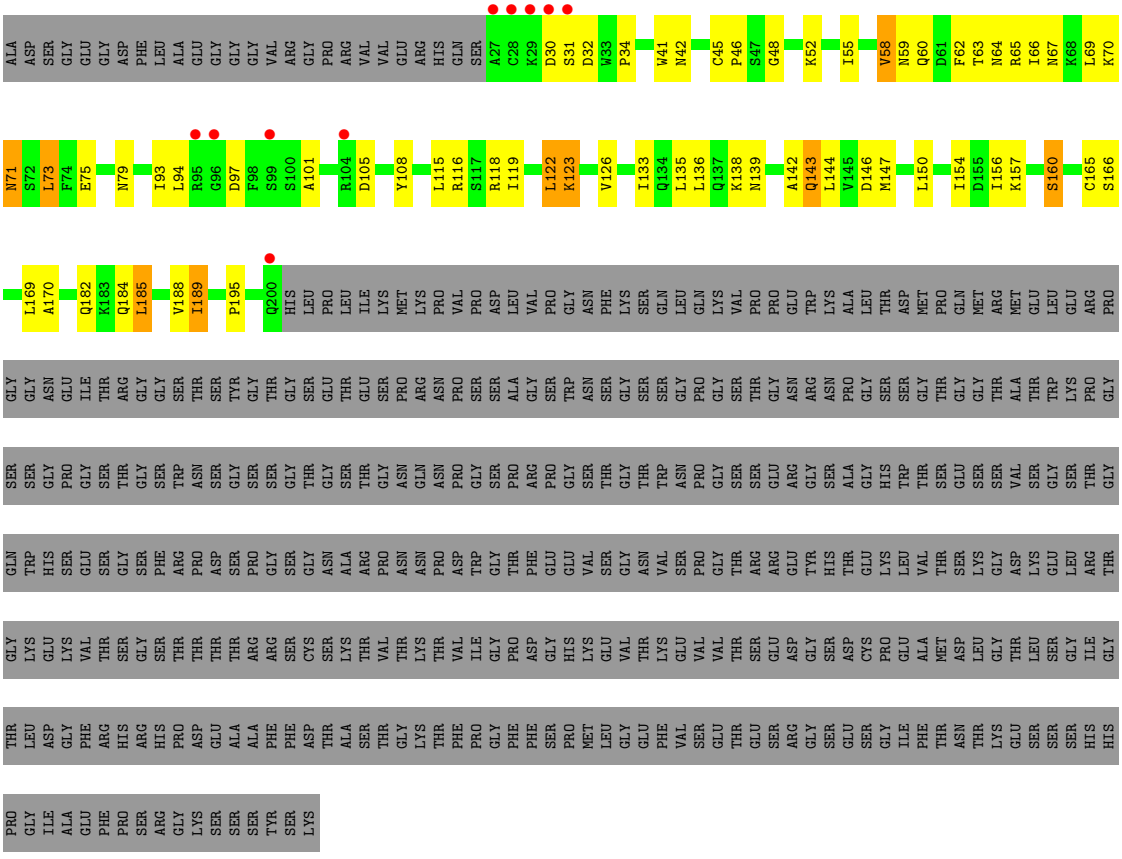
• Molecule 1: Fibrinogen alpha chain





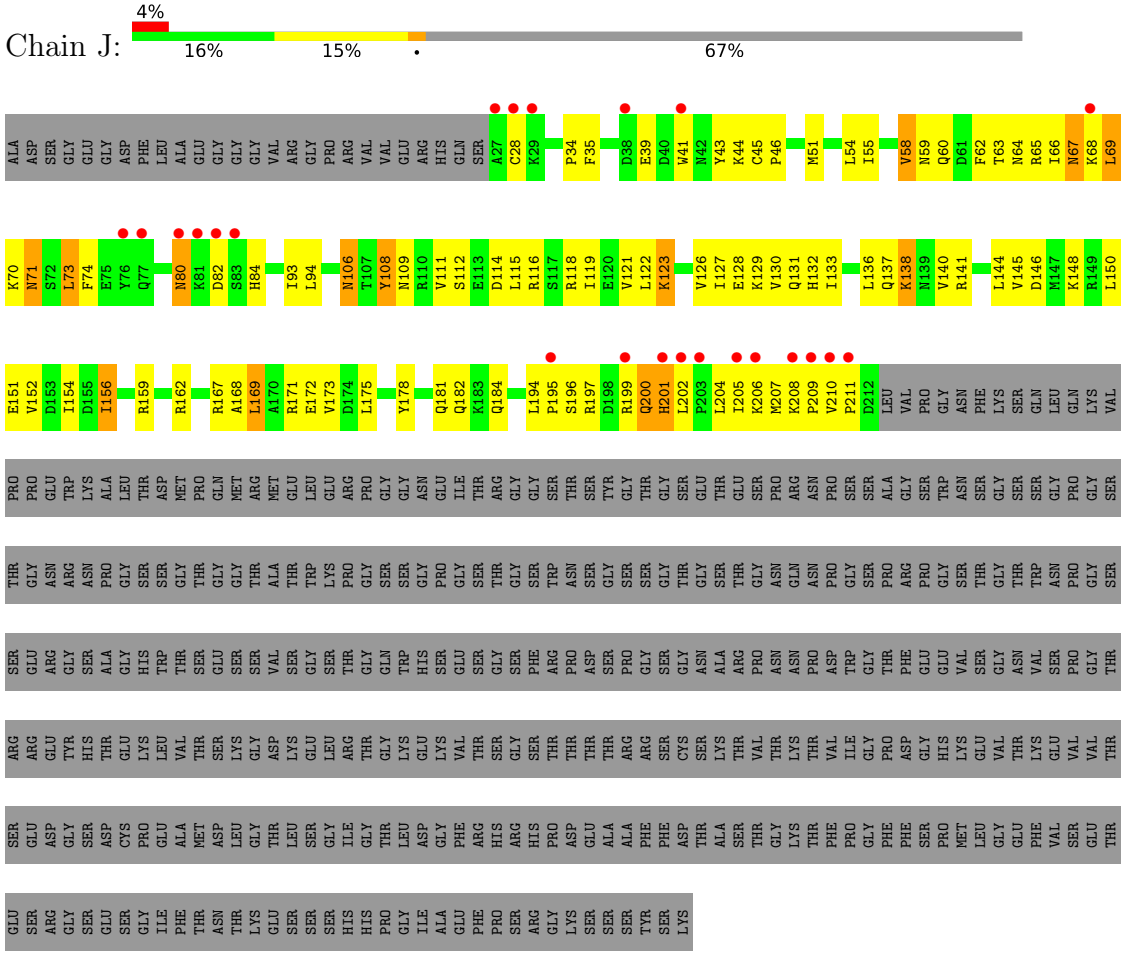
• Molecule 1: Fibrinogen alpha chain

Chain G:



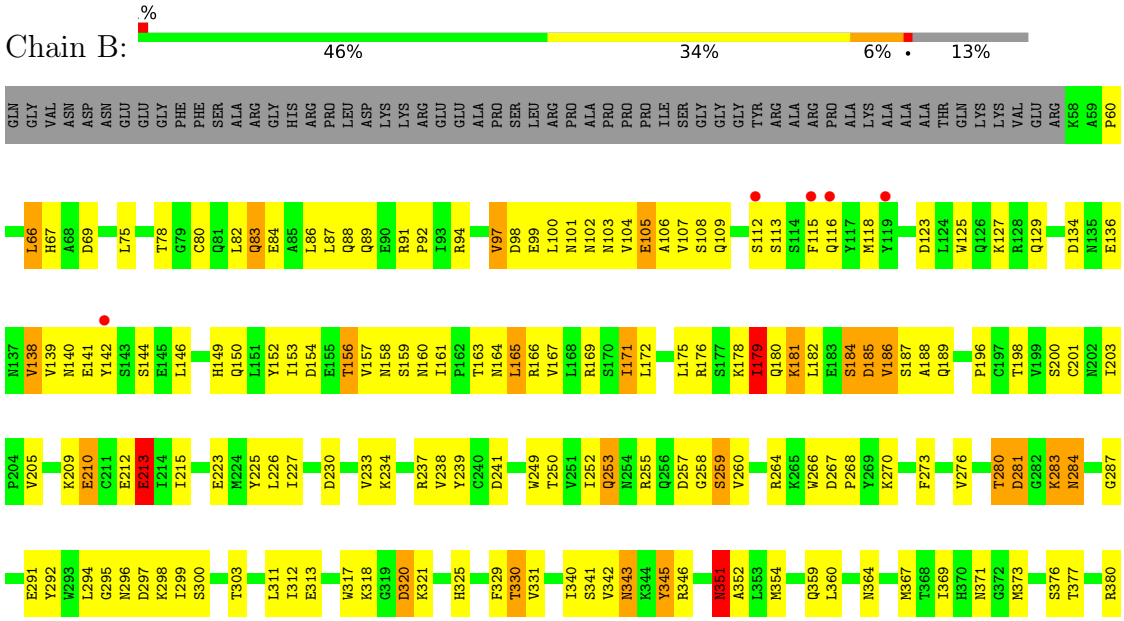
• Molecule 1: Fibrinogen alpha chain

Chain J:



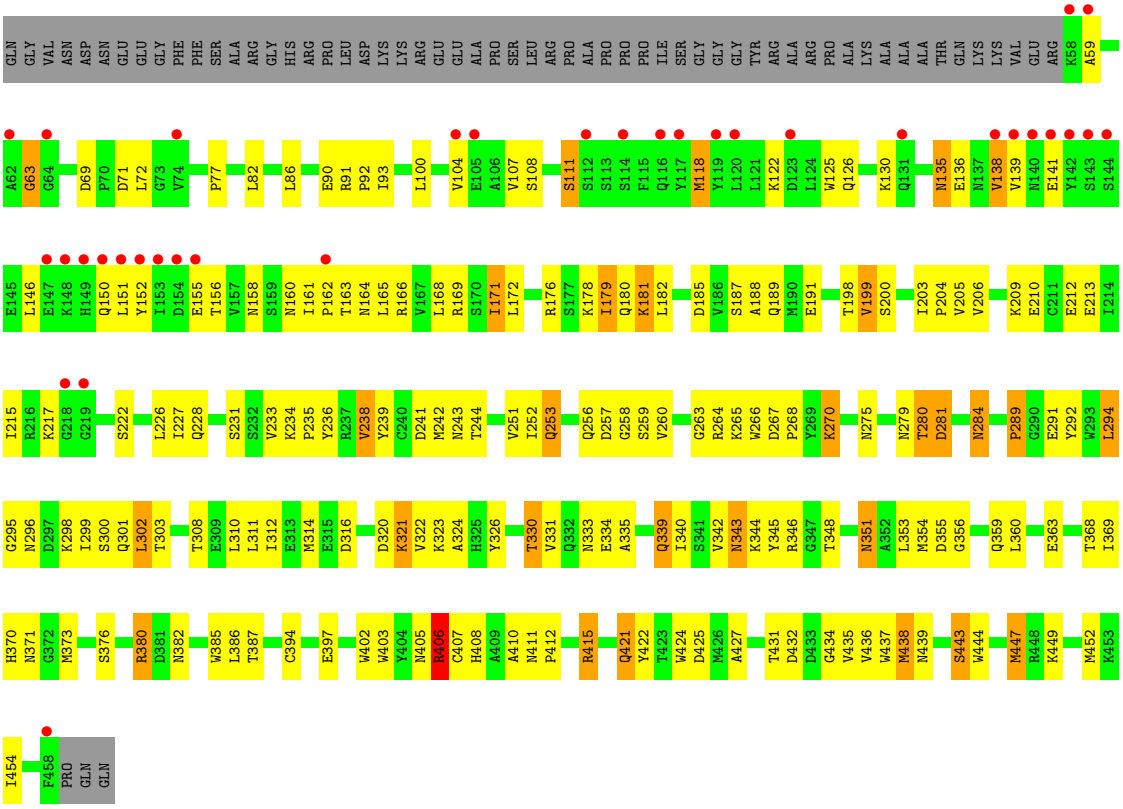
• Molecule 2: Fibrinogen beta chain

Chain B:



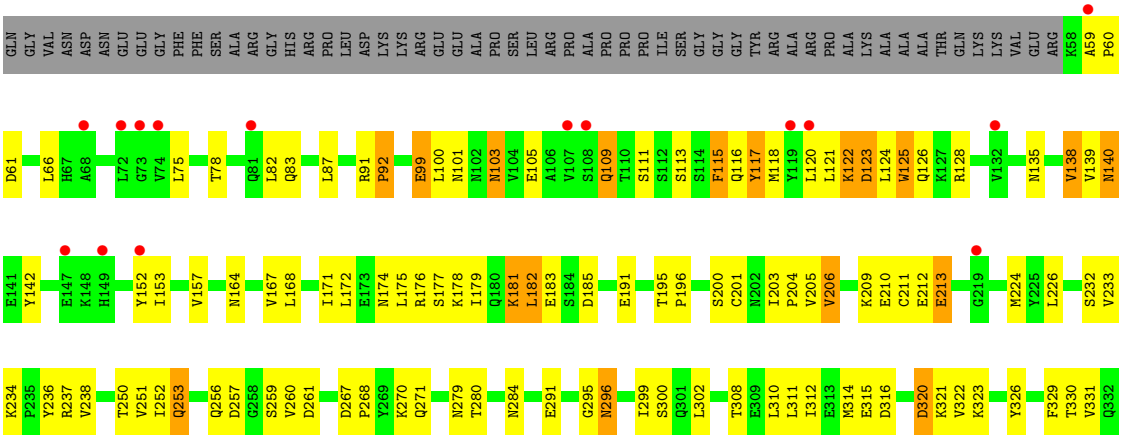
• Molecule 2: Fibrinogen beta chain

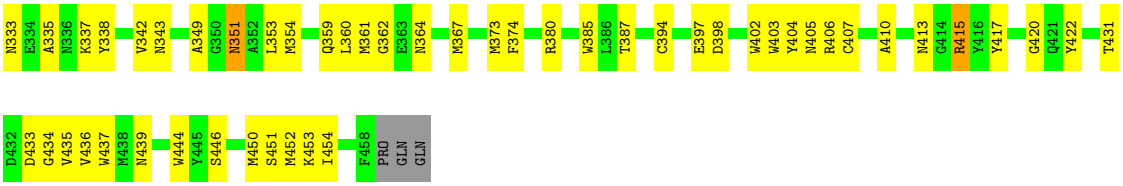
Chain E:



• Molecule 2: Fibrinogen beta chain

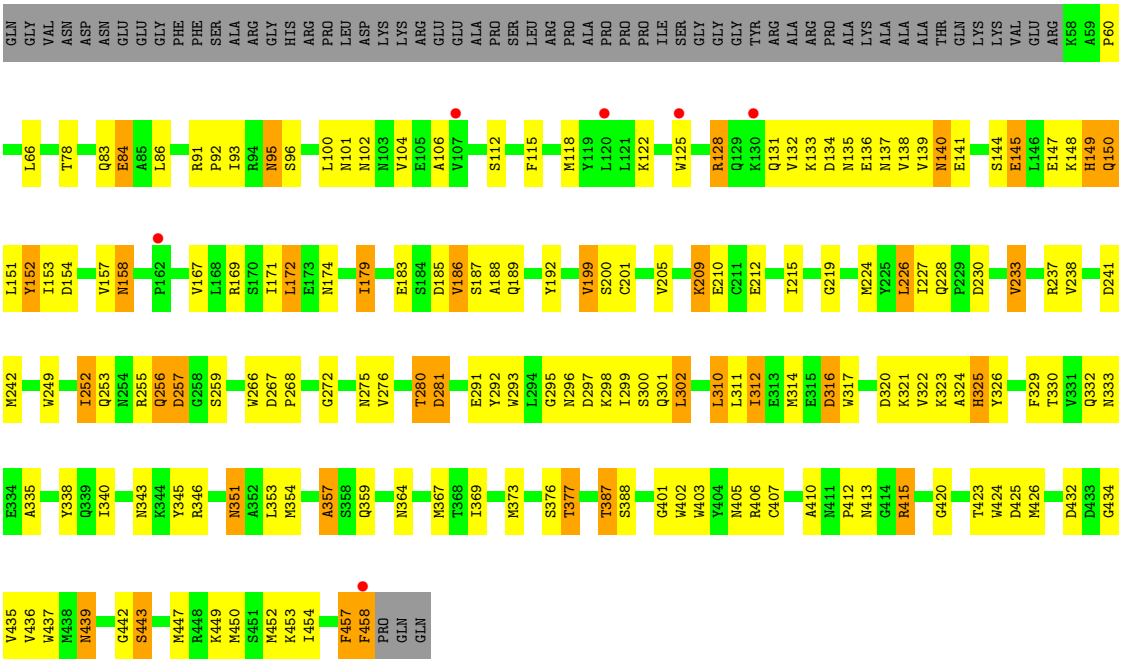
Chain H:





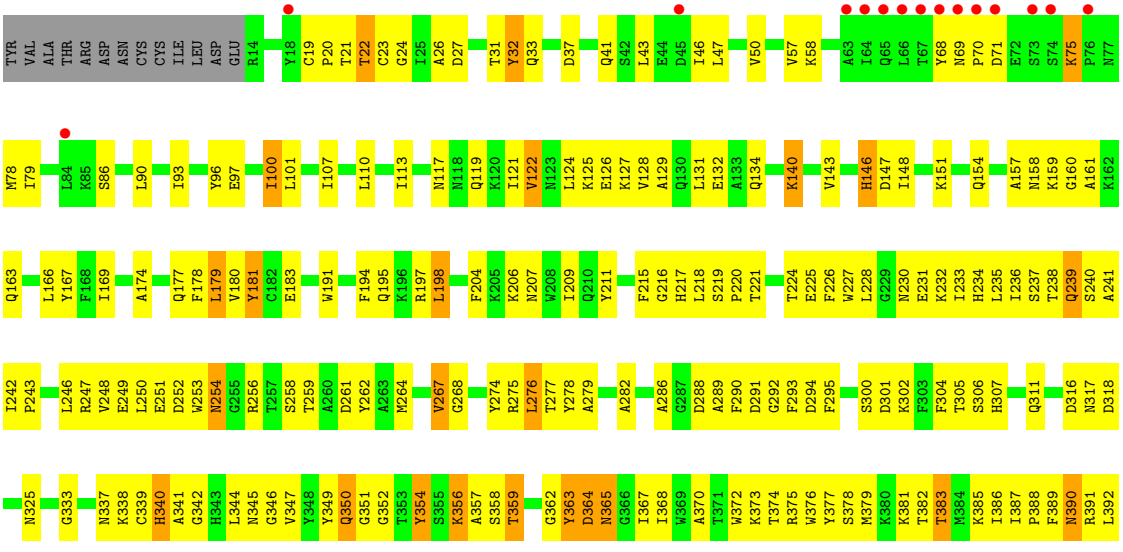
• Molecule 2: Fibrinogen beta chain

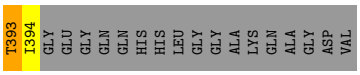
Chain K:



• Molecule 3: Fibrinogen gamma chain

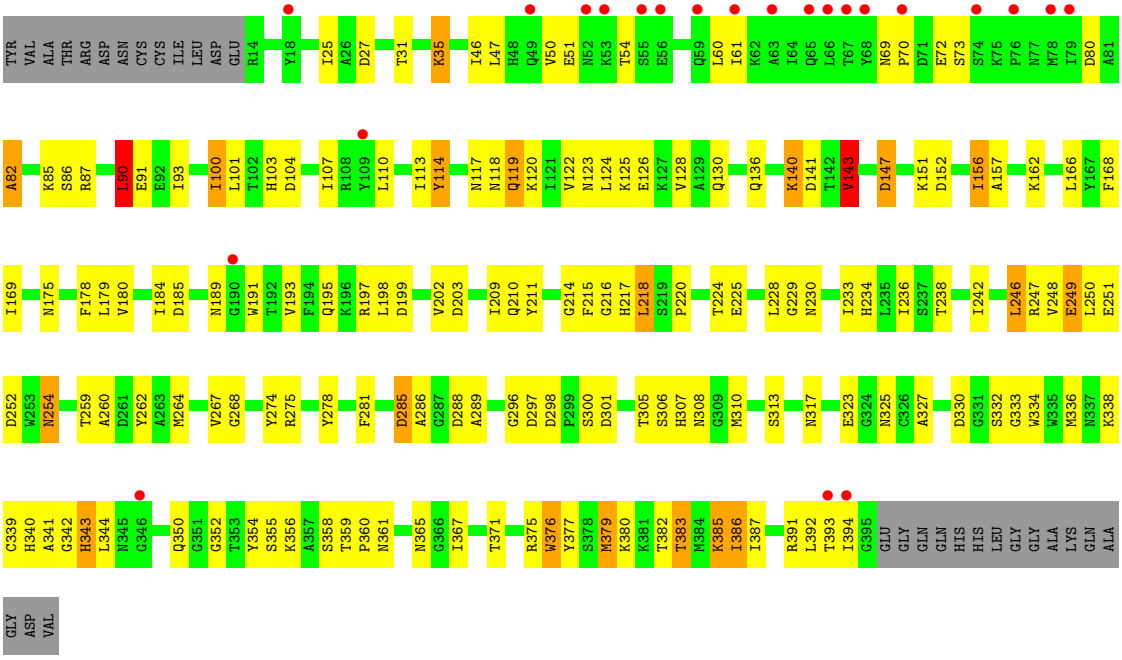
Chain C:





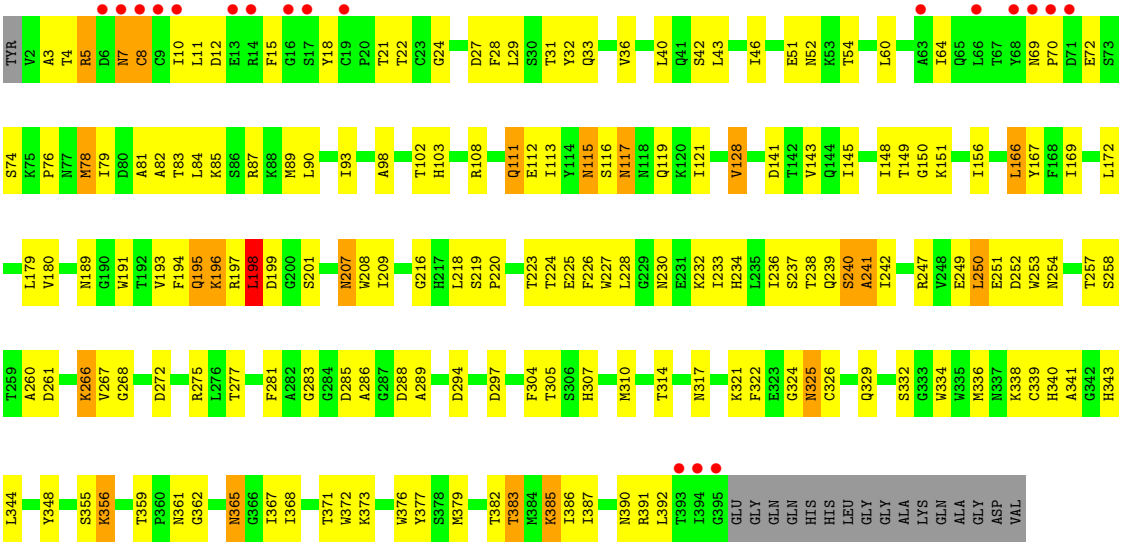
• Molecule 3: Fibrinogen gamma chain

Chain F:



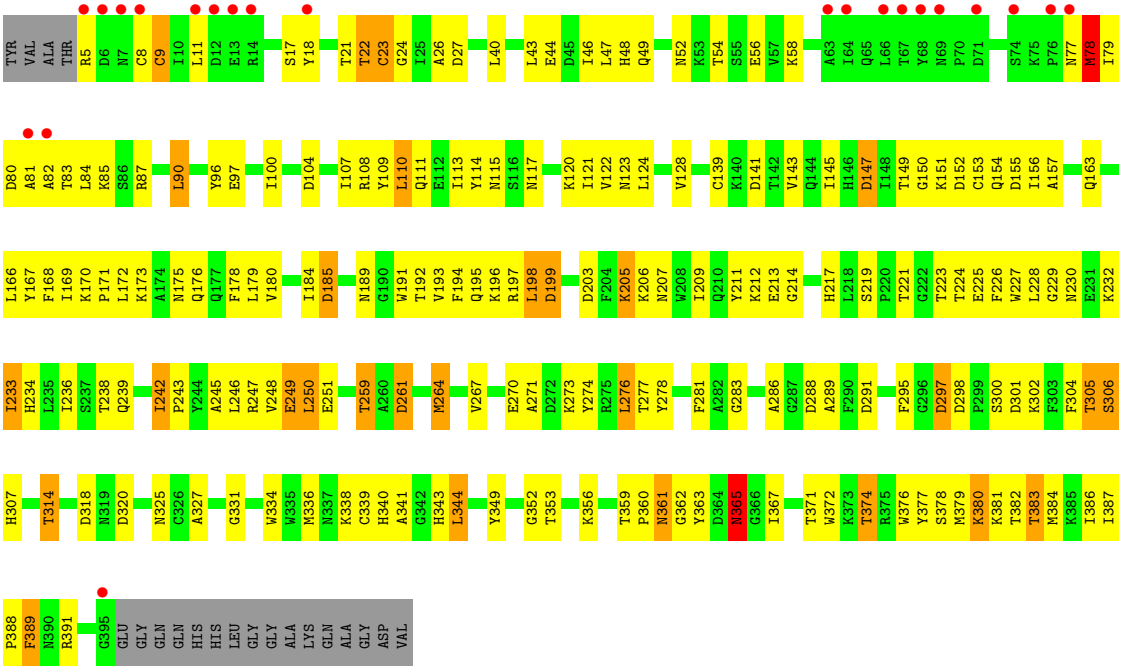
• Molecule 3: Fibrinogen gamma chain

Chain I:



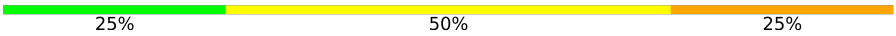
• Molecule 3: Fibrinogen gamma chain

Chain L:



- Molecule 4: A knob

Chain M:



- Molecule 4: A knob

Chain N:

- Molecule 4: A knob

Chain Q:

- Molecule 4: A knob

Chain R:

- Molecule 5: B knob

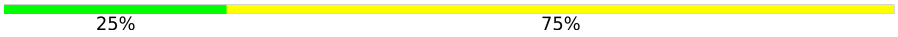
Chain O:

• Molecule 5: B knob

Chain P:

• Molecule 5: B knob

Chain S:



• Molecule 5: B knob

Chain T:

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

Chain U:

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

Chain V:

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

Chain X:

• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.24Å 94.87Å 300.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.90) 69.4 (19.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.252 , 0.309 0.259 , 0.311	Depositor DCC
R_{free} test set	5820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 75.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31833	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2228e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, MAN, BMA, GAL, NAG, CA

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	0.45	0/1447	0.61	0/1939
1	D	0.44	0/1447	0.56	0/1939
1	G	0.40	0/1447	0.54	0/1939
1	J	0.46	0/1547	0.62	0/2076
2	B	0.59	0/3283	0.73	0/4438
2	E	0.52	0/3283	0.62	0/4438
2	H	0.52	0/3283	0.65	0/4438
2	K	0.51	0/3283	0.65	0/4438
3	C	0.83	2/3125 (0.1%)	0.84	2/4224 (0.0%)
3	F	0.46	0/3129	0.57	1/4229 (0.0%)
3	I	0.53	0/3220	0.63	0/4353
3	L	0.55	0/3201	0.65	0/4326
4	M	0.80	0/31	0.89	0/40
4	N	0.46	0/31	0.62	0/40
4	Q	0.74	0/31	0.62	0/40
4	R	0.74	0/31	0.59	0/40
5	O	0.57	0/34	0.72	0/43
5	P	0.48	0/34	0.67	0/43
5	S	0.47	0/34	0.59	0/43
5	T	0.56	0/34	0.86	0/43
All	All	0.55	2/31955 (0.0%)	0.66	3/43109 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	TYR	CG-CD1	-5.83	1.31	1.39
3	C	181	TYR	CG-CD2	-5.10	1.32	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	90	LEU	CA-CB-CG	5.60	128.18	115.30
3	C	364	ASP	CB-CG-OD1	5.47	123.22	118.30
3	C	363	TYR	CA-CB-CG	5.25	123.38	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1431	0	1424	104	0
1	D	1431	0	1424	72	0
1	G	1431	0	1424	78	0
1	J	1527	0	1533	140	1
2	B	3209	0	3042	210	0
2	E	3209	0	3042	181	0
2	H	3209	0	3041	159	0
2	K	3209	0	3043	192	0
3	C	3050	0	2906	209	0
3	F	3054	0	2909	157	0
3	I	3145	0	2993	186	1
3	L	3126	0	2972	239	0
4	M	30	0	32	2	0
4	N	30	0	32	0	0
4	Q	30	0	32	0	0
4	R	30	0	32	1	0
5	O	33	0	32	3	0
5	P	33	0	32	2	0
5	S	33	0	32	4	0
5	T	33	0	32	4	0
6	U	151	0	126	24	0
6	V	151	0	126	17	0
6	X	151	0	126	19	0
7	W	61	0	52	8	0
8	Y	28	0	25	12	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
All	All	31833	0	30464	1668	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (1668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:364:ASN:HD21	6:X:1:NAG:C1	1.17	1.55
2:B:364:ASN:ND2	6:U:1:NAG:C1	1.70	1.52
2:K:364:ASN:ND2	6:X:1:NAG:C1	1.85	1.38
3:L:56:GLU:HB2	8:Y:1:NAG:O3	1.20	1.32
2:H:172:LEU:HD21	3:I:113:ILE:CG2	1.70	1.19
1:J:108:TYR:OH	3:L:83:THR:C	1.85	1.15
1:J:115:LEU:CD2	3:L:90:LEU:HD21	1.78	1.14
1:A:115:LEU:HD21	3:C:90:LEU:HD13	1.23	1.13
3:I:10:ILE:O	3:I:18:TYR:OH	1.65	1.12
2:K:302:LEU:HD22	2:K:454:ILE:HD11	1.31	1.11
1:G:108:TYR:CE2	3:I:82:ALA:HB1	1.86	1.11
3:I:12:ASP:HB3	3:I:15:PHE:HD1	0.99	1.09
3:I:12:ASP:CB	3:I:15:PHE:HD1	1.65	1.08
1:G:154:ILE:HD11	3:I:128:VAL:HG21	1.28	1.07
1:J:108:TYR:OH	3:L:84:LEU:N	1.87	1.07
3:I:12:ASP:HB3	3:I:15:PHE:CD1	1.90	1.06
1:A:55:ILE:HG23	2:B:86:LEU:HD21	1.35	1.06
3:I:27:ASP:O	3:I:31:THR:HG23	1.56	1.06
1:J:115:LEU:HD21	3:L:90:LEU:HD21	1.12	1.06
1:A:108:TYR:O	1:A:112:SER:OG	1.74	1.05
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.34	1.04
3:L:49:GLN:NE2	8:Y:1:NAG:H81	1.72	1.02
3:L:359:THR:HG21	3:L:363:TYR:O	1.59	1.02
1:G:119:ILE:HD11	3:I:93:ILE:CD1	1.89	1.01
1:A:119:ILE:HD13	3:C:93:ILE:HD13	1.43	1.01
2:B:252:ILE:HD11	2:B:454:ILE:HD13	1.02	1.01
2:H:172:LEU:HD21	3:I:113:ILE:HG21	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:52:ASN:ND2	8:Y:1:NAG:C1	2.24	1.01
1:G:154:ILE:CD1	3:I:128:VAL:HG21	1.90	0.99
1:D:135:LEU:HD22	1:D:136:LEU:HD22	1.43	0.99
1:G:105:ASP:OD1	3:I:79:ILE:HD11	1.63	0.98
2:B:154:ASP:OD1	3:C:96:TYR:OH	1.79	0.98
1:J:60:GLN:O	1:J:64:ASN:OD1	1.81	0.98
1:A:115:LEU:CD2	3:C:90:LEU:HD13	1.94	0.97
1:J:108:TYR:CE1	3:L:83:THR:HB	1.99	0.97
1:J:207:MET:HB2	2:K:135:ASN:HD21	1.21	0.97
1:G:55:ILE:HD12	2:H:82:LEU:HD22	1.44	0.97
3:I:8:CYS:SG	3:I:18:TYR:CD2	2.58	0.97
3:I:8:CYS:SG	3:I:18:TYR:CE2	2.58	0.97
1:G:119:ILE:HD11	3:I:93:ILE:HD11	1.48	0.95
3:L:56:GLU:HB2	8:Y:1:NAG:HO3	1.21	0.95
3:L:219:SER:H	3:L:224:THR:HG21	1.29	0.95
2:B:159:SER:O	2:B:163:THR:HG23	1.67	0.95
3:L:56:GLU:CB	8:Y:1:NAG:O3	2.15	0.94
2:E:241:ASP:OD1	2:E:244:THR:OG1	1.85	0.94
1:J:115:LEU:HD13	3:L:90:LEU:HD11	1.50	0.93
2:B:252:ILE:HD11	2:B:454:ILE:CD1	1.97	0.93
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.51	0.92
2:H:310:LEU:HD12	2:H:311:LEU:N	1.85	0.92
2:E:222:SER:OG	2:E:242:MET:N	2.01	0.92
2:H:252:ILE:HD12	2:H:454:ILE:HG23	1.50	0.92
2:B:239:TYR:OH	2:B:287:GLY:O	1.85	0.91
2:B:230:ASP:O	2:B:233:VAL:HG12	1.69	0.91
3:I:12:ASP:CB	3:I:15:PHE:CD1	2.51	0.90
3:C:390:ASN:HD22	3:C:391:ARG:N	1.69	0.90
1:J:115:LEU:HD21	3:L:90:LEU:CD2	2.00	0.90
2:B:252:ILE:CD1	2:B:454:ILE:HD13	1.96	0.89
3:F:323:GLU:N	3:F:323:GLU:OE2	2.05	0.89
2:H:172:LEU:CD2	3:I:113:ILE:HG21	2.02	0.89
3:C:307:HIS:HE1	3:C:342:GLY:H	1.21	0.88
3:L:52:ASN:ND2	8:Y:1:NAG:O5	2.07	0.88
1:A:55:ILE:HD12	2:B:82:LEU:HD22	1.53	0.88
1:A:144:LEU:HD13	2:B:175:LEU:HD11	1.54	0.88
1:J:108:TYR:HH	3:L:84:LEU:N	1.69	0.88
2:B:172:LEU:HB3	3:C:113:ILE:HG21	1.57	0.87
2:H:135:ASN:O	2:H:139:VAL:HG23	1.74	0.87
1:J:184:GLN:HE21	2:K:167:VAL:HG23	1.37	0.87
3:L:219:SER:OG	3:L:224:THR:HG22	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:201:CYS:O	3:L:143:VAL:HG21	1.74	0.86
1:A:55:ILE:HG23	2:B:86:LEU:CD2	2.04	0.85
1:J:169:LEU:HB2	2:K:189:GLN:HE22	1.41	0.85
1:J:148:LYS:HZ1	2:K:425:ASP:CG	1.79	0.85
2:E:222:SER:HG	2:E:242:MET:H	1.19	0.85
3:I:219:SER:OG	3:I:224:THR:HG22	1.77	0.85
3:L:49:GLN:NE2	8:Y:1:NAG:C8	2.39	0.85
2:H:210:GLU:OE2	2:H:212:GLU:N	2.09	0.84
1:J:69:LEU:HD11	2:K:100:LEU:HD13	1.56	0.84
1:A:122:LEU:HD11	2:B:153:ILE:HG21	1.60	0.83
1:A:73:LEU:HD23	2:B:104:VAL:HG22	1.60	0.83
3:F:246:LEU:HD11	3:F:248:VAL:HG23	1.59	0.83
2:H:172:LEU:HD21	3:I:113:ILE:CB	2.08	0.83
6:X:2:NAG:H62	6:X:5:NAG:H83	1.60	0.83
6:X:2:NAG:H62	6:X:5:NAG:C8	2.09	0.83
2:E:172:LEU:CD2	3:F:113:ILE:HG23	2.07	0.83
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.61	0.83
2:H:302:LEU:HD22	2:H:454:ILE:CD1	2.09	0.82
2:K:310:LEU:HD12	2:K:311:LEU:N	1.94	0.82
3:L:52:ASN:HD22	8:Y:1:NAG:C1	1.91	0.82
3:C:194:PHE:CD1	3:C:233:ILE:CD1	2.63	0.82
1:A:59:ASN:HD21	2:B:86:LEU:HD23	1.41	0.82
2:B:364:ASN:CG	6:U:1:NAG:C1	2.46	0.82
2:H:252:ILE:HD11	2:H:454:ILE:HD13	1.60	0.82
1:J:207:MET:HB2	2:K:135:ASN:ND2	1.95	0.82
2:K:133:LYS:O	2:K:136:GLU:HG2	1.79	0.82
2:K:343:ASN:HA	2:K:354:MET:SD	2.21	0.81
1:J:115:LEU:HD13	3:L:90:LEU:CD1	2.11	0.80
2:E:212:GLU:O	2:E:215:ILE:HG22	1.81	0.80
3:C:254:ASN:HD22	3:C:254:ASN:N	1.79	0.80
2:H:310:LEU:HD12	2:H:311:LEU:H	1.46	0.80
2:K:423:THR:OG1	2:K:425:ASP:OD1	1.99	0.80
1:A:123:LYS:HA	1:A:126:VAL:HG12	1.62	0.80
1:G:93:ILE:HG22	1:G:94:LEU:HD12	1.62	0.80
3:C:215:PHE:CE2	3:C:227:TRP:HB3	2.17	0.80
3:C:179:LEU:HD22	3:C:218:LEU:HD13	1.63	0.79
3:F:234:HIS:ND1	3:F:267:VAL:O	2.11	0.79
3:I:208:TRP:HA	3:I:314:THR:HG21	1.64	0.79
2:B:354:MET:O	2:B:369:ILE:HD13	1.81	0.79
1:D:119:ILE:HD11	3:F:93:ILE:HD13	1.64	0.79
3:C:253:TRP:C	3:C:254:ASN:HD22	1.85	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.62	0.79
2:H:252:ILE:CD1	2:H:454:ILE:HG23	2.12	0.79
2:K:295:GLY:O	2:K:299:ILE:HG13	1.83	0.79
3:F:46:ILE:O	3:F:50:VAL:HG22	1.83	0.79
1:A:119:ILE:HD13	3:C:93:ILE:CD1	2.14	0.78
3:C:307:HIS:CE1	3:C:342:GLY:H	2.02	0.78
1:G:58:VAL:HG21	3:I:29:LEU:HD11	1.66	0.78
2:B:179:ILE:HG23	2:B:180:GLN:N	1.98	0.78
1:J:108:TYR:CZ	3:L:83:THR:HB	2.18	0.78
1:J:205:ILE:HG13	2:K:138:VAL:HG11	1.65	0.78
2:B:351:ASN:C	2:B:351:ASN:HD22	1.87	0.78
2:E:343:ASN:HA	2:E:354:MET:SD	2.24	0.78
1:A:69:LEU:HD12	2:B:100:LEU:HD13	1.67	0.77
2:E:326:TYR:CE1	2:E:353:LEU:HD12	2.19	0.77
2:E:165:LEU:HD21	3:F:107:ILE:HD12	1.64	0.77
1:A:71:ASN:HD22	1:A:72:SER:N	1.82	0.77
3:F:296:GLY:N	3:F:301:ASP:OD2	2.18	0.77
2:B:252:ILE:HD12	2:B:454:ILE:HG23	1.67	0.77
1:J:46:PRO:O	3:L:22:THR:HG21	1.85	0.77
2:E:203:ILE:HG22	2:E:204:PRO:O	1.85	0.77
2:H:78:THR:HG23	1:J:43:TYR:O	1.84	0.76
2:K:210:GLU:OE2	2:K:212:GLU:N	2.14	0.76
2:B:165:LEU:HD11	3:C:107:ILE:CD1	2.15	0.76
3:I:8:CYS:SG	3:I:18:TYR:HD2	2.06	0.76
1:A:55:ILE:CD1	2:B:82:LEU:HD22	2.16	0.76
3:C:246:LEU:HD21	3:C:248:VAL:CG2	2.16	0.76
3:C:364:ASP:OD1	3:C:364:ASP:O	2.04	0.76
3:I:8:CYS:SG	3:I:18:TYR:HE2	2.06	0.76
3:I:281:PHE:CE2	3:I:283:GLY:HA2	2.20	0.76
3:F:246:LEU:HD12	3:F:247:ARG:N	2.00	0.76
3:I:143:VAL:O	3:I:143:VAL:HG23	1.84	0.76
2:K:312:ILE:HB	2:K:324:ALA:HB3	1.67	0.76
1:A:122:LEU:HD11	2:B:153:ILE:CG2	2.16	0.76
2:H:434:GLY:O	2:H:436:VAL:HG23	1.85	0.75
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.66	0.75
1:J:63:THR:HA	1:J:66:ILE:HG22	1.68	0.75
1:G:69:LEU:HD12	2:H:100:LEU:HD13	1.68	0.75
2:K:149:HIS:ND1	2:K:149:HIS:C	2.39	0.75
3:L:246:LEU:HD12	3:L:247:ARG:N	2.02	0.75
3:F:90:LEU:HD22	3:F:91:GLU:N	2.02	0.75
2:B:320:ASP:OD2	2:B:320:ASP:N	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:252:ILE:HD12	2:K:452:MET:C	2.08	0.74
1:A:122:LEU:CD1	2:B:153:ILE:HG21	2.17	0.74
3:L:77:ASN:HA	3:L:82:ALA:HB2	1.69	0.74
2:H:367:MET:SD	2:H:406:ARG:HD3	2.28	0.74
1:J:69:LEU:C	1:J:69:LEU:HD13	2.08	0.74
3:C:90:LEU:O	3:C:93:ILE:HG22	1.87	0.74
3:I:207:ASN:HD21	3:I:209:ILE:HD13	1.51	0.74
1:J:128:GLU:O	1:J:132:HIS:ND1	2.21	0.74
2:K:439:ASN:HD22	2:K:439:ASN:N	1.86	0.74
2:B:205:VAL:O	2:B:205:VAL:HG12	1.87	0.73
2:E:181:LYS:O	2:E:185:ASP:HB2	1.87	0.73
3:I:141:ASP:CG	3:I:143:VAL:HG22	2.07	0.73
3:L:198:LEU:HD13	3:L:199:ASP:N	2.02	0.73
1:D:55:ILE:HG23	2:E:86:LEU:HD13	1.69	0.73
2:B:381:ASP:HB2	2:B:393:GLN:HE21	1.54	0.73
2:B:169:ARG:HA	3:C:110:LEU:HD21	1.69	0.73
1:J:66:ILE:HG23	1:J:67:ASN:HD22	1.54	0.73
2:K:412:PRO:HG3	2:K:450:MET:HE3	1.71	0.73
6:X:1:NAG:O3	6:X:2:NAG:H2	1.90	0.72
2:H:172:LEU:CD2	3:I:113:ILE:CG2	2.58	0.72
2:H:59:ALA:HB1	2:H:60:PRO:HD2	1.70	0.72
2:H:201:CYS:O	3:I:143:VAL:HG21	1.88	0.72
3:C:368:ILE:CG2	3:C:377:TYR:O	2.37	0.72
3:F:218:LEU:N	3:F:218:LEU:HD23	2.04	0.72
3:I:219:SER:OG	3:I:224:THR:CG2	2.37	0.72
3:L:203:ASP:O	3:L:206:LYS:NZ	2.23	0.72
1:D:86:LEU:HD23	3:F:61:ILE:HD12	1.71	0.72
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.72	0.71
2:K:364:ASN:ND2	6:X:1:NAG:C2	2.52	0.71
3:L:334:TRP:HH2	3:L:344:LEU:HD12	1.54	0.71
1:J:129:LYS:O	1:J:133:ILE:HD13	1.91	0.71
2:K:172:LEU:HD22	3:L:113:ILE:HG23	1.70	0.71
3:L:344:LEU:HA	3:L:367:ILE:HG23	1.72	0.71
3:L:213:GLU:O	3:L:232:LYS:NZ	2.20	0.71
1:J:127:ILE:HA	1:J:130:VAL:HG12	1.70	0.71
3:L:318:ASP:OD1	3:L:325:ASN:ND2	2.22	0.71
3:C:194:PHE:CD1	3:C:233:ILE:HD13	2.25	0.71
3:C:295:PHE:CE1	3:C:305:THR:HG21	2.25	0.71
1:J:148:LYS:NZ	2:K:425:ASP:CG	2.42	0.71
1:J:169:LEU:HB2	2:K:189:GLN:NE2	2.06	0.71
2:E:316:ASP:OD2	2:E:320:ASP:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:H	2:E:407:CYS:HA	1.56	0.71
3:F:301:ASP:O	3:F:305:THR:HG23	1.89	0.71
1:J:67:ASN:HA	1:J:70:LYS:HE2	1.73	0.71
1:A:175:LEU:HD12	2:B:426:MET:CE	2.21	0.70
1:G:55:ILE:CD1	2:H:82:LEU:HD22	2.20	0.70
2:K:149:HIS:ND1	2:K:150:GLN:N	2.39	0.70
3:C:194:PHE:CG	3:C:233:ILE:HD13	2.27	0.70
3:I:3:ALA:HB2	3:L:11:LEU:HD12	1.73	0.70
3:F:147:ASP:OD1	3:F:147:ASP:N	2.23	0.70
2:H:302:LEU:HD22	2:H:454:ILE:HD11	1.73	0.70
1:G:123:LYS:HA	1:G:126:VAL:HG12	1.72	0.70
1:A:71:ASN:HD22	1:A:71:ASN:C	1.95	0.70
3:L:195:GLN:NE2	3:L:197:ARG:HG3	2.06	0.70
2:E:169:ARG:HA	3:F:110:LEU:HD11	1.74	0.70
3:F:169:ILE:HD11	3:F:180:VAL:HG21	1.74	0.70
3:C:75:LYS:HB3	3:C:78:MET:HE3	1.72	0.70
1:A:129:LYS:O	1:A:133:ILE:HD13	1.91	0.70
3:C:276:LEU:HD23	3:C:276:LEU:C	2.12	0.70
3:L:9:CYS:O	3:L:17:SER:HA	1.92	0.70
2:B:101:ASN:OD1	3:C:43:LEU:HD21	1.92	0.69
5:S:4:PRO:HB3	7:W:1:NAG:H62	1.73	0.69
1:A:119:ILE:CD1	3:C:93:ILE:HD13	2.18	0.69
2:B:364:ASN:HD22	6:U:1:NAG:C1	1.96	0.69
3:C:100:ILE:HG23	3:C:101:LEU:HD23	1.74	0.69
2:E:168:LEU:HD22	3:F:110:LEU:CD2	2.21	0.69
2:K:118:MET:O	2:K:122:LYS:HB3	1.93	0.69
3:L:219:SER:OG	3:L:224:THR:CG2	2.38	0.69
1:A:59:ASN:HD21	2:B:86:LEU:CD2	2.05	0.69
1:D:118:ARG:HH22	3:F:90:LEU:HD23	1.56	0.69
2:E:351:ASN:HD21	2:E:354:MET:H	1.39	0.69
1:J:207:MET:O	1:J:211:PRO:HD3	1.93	0.69
2:H:224:MET:HE2	2:H:237:ARG:HD3	1.75	0.69
3:I:81:ALA:O	3:I:85:LYS:N	2.23	0.69
3:C:368:ILE:HG22	3:C:377:TYR:O	1.92	0.69
1:J:115:LEU:O	1:J:119:ILE:HG12	1.93	0.69
2:K:179:ILE:HD11	3:L:121:ILE:HG13	1.75	0.69
6:U:7:SIA:O10	6:U:7:SIA:H7	1.93	0.69
2:B:253:GLN:HE21	2:B:253:GLN:C	1.96	0.69
1:A:111:VAL:O	1:A:115:LEU:HD12	1.93	0.69
6:U:10:GAL:H5	6:U:11:SIA:H32	1.74	0.69
3:F:246:LEU:HD11	3:F:248:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:ASN:HA	1:J:74:PHE:CD2	2.28	0.68
2:B:252:ILE:CD1	2:B:454:ILE:HG23	2.23	0.68
3:C:166:LEU:HB3	3:C:179:LEU:HD21	1.75	0.68
3:C:197:ARG:NH1	3:C:367:ILE:HD11	2.08	0.68
2:H:342:VAL:HG11	2:H:353:LEU:HD13	1.74	0.68
1:J:145:VAL:HG13	1:J:146:ASP:N	2.07	0.68
2:K:212:GLU:O	2:K:215:ILE:HG22	1.92	0.68
2:K:432:ASP:OD1	2:K:443:SER:OG	2.10	0.68
3:C:248:VAL:HG12	3:C:250:LEU:HD11	1.73	0.68
1:A:115:LEU:HD21	3:C:90:LEU:CD1	2.14	0.68
2:E:436:VAL:HG11	2:E:443:SER:HA	1.75	0.68
1:G:115:LEU:HD11	3:I:89:MET:HB2	1.75	0.68
3:F:27:ASP:O	3:F:31:THR:HB	1.94	0.68
2:K:345:TYR:HB2	2:K:354:MET:HE2	1.74	0.68
1:A:63:THR:HA	1:A:66:ILE:HG22	1.75	0.68
3:C:291:ASP:O	3:C:302:LYS:NZ	2.27	0.68
3:F:260:ALA:HB2	3:F:286:ALA:CB	2.20	0.67
2:H:172:LEU:HD21	3:I:113:ILE:HB	1.75	0.67
1:J:144:LEU:HD22	2:K:171:ILE:HD11	1.75	0.67
1:J:69:LEU:HD11	2:K:100:LEU:CD1	2.24	0.67
1:J:121:VAL:HG12	1:J:122:LEU:HD22	1.74	0.67
2:K:102:ASN:O	2:K:106:ALA:HB3	1.94	0.67
3:L:379:MET:HA	3:L:379:MET:HE3	1.75	0.67
2:B:406:ARG:N	2:B:407:CYS:HA	2.08	0.67
1:D:55:ILE:CG2	2:E:86:LEU:HD13	2.24	0.67
3:L:288:ASP:C	3:L:371:THR:HG21	2.14	0.67
3:L:314:THR:C	3:L:327:ALA:HB1	2.15	0.67
2:B:408:HIS:O	5:O:1:GLY:N	2.24	0.67
3:C:350:GLN:O	3:C:352:GLY:N	2.21	0.67
2:K:364:ASN:CG	6:X:1:NAG:C1	2.61	0.67
1:A:115:LEU:HD11	3:C:90:LEU:HB2	1.76	0.67
3:C:181:TYR:HE1	3:C:220:PRO:O	1.77	0.67
1:A:175:LEU:HD12	2:B:426:MET:HE2	1.76	0.67
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.77	0.67
2:H:135:ASN:HA	2:H:138:VAL:HG12	1.77	0.67
3:I:79:ILE:HA	3:I:82:ALA:HB3	1.76	0.67
3:I:199:ASP:OD1	3:I:201:SER:N	2.27	0.66
2:K:351:ASN:HD21	2:K:354:MET:HG3	1.59	0.66
2:B:367:MET:SD	2:B:406:ARG:HD3	2.35	0.66
3:C:225:GLU:O	3:C:226:PHE:HB3	1.96	0.66
2:H:360:LEU:HD11	5:S:2:HIS:ND1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:361:MET:HB2	7:W:1:NAG:H81	1.78	0.66
3:L:185:ASP:OD2	3:L:189:ASN:N	2.25	0.66
3:I:11:LEU:HD23	3:I:12:ASP:N	2.11	0.66
3:C:276:LEU:HD21	3:C:278:TYR:CD2	2.31	0.66
2:E:406:ARG:N	2:E:407:CYS:HA	2.10	0.66
3:L:242:ILE:HG23	3:L:243:PRO:HD2	1.76	0.66
6:U:5:NAG:H4	6:U:6:GAL:O2	1.95	0.66
3:C:365:ASN:HD22	3:C:365:ASN:H	1.43	0.66
6:U:2:NAG:O6	6:U:5:NAG:H2	1.94	0.66
3:C:194:PHE:CD1	3:C:233:ILE:HD11	2.29	0.66
1:J:51:MET:HG3	3:L:22:THR:HG22	1.77	0.66
1:J:208:LYS:HB2	1:J:209:PRO:HD3	1.78	0.66
3:L:11:LEU:HB3	3:L:18:TYR:CE1	2.31	0.66
3:C:179:LEU:HD23	3:C:180:VAL:N	2.10	0.66
3:C:364:ASP:OD2	4:M:1:GLY:N	2.28	0.66
1:G:119:ILE:HD11	3:I:93:ILE:HD13	1.78	0.66
1:D:109:ASN:OD1	1:D:110:ARG:N	2.29	0.65
2:H:182:LEU:O	2:H:185:ASP:N	2.29	0.65
2:B:294:LEU:HD12	2:B:295:GLY:H	1.62	0.65
2:H:257:ASP:OD1	2:H:259:SER:OG	2.10	0.65
3:F:27:ASP:O	3:F:31:THR:CB	2.45	0.65
1:G:123:LYS:NZ	2:H:153:ILE:HG21	2.10	0.65
2:B:354:MET:O	2:B:369:ILE:HG23	1.96	0.65
3:C:197:ARG:HD2	3:C:344:LEU:O	1.97	0.65
2:E:340:ILE:HD12	2:E:403:TRP:CZ3	2.31	0.65
2:H:302:LEU:HD22	2:H:454:ILE:HD12	1.77	0.65
3:I:42:SER:O	3:I:46:ILE:HD13	1.96	0.65
3:L:236:ILE:HG21	3:L:386:ILE:HD11	1.77	0.65
3:L:264:MET:O	3:L:278:TYR:HA	1.96	0.65
8:Y:1:NAG:H62	8:Y:2:NAG:H61	1.77	0.65
2:K:276:VAL:HA	2:K:292:TYR:CD2	2.32	0.65
6:U:8:MAN:H4	6:U:9:NAG:N2	2.12	0.65
2:E:205:VAL:HG22	3:F:218:LEU:HD21	1.78	0.65
3:I:193:VAL:HG22	3:I:385:LYS:HB3	1.77	0.65
3:C:146:HIS:HD2	3:C:167:TYR:CZ	2.14	0.64
1:D:144:LEU:HD21	1:D:182:GLN:HA	1.78	0.64
3:L:169:ILE:CD1	3:L:180:VAL:HG11	2.27	0.64
1:A:134:GLN:NE2	1:A:193:LEU:HD23	2.12	0.64
2:E:296:ASN:O	2:E:299:ILE:N	2.28	0.64
2:H:252:ILE:CD1	2:H:454:ILE:CG2	2.75	0.64
2:B:154:ASP:CG	3:C:96:TYR:OH	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.33	0.64
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.31	0.64
2:H:316:ASP:OD2	2:H:320:ASP:N	2.20	0.64
3:L:246:LEU:HD12	3:L:247:ARG:H	1.63	0.64
3:L:219:SER:N	3:L:224:THR:HG21	2.09	0.64
2:B:171:ILE:HG22	2:B:172:LEU:HD13	1.80	0.64
2:B:205:VAL:HG22	3:C:218:LEU:HG	1.79	0.64
1:J:69:LEU:HD13	1:J:70:LYS:N	2.13	0.64
2:E:160:ASN:O	2:E:164:ASN:N	2.20	0.64
2:H:66:LEU:N	1:J:34:PRO:O	2.31	0.64
1:J:71:ASN:HA	1:J:74:PHE:CE2	2.33	0.64
6:U:1:NAG:O3	6:U:2:NAG:H2	1.98	0.64
7:W:2:NAG:O7	7:W:2:NAG:H3	1.98	0.64
3:L:152:ASP:OD1	3:L:155:ASP:N	2.30	0.64
1:G:97:ASP:O	1:G:101:ALA:CB	2.46	0.64
2:B:165:LEU:HD11	3:C:107:ILE:HD12	1.79	0.64
3:C:365:ASN:HD22	3:C:365:ASN:N	1.96	0.64
3:C:174:ALA:HB2	3:C:235:LEU:HD13	1.79	0.63
3:C:340:HIS:ND1	3:C:340:HIS:O	2.30	0.63
2:E:199:VAL:O	3:F:141:ASP:OD2	2.16	0.63
3:L:209:ILE:H	3:L:209:ILE:HD12	1.63	0.63
3:F:250:LEU:HD23	3:F:379:MET:CE	2.28	0.63
2:H:153:ILE:O	2:H:153:ILE:HG22	1.97	0.63
3:I:189:ASN:HB3	3:I:387:ILE:HD11	1.78	0.63
1:A:134:GLN:HE22	1:A:193:LEU:HD23	1.63	0.63
1:A:169:LEU:HD23	1:A:171:ARG:HD2	1.80	0.63
3:I:5:ARG:HB2	3:I:11:LEU:HD13	1.80	0.63
2:K:199:VAL:HG23	3:L:141:ASP:HA	1.80	0.63
3:I:12:ASP:OD2	3:I:15:PHE:CD1	2.52	0.63
1:J:132:HIS:CB	3:L:107:ILE:HD11	2.28	0.63
2:K:332:GLN:O	2:K:338:TYR:HA	1.98	0.63
3:L:197:ARG:NH1	3:L:367:ILE:HD11	2.14	0.63
2:B:238:VAL:HG11	2:B:250:THR:HG23	1.81	0.63
3:C:121:ILE:HG22	3:C:122:VAL:N	2.12	0.63
3:C:261:ASP:HB3	3:C:282:ALA:HB3	1.81	0.63
2:E:172:LEU:HD21	3:F:113:ILE:HG23	1.79	0.63
2:E:314:MET:CG	2:E:322:VAL:HG23	2.28	0.63
2:K:436:VAL:HG11	2:K:442:GLY:O	1.99	0.63
2:B:172:LEU:HB3	3:C:113:ILE:CG2	2.27	0.63
1:D:50:ARG:HD3	2:E:59:ALA:HB1	1.81	0.63
1:G:118:ARG:NH2	3:I:90:LEU:HD21	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:356:LYS:HA	3:I:359:THR:HG23	1.80	0.63
1:G:184:GLN:HE21	2:H:167:VAL:HG23	1.64	0.62
3:I:242:ILE:HD12	3:I:242:ILE:O	1.98	0.62
2:B:281:ASP:O	2:B:281:ASP:OD2	2.18	0.62
2:E:226:LEU:HD11	2:E:235:PRO:HB2	1.80	0.62
2:E:385:TRP:O	2:E:387:THR:N	2.29	0.62
1:J:115:LEU:CD2	3:L:90:LEU:CD2	2.66	0.62
2:K:172:LEU:CD2	3:L:113:ILE:HG23	2.29	0.62
3:C:246:LEU:HA	3:C:386:ILE:HG22	1.80	0.62
3:C:349:TYR:CE1	3:C:354:TYR:CE1	2.88	0.62
2:H:87:LEU:HD23	2:H:87:LEU:O	2.00	0.62
1:G:62:PHE:CE1	3:I:36:VAL:HG12	2.35	0.62
1:J:137:GLN:O	1:J:140:VAL:HG22	1.99	0.62
1:J:156:ILE:O	1:J:159:ARG:N	2.32	0.62
2:K:373:MET:SD	2:K:405:ASN:HB2	2.38	0.62
2:K:406:ARG:N	2:K:407:CYS:HA	2.13	0.62
1:D:86:LEU:CD2	3:F:61:ILE:HG21	2.30	0.62
1:D:118:ARG:NH2	3:F:90:LEU:HD23	2.13	0.62
2:E:171:ILE:CG2	2:E:172:LEU:N	2.62	0.62
2:E:205:VAL:HG23	3:F:216:GLY:O	1.98	0.62
3:I:169:ILE:HD11	3:I:180:VAL:HG11	1.80	0.62
2:K:376:SER:O	2:K:401:GLY:HA2	1.99	0.62
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.29	0.62
3:C:261:ASP:CB	3:C:282:ALA:HB3	2.30	0.61
2:H:171:ILE:HG23	2:H:172:LEU:N	2.15	0.61
1:J:106:ASN:ND2	1:J:106:ASN:C	2.54	0.61
3:C:333:GLY:O	3:C:345:ASN:ND2	2.32	0.61
2:E:340:ILE:HD12	2:E:403:TRP:CE3	2.36	0.61
1:J:154:ILE:HD11	3:L:128:VAL:HG21	1.80	0.61
3:C:295:PHE:HE1	3:C:305:THR:HG21	1.63	0.61
2:E:165:LEU:HD21	3:F:107:ILE:CD1	2.30	0.61
2:H:122:LYS:HZ3	3:I:60:LEU:HB3	1.66	0.61
2:K:326:TYR:CE1	2:K:353:LEU:HD12	2.35	0.61
1:D:137:GLN:O	1:D:140:VAL:HG22	1.99	0.61
2:B:102:ASN:O	2:B:106:ALA:HB3	2.00	0.61
3:F:124:LEU:O	3:F:128:VAL:HG23	1.99	0.61
2:K:137:ASN:HA	2:K:140:ASN:HD21	1.64	0.61
3:C:240:SER:O	3:C:242:ILE:N	2.28	0.61
1:G:185:LEU:HD11	1:G:189:ILE:HD11	1.82	0.61
2:H:253:GLN:HE21	2:H:253:GLN:C	2.03	0.61
2:B:172:LEU:HD22	3:C:110:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:O	2:E:179:ILE:HG22	2.01	0.61
3:L:56:GLU:CB	8:Y:1:NAG:HO3	2.03	0.61
1:D:135:LEU:HD22	1:D:136:LEU:CD2	2.24	0.61
3:I:116:SER:O	3:I:119:GLN:N	2.33	0.61
3:I:141:ASP:OD2	3:I:143:VAL:HG22	2.01	0.61
2:K:410:ALA:HB1	2:K:437:TRP:CE3	2.36	0.61
1:J:118:ARG:O	1:J:122:LEU:HD23	2.01	0.61
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.82	0.60
2:E:226:LEU:HD11	2:E:235:PRO:CB	2.30	0.60
2:H:75:LEU:HD22	1:J:46:PRO:N	2.16	0.60
1:J:63:THR:HA	1:J:66:ILE:CG2	2.31	0.60
3:L:143:VAL:HG23	3:L:143:VAL:O	2.00	0.60
2:B:260:VAL:HG21	2:B:291:GLU:O	2.01	0.60
2:E:312:ILE:HD11	2:E:452:MET:HE2	1.83	0.60
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.35	0.60
1:G:154:ILE:HD11	3:I:128:VAL:CG2	2.19	0.60
3:L:21:THR:HG23	3:L:24:GLY:H	1.66	0.60
3:L:236:ILE:CG2	3:L:386:ILE:HD11	2.30	0.60
3:C:367:ILE:O	3:C:378:SER:HA	2.01	0.60
1:G:58:VAL:HG12	1:G:59:ASN:N	2.16	0.60
2:H:172:LEU:HD21	3:I:113:ILE:HG22	1.78	0.60
3:I:209:ILE:H	3:I:209:ILE:HD12	1.66	0.60
3:C:359:THR:HG21	3:C:363:TYR:O	2.01	0.60
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.82	0.60
3:C:191:TRP:CH2	3:C:387:ILE:HG21	2.37	0.60
2:H:406:ARG:N	2:H:407:CYS:HA	2.16	0.60
3:L:153:CYS:HB2	3:L:192:THR:OG1	2.02	0.60
1:A:139:ASN:O	1:A:142:ALA:HB3	2.00	0.60
2:B:75:LEU:HD13	1:D:44:LYS:O	2.00	0.60
1:J:207:MET:HE2	2:K:131:GLN:HE22	1.66	0.60
2:B:238:VAL:HG11	2:B:250:THR:CG2	2.32	0.60
3:F:246:LEU:CD1	3:F:248:VAL:HG23	2.30	0.60
2:H:312:ILE:HG23	2:H:451:SER:O	2.02	0.60
3:F:298:ASP:OD2	3:F:300:SER:N	2.35	0.60
2:H:374:PHE:O	2:H:403:TRP:HA	2.02	0.60
2:K:412:PRO:HG3	2:K:450:MET:CE	2.31	0.60
3:I:387:ILE:HG23	3:I:387:ILE:O	2.02	0.60
2:K:139:VAL:HG21	3:L:79:ILE:HG21	1.84	0.60
2:K:169:ARG:HA	3:L:110:LEU:HD11	1.84	0.60
2:K:199:VAL:HG23	3:L:141:ASP:CA	2.31	0.60
2:E:126:GLN:O	2:E:130:LYS:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:HIS:HB3	3:L:107:ILE:HD11	1.83	0.60
3:C:293:PHE:CD1	3:C:370:ALA:HB1	2.37	0.59
3:I:79:ILE:O	3:I:83:THR:N	2.25	0.59
6:V:5:NAG:H62	6:V:6:GAL:C1	2.32	0.59
2:B:179:ILE:CG2	2:B:180:GLN:N	2.64	0.59
2:E:253:GLN:HE21	2:E:253:GLN:C	2.06	0.59
2:E:405:ASN:O	2:E:406:ARG:CB	2.50	0.59
1:G:166:SER:HB3	2:H:195:THR:OG1	2.02	0.59
3:I:98:ALA:O	3:I:102:THR:HG23	2.02	0.59
2:K:266:TRP:HA	2:K:377:THR:HG21	1.84	0.59
3:L:349:TYR:OH	3:L:365:ASN:ND2	2.32	0.59
3:I:51:GLU:O	3:I:54:THR:OG1	2.16	0.59
2:K:171:ILE:HG23	2:K:172:LEU:N	2.17	0.59
6:X:11:SIA:O10	6:X:11:SIA:H7	2.01	0.59
3:F:197:ARG:NH2	3:F:367:ILE:HD11	2.18	0.59
3:I:227:TRP:HE1	3:I:230:ASN:HD22	1.50	0.59
2:B:210:GLU:OE2	2:B:212:GLU:N	2.31	0.59
3:C:390:ASN:HD22	3:C:390:ASN:C	2.05	0.59
2:E:238:VAL:HG13	2:E:239:TYR:O	2.02	0.59
1:G:188:VAL:HG11	2:H:164:ASN:ND2	2.18	0.59
2:K:139:VAL:HG21	3:L:79:ILE:CG2	2.33	0.59
3:L:219:SER:HG	3:L:224:THR:HG22	1.67	0.59
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.03	0.59
2:E:146:LEU:O	2:E:150:GLN:N	2.25	0.59
2:H:333:ASN:OD1	2:H:335:ALA:HB3	2.03	0.59
1:A:185:LEU:O	1:A:185:LEU:HD22	2.01	0.59
2:E:432:ASP:OD1	2:E:443:SER:OG	2.19	0.59
2:H:211:CYS:SG	2:H:250:THR:HG23	2.43	0.59
3:I:11:LEU:HA	3:I:18:TYR:OH	2.02	0.59
2:B:257:ASP:N	2:B:257:ASP:OD1	2.35	0.59
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.51	0.59
1:G:30:ASP:O	1:G:32:ASP:N	2.35	0.59
1:G:75:GLU:O	1:G:79:ASN:HB2	2.03	0.59
2:B:351:ASN:HD21	2:B:354:MET:H	1.50	0.59
3:C:126:GLU:O	3:C:129:ALA:HB3	2.03	0.59
1:D:55:ILE:HG23	2:E:86:LEU:CD1	2.32	0.59
1:J:127:ILE:O	1:J:130:VAL:HG12	2.03	0.59
2:B:434:GLY:O	2:B:436:VAL:N	2.36	0.58
3:C:246:LEU:HG	3:C:247:ARG:N	2.17	0.58
3:L:44:GLU:O	3:L:48:HIS:HB2	2.03	0.58
3:L:224:THR:HG23	3:L:224:THR:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:367:ILE:HG21	3:C:382:THR:HG21	1.85	0.58
1:A:169:LEU:HD21	2:B:185:ASP:OD2	2.04	0.58
3:C:206:LYS:HB2	3:C:211:TYR:CE1	2.38	0.58
2:E:171:ILE:HG22	2:E:172:LEU:N	2.19	0.58
1:G:115:LEU:HD11	3:I:89:MET:CB	2.33	0.58
1:A:147:MET:SD	3:C:121:ILE:HD11	2.43	0.58
2:H:176:ARG:NH1	3:I:113:ILE:HG23	2.18	0.58
3:I:84:LEU:HD12	3:I:87:ARG:HD2	1.84	0.58
1:A:119:ILE:O	1:A:122:LEU:HB3	2.04	0.58
2:B:351:ASN:C	2:B:351:ASN:ND2	2.56	0.58
2:E:185:ASP:O	2:E:188:ALA:HB3	2.03	0.58
3:I:166:LEU:HD23	3:I:218:LEU:HB3	1.85	0.58
2:K:141:GLU:O	2:K:145:GLU:HB2	2.04	0.58
3:L:367:ILE:HG21	3:L:382:THR:HG21	1.85	0.58
1:A:115:LEU:CD1	3:C:90:LEU:HB2	2.33	0.58
3:C:179:LEU:HD23	3:C:180:VAL:H	1.69	0.58
3:F:236:ILE:HG21	3:F:386:ILE:HD11	1.86	0.58
1:J:123:LYS:HA	1:J:126:VAL:HG12	1.85	0.58
1:J:207:MET:HA	1:J:210:VAL:HG12	1.86	0.58
3:F:393:THR:HG23	3:F:394:ILE:HD12	1.85	0.58
1:J:73:LEU:HD13	1:J:73:LEU:C	2.24	0.58
2:K:215:ILE:HD12	2:K:219:GLY:O	2.04	0.58
2:B:66:LEU:HD12	1:D:31:SER:HB3	1.86	0.58
2:B:186:VAL:HG12	2:B:187:SER:N	2.18	0.58
2:B:325:HIS:HB3	2:B:346:ARG:HG2	1.85	0.58
3:C:121:ILE:O	3:C:124:LEU:N	2.37	0.58
2:E:213:GLU:OE2	2:E:217:LYS:HE3	2.03	0.58
1:G:105:ASP:OD1	3:I:79:ILE:CD1	2.46	0.58
1:G:122:LEU:HB3	1:G:123:LYS:HZ2	1.69	0.58
2:K:144:SER:HB3	2:K:148:LYS:HZ1	1.68	0.58
3:L:169:ILE:HD13	3:L:180:VAL:HG11	1.85	0.58
1:A:91:MET:O	1:A:95:ARG:N	2.37	0.57
2:B:142:TYR:O	2:B:146:LEU:HG	2.04	0.57
3:F:90:LEU:HD22	3:F:90:LEU:C	2.24	0.57
2:H:178:LYS:O	2:H:181:LYS:HG3	2.03	0.57
2:H:205:VAL:HG23	3:I:216:GLY:O	2.04	0.57
2:K:345:TYR:CB	2:K:354:MET:HE2	2.33	0.57
1:A:149:ARG:O	1:A:152:VAL:CG1	2.52	0.57
1:J:133:ILE:O	1:J:137:GLN:HG3	2.04	0.57
2:H:415:ARG:O	2:H:434:GLY:HA2	2.05	0.57
1:J:184:GLN:HE21	2:K:167:VAL:CG2	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:210:VAL:HG21	2:K:131:GLN:HG3	1.86	0.57
3:C:97:GLU:O	3:C:100:ILE:HG22	2.05	0.57
2:E:394:CYS:SG	2:E:406:ARG:HA	2.45	0.57
3:I:289:ALA:HA	3:I:371:THR:HG23	1.87	0.57
2:B:205:VAL:O	2:B:205:VAL:CG1	2.53	0.57
1:D:122:LEU:HD12	1:D:123:LYS:HE3	1.86	0.57
3:F:197:ARG:CZ	3:F:367:ILE:HD11	2.35	0.57
1:G:150:LEU:O	1:G:154:ILE:HD13	2.04	0.57
2:H:251:VAL:HG22	2:H:453:LYS:HE2	1.86	0.57
2:E:312:ILE:HD11	2:E:452:MET:CE	2.35	0.57
1:G:108:TYR:CZ	3:I:82:ALA:HB1	2.38	0.57
1:J:58:VAL:HG22	1:J:62:PHE:CE1	2.39	0.57
1:A:70:LYS:HG2	2:B:100:LEU:HD21	1.86	0.57
2:B:179:ILE:HG23	2:B:180:GLN:H	1.70	0.57
1:D:111:VAL:HG11	3:F:87:ARG:HB2	1.85	0.57
2:E:210:GLU:OE1	2:E:213:GLU:N	2.30	0.57
2:E:310:LEU:HD12	2:E:311:LEU:N	2.19	0.57
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.53	0.57
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.85	0.57
1:J:136:LEU:O	1:J:140:VAL:HG13	2.05	0.57
2:K:140:ASN:N	2:K:140:ASN:OD1	2.38	0.57
2:K:312:ILE:HD13	2:K:452:MET:HG2	1.86	0.57
2:K:333:ASN:ND2	2:K:335:ALA:HB3	2.20	0.57
2:B:311:LEU:HD12	2:B:312:ILE:N	2.20	0.57
1:D:94:LEU:HD13	2:E:125:TRP:CD1	2.40	0.57
3:F:250:LEU:HD23	3:F:379:MET:HE2	1.86	0.57
3:L:143:VAL:O	3:L:143:VAL:CG2	2.53	0.57
2:B:153:ILE:O	2:B:153:ILE:HG22	2.05	0.56
3:I:10:ILE:O	3:I:18:TYR:CZ	2.57	0.56
3:I:334:TRP:HB3	3:I:336:MET:HE1	1.87	0.56
6:X:8:MAN:C1	6:X:9:NAG:O5	2.53	0.56
2:B:115:PHE:CE2	3:C:50:VAL:HG13	2.40	0.56
2:B:296:ASN:O	2:B:299:ILE:N	2.34	0.56
6:V:8:MAN:H62	6:V:10:GAL:H2	1.86	0.56
6:X:6:GAL:H5	6:X:7:SIA:O6	2.04	0.56
3:C:228:LEU:HD11	3:C:232:LYS:HD2	1.85	0.56
2:E:340:ILE:HG22	2:E:373:MET:O	2.05	0.56
3:F:217:HIS:C	3:F:218:LEU:HD23	2.26	0.56
3:I:338:LYS:N	3:I:339:CYS:HA	2.20	0.56
2:K:209:LYS:HA	2:K:228:GLN:O	2.04	0.56
3:L:228:LEU:HD11	3:L:232:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:8:MAN:C3	6:U:9:NAG:HN2	2.17	0.56
1:A:169:LEU:H	2:B:189:GLN:NE2	2.04	0.56
3:C:246:LEU:HD21	3:C:248:VAL:HG22	1.88	0.56
1:D:94:LEU:HD22	2:E:125:TRP:NE1	2.20	0.56
3:L:259:THR:O	3:L:286:ALA:HB3	2.06	0.56
2:H:224:MET:CE	2:H:237:ARG:HD3	2.36	0.56
2:H:351:ASN:HD21	2:H:354:MET:HG3	1.70	0.56
1:J:69:LEU:CD1	2:K:100:LEU:CD1	2.83	0.56
3:L:78:MET:O	3:L:81:ALA:N	2.38	0.56
6:V:7:SIA:H112	6:V:7:SIA:H7	1.88	0.56
6:V:9:NAG:H83	6:V:9:NAG:O3	2.06	0.56
1:A:70:LYS:HG3	2:B:100:LEU:HD11	1.87	0.56
1:A:122:LEU:C	1:A:122:LEU:HD13	2.26	0.56
1:D:169:LEU:HB2	2:E:189:GLN:HE22	1.70	0.56
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.40	0.56
3:F:289:ALA:HA	3:F:371:THR:HG23	1.87	0.56
1:G:58:VAL:HG13	1:G:62:PHE:CE2	2.40	0.56
3:I:209:ILE:HD12	3:I:209:ILE:N	2.21	0.56
2:K:101:ASN:OD1	3:L:43:LEU:HD13	2.06	0.56
3:F:249:GLU:C	3:F:250:LEU:HD12	2.26	0.56
1:J:162:ARG:HA	1:J:168:ALA:HB2	1.85	0.56
2:B:112:SER:HA	2:B:115:PHE:CD2	2.41	0.56
2:E:402:TRP:CZ3	2:E:412:PRO:HG2	2.41	0.56
3:I:297:ASP:OD1	3:I:297:ASP:N	2.38	0.56
2:E:402:TRP:CH2	2:E:412:PRO:HG3	2.41	0.56
3:I:143:VAL:O	3:I:143:VAL:CG2	2.53	0.56
3:I:344:LEU:HA	3:I:367:ILE:HG23	1.86	0.56
1:J:108:TYR:CE1	3:L:83:THR:CB	2.84	0.56
2:K:185:ASP:O	2:K:188:ALA:HB3	2.05	0.56
2:B:104:VAL:HG12	2:B:105:GLU:OE2	2.06	0.55
2:K:171:ILE:CG2	2:K:172:LEU:N	2.69	0.55
2:B:179:ILE:C	2:B:179:ILE:HD13	2.26	0.55
3:C:197:ARG:HH11	3:C:367:ILE:HD11	1.70	0.55
2:E:303:THR:HG22	2:E:308:THR:HG21	1.88	0.55
2:H:252:ILE:HD11	2:H:454:ILE:CG2	2.36	0.55
3:I:7:ASN:O	3:L:9:CYS:HA	2.07	0.55
1:J:108:TYR:OH	3:L:83:THR:CA	2.53	0.55
2:H:402:TRP:HB3	2:H:404:TYR:CE2	2.41	0.55
2:K:157:VAL:C	2:K:158:ASN:HD22	2.10	0.55
1:A:137:GLN:HB3	1:A:189:ILE:HD13	1.89	0.55
3:C:295:PHE:HB3	3:C:375:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:LYS:HZ3	2:H:153:ILE:HG21	1.70	0.55
3:I:310:MET:CE	3:I:321:LYS:HZ1	2.19	0.55
1:J:66:ILE:O	1:J:70:LYS:HG3	2.07	0.55
2:K:415:ARG:O	2:K:434:GLY:HA2	2.06	0.55
1:A:105:ASP:O	1:A:109:ASN:N	2.35	0.55
1:A:184:GLN:NE2	2:B:167:VAL:HG23	2.21	0.55
2:E:227:ILE:HD11	2:E:236:TYR:HE2	1.70	0.55
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.89	0.55
3:I:387:ILE:O	3:I:387:ILE:CG2	2.55	0.55
6:X:2:NAG:H5	6:X:3:BMA:C2	2.37	0.55
2:B:156:THR:HG22	2:B:157:VAL:N	2.22	0.55
3:C:276:LEU:HD21	3:C:278:TYR:HD2	1.68	0.55
3:I:151:LYS:HE2	3:I:172:LEU:HD13	1.89	0.55
3:F:218:LEU:N	3:F:218:LEU:CD2	2.70	0.55
1:J:207:MET:HE1	2:K:131:GLN:OE1	2.06	0.55
3:L:189:ASN:HD22	3:L:391:ARG:HE	1.54	0.55
2:H:117:TYR:CD1	2:H:120:LEU:HD12	2.42	0.55
3:L:334:TRP:CH2	3:L:344:LEU:HD12	2.40	0.55
3:C:390:ASN:ND2	3:C:391:ARG:N	2.48	0.54
3:F:191:TRP:CH2	3:F:247:ARG:HB2	2.42	0.54
1:A:149:ARG:O	1:A:152:VAL:HG12	2.08	0.54
2:K:340:ILE:HG22	2:K:403:TRP:CD1	2.42	0.54
2:B:123:ASP:O	2:B:127:LYS:N	2.40	0.54
2:B:176:ARG:O	2:B:179:ILE:HG22	2.07	0.54
1:D:169:LEU:HB2	2:E:189:GLN:NE2	2.23	0.54
2:E:182:LEU:O	2:E:185:ASP:N	2.40	0.54
3:F:289:ALA:HB1	3:F:341:ALA:O	2.08	0.54
1:J:140:VAL:HG23	1:J:141:ARG:N	2.23	0.54
3:L:79:ILE:HD12	3:L:79:ILE:H	1.73	0.54
3:L:338:LYS:N	3:L:339:CYS:HA	2.21	0.54
2:B:311:LEU:HD11	2:B:313:GLU:HG2	1.88	0.54
3:C:23:CYS:O	3:C:26:ALA:N	2.40	0.54
1:G:46:PRO:O	3:I:22:THR:CB	2.56	0.54
3:C:121:ILE:O	3:C:122:VAL:C	2.46	0.54
2:E:376:SER:OG	2:E:382:ASN:N	2.34	0.54
2:H:315:GLU:HA	2:H:320:ASP:O	2.06	0.54
3:L:110:LEU:HA	3:L:113:ILE:CG2	2.36	0.54
3:L:276:LEU:HD23	3:L:277:THR:N	2.22	0.54
2:B:300:SER:HB2	2:B:331:VAL:O	2.07	0.54
3:C:148:ILE:HD12	3:C:161:ALA:HB2	1.90	0.54
3:F:189:ASN:HB3	3:F:387:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:LYS:HE2	3:L:104:ASP:HB3	1.89	0.54
3:F:233:ILE:CG2	3:F:267:VAL:HG21	2.37	0.54
1:G:46:PRO:O	3:I:22:THR:OG1	2.21	0.54
3:L:234:HIS:HB2	3:L:267:VAL:HG12	1.88	0.54
3:L:352:GLY:O	3:L:377:TYR:HA	2.08	0.54
3:C:364:ASP:OD2	3:C:375:ARG:HG3	2.07	0.54
3:C:372:TRP:HZ3	3:C:379:MET:CE	2.21	0.54
1:D:89:ASN:O	1:D:93:ILE:HG23	2.06	0.54
2:H:59:ALA:HB1	2:H:60:PRO:CD	2.36	0.54
2:H:398:ASP:OD1	5:S:3:ARG:NH1	2.40	0.54
1:J:132:HIS:CG	3:L:107:ILE:HD11	2.43	0.54
1:A:181:GLN:HB3	2:B:171:ILE:HD11	1.90	0.54
2:B:299:ILE:O	2:B:303:THR:HG23	2.07	0.54
2:E:424:TRP:CH2	6:V:7:SIA:H31	2.43	0.54
3:I:238:THR:HG22	3:I:266:LYS:HG3	1.88	0.54
2:K:135:ASN:O	2:K:139:VAL:HG23	2.08	0.54
1:J:115:LEU:CD1	3:L:90:LEU:HD11	2.30	0.54
2:K:252:ILE:HG21	2:K:299:ILE:HG23	1.89	0.54
3:L:314:THR:C	3:L:327:ALA:CB	2.76	0.54
1:A:94:LEU:HD13	2:B:125:TRP:CZ3	2.43	0.53
3:C:349:TYR:CE1	3:C:354:TYR:CD1	2.96	0.53
2:E:275:ASN:N	2:E:291:GLU:O	2.41	0.53
3:L:84:LEU:HD23	3:L:84:LEU:C	2.28	0.53
3:L:152:ASP:OD1	3:L:154:GLN:N	2.40	0.53
6:U:7:SIA:H7	6:U:7:SIA:C10	2.39	0.53
1:A:188:VAL:CG1	2:B:164:ASN:ND2	2.71	0.53
1:G:73:LEU:O	1:G:73:LEU:HD22	2.08	0.53
2:H:351:ASN:C	2:H:351:ASN:HD22	2.10	0.53
3:I:10:ILE:C	3:I:18:TYR:HH	1.93	0.53
1:J:65:ARG:NH2	3:L:44:GLU:OE2	2.38	0.53
1:A:135:LEU:CD2	1:A:136:LEU:HD22	2.38	0.53
2:E:405:ASN:O	2:E:406:ARG:HB3	2.07	0.53
1:J:106:ASN:C	1:J:106:ASN:HD22	2.12	0.53
1:J:127:ILE:O	1:J:131:GLN:N	2.34	0.53
3:L:150:GLY:HA3	3:L:155:ASP:OD1	2.09	0.53
6:X:2:NAG:H5	6:X:3:BMA:H2	1.90	0.53
2:B:317:TRP:HB2	2:B:445:TYR:OH	2.08	0.53
2:E:135:ASN:HA	2:E:138:VAL:HG12	1.91	0.53
1:G:166:SER:CB	2:H:195:THR:OG1	2.56	0.53
2:H:326:TYR:OH	2:H:351:ASN:ND2	2.41	0.53
2:K:310:LEU:HD22	2:K:329:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.90	0.53
2:E:435:VAL:O	2:E:435:VAL:HG12	2.09	0.53
2:H:118:MET:O	2:H:123:ASP:N	2.40	0.53
3:I:191:TRP:CE3	3:I:385:LYS:HD2	2.43	0.53
3:I:249:GLU:HB2	3:I:383:THR:HG23	1.89	0.53
1:J:145:VAL:CG1	1:J:146:ASP:N	2.71	0.53
1:J:210:VAL:N	1:J:211:PRO:CD	2.72	0.53
2:K:252:ILE:HG21	2:K:299:ILE:CG2	2.37	0.53
3:L:23:CYS:O	3:L:26:ALA:N	2.37	0.53
1:A:71:ASN:C	1:A:71:ASN:ND2	2.62	0.53
3:C:217:HIS:O	3:C:224:THR:CG2	2.56	0.53
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.90	0.53
3:F:193:VAL:CG1	3:F:195:GLN:O	2.56	0.53
3:F:233:ILE:HG22	3:F:267:VAL:HG21	1.91	0.53
3:F:288:ASP:C	3:F:371:THR:HG21	2.29	0.53
1:G:97:ASP:O	1:G:101:ALA:HB3	2.08	0.53
3:L:120:LYS:O	3:L:123:ASN:HB2	2.09	0.53
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.90	0.53
3:C:249:GLU:C	3:C:250:LEU:HD12	2.29	0.53
1:D:64:ASN:C	1:D:64:ASN:HD22	2.12	0.53
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.91	0.53
2:H:405:ASN:O	2:H:406:ARG:HB3	2.09	0.53
3:L:229:GLY:O	3:L:233:ILE:HG13	2.08	0.53
2:E:369:ILE:H	2:E:405:ASN:HD22	1.55	0.53
2:H:122:LYS:NZ	3:I:60:LEU:HB3	2.23	0.53
2:K:137:ASN:HA	2:K:140:ASN:ND2	2.24	0.53
3:C:354:TYR:CE2	3:C:376:TRP:HA	2.44	0.53
3:C:372:TRP:CZ3	3:C:379:MET:HE2	2.44	0.53
2:E:421:GLN:HE21	2:E:421:GLN:HA	1.74	0.53
2:H:115:PHE:CZ	3:I:54:THR:HG22	2.43	0.53
2:B:373:MET:CG	2:B:405:ASN:HB2	2.35	0.52
3:C:251:GLU:HA	3:C:256:ARG:O	2.09	0.52
3:I:191:TRP:CE3	3:I:387:ILE:HB	2.44	0.52
2:K:351:ASN:C	2:K:351:ASN:HD22	2.11	0.52
4:M:3:ARG:HG3	4:M:4:PRO:O	2.08	0.52
6:X:8:MAN:H4	6:X:9:NAG:HN2	1.72	0.52
3:C:46:ILE:HG22	3:C:46:ILE:O	2.10	0.52
3:C:191:TRP:CZ3	3:C:387:ILE:CG2	2.92	0.52
3:C:340:HIS:C	3:C:340:HIS:HD1	2.13	0.52
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.07	0.52
3:L:167:TYR:O	3:L:179:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:OG	3:C:127:LYS:NZ	2.39	0.52
2:E:168:LEU:HD22	3:F:110:LEU:HD23	1.90	0.52
3:F:285:ASP:OD1	3:F:285:ASP:N	2.26	0.52
2:B:87:LEU:HD23	2:B:87:LEU:C	2.29	0.52
2:K:354:MET:O	2:K:369:ILE:HD13	2.10	0.52
1:A:73:LEU:HD22	1:A:73:LEU:O	2.10	0.52
2:K:280:THR:HG22	2:K:281:ASP:H	1.75	0.52
3:L:195:GLN:OE1	3:L:384:MET:HG3	2.09	0.52
2:E:172:LEU:HD23	3:F:113:ILE:HG23	1.88	0.52
2:E:280:THR:HG22	2:E:281:ASP:OD2	2.08	0.52
3:F:268:GLY:N	3:F:275:ARG:O	2.39	0.52
3:F:355:SER:O	3:F:359:THR:HG23	2.10	0.52
2:H:75:LEU:HD13	1:J:44:LYS:O	2.10	0.52
2:K:325:HIS:O	2:K:345:TYR:HA	2.09	0.52
3:L:246:LEU:HA	3:L:386:ILE:HG22	1.91	0.52
1:A:55:ILE:HG12	2:B:86:LEU:HD11	1.91	0.52
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.24	0.52
1:G:59:ASN:O	1:G:63:THR:HG23	2.09	0.52
2:H:342:VAL:HG23	2:H:354:MET:HG2	1.91	0.52
2:K:136:GLU:HB2	3:L:79:ILE:HD11	1.92	0.52
2:B:317:TRP:CD1	2:B:420:GLY:HA3	2.45	0.52
2:E:270:LYS:NZ	2:E:334:GLU:OE1	2.24	0.52
3:I:209:ILE:H	3:I:209:ILE:CD1	2.23	0.52
1:J:59:ASN:OD1	2:K:93:ILE:HD12	2.10	0.52
1:J:138:LYS:C	1:J:138:LYS:HD3	2.30	0.52
6:V:2:NAG:H5	6:V:3:BMA:O2	2.10	0.52
2:B:203:ILE:HD12	2:B:203:ILE:N	2.25	0.52
2:B:253:GLN:C	2:B:253:GLN:NE2	2.62	0.52
2:E:168:LEU:C	2:E:168:LEU:HD23	2.31	0.52
3:F:209:ILE:H	3:F:209:ILE:HD12	1.74	0.52
2:H:174:ASN:O	2:H:177:SER:OG	2.24	0.52
2:K:200:SER:HA	3:L:141:ASP:OD2	2.10	0.52
6:V:11:SIA:H7	6:V:11:SIA:C10	2.39	0.52
2:B:94:ARG:O	2:B:97:VAL:HG12	2.09	0.52
1:D:48:GLY:HA2	2:E:82:LEU:HD11	1.92	0.52
2:E:264:ARG:HG2	3:F:136:GLN:HE22	1.73	0.52
1:J:209:PRO:C	1:J:211:PRO:HD2	2.30	0.52
3:L:288:ASP:O	3:L:371:THR:HG21	2.09	0.52
2:B:212:GLU:O	2:B:213:GLU:C	2.48	0.51
2:E:82:LEU:CB	3:F:25:ILE:HD13	2.40	0.51
2:E:251:VAL:HB	2:E:292:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:260:VAL:HG23	2:E:291:GLU:HB2	1.92	0.51
3:F:268:GLY:O	3:F:274:TYR:HA	2.10	0.51
2:K:151:LEU:HD23	2:K:151:LEU:C	2.30	0.51
3:L:261:ASP:OD2	3:L:261:ASP:N	2.43	0.51
3:L:356:LYS:HG2	3:L:362:GLY:O	2.09	0.51
2:B:171:ILE:CG2	2:B:172:LEU:N	2.74	0.51
1:D:181:GLN:HB3	2:E:171:ILE:HD11	1.91	0.51
3:F:110:LEU:HD12	3:F:113:ILE:HG21	1.91	0.51
3:F:156:ILE:HG22	3:F:157:ALA:N	2.25	0.51
3:I:233:ILE:HA	3:I:236:ILE:HD12	1.92	0.51
2:K:252:ILE:HD11	2:K:454:ILE:HG23	1.93	0.51
6:U:6:GAL:H4	6:U:7:SIA:O6	2.10	0.51
6:V:6:GAL:H4	6:V:7:SIA:O4	2.11	0.51
1:A:48:GLY:CA	2:B:82:LEU:HD11	2.40	0.51
1:A:175:LEU:HD12	2:B:426:MET:HE1	1.91	0.51
1:D:86:LEU:HD23	3:F:61:ILE:HG21	1.91	0.51
2:E:252:ILE:HG21	2:E:299:ILE:HG23	1.92	0.51
2:E:340:ILE:CD1	2:E:403:TRP:CE3	2.93	0.51
3:I:179:LEU:HD23	3:I:218:LEU:CD1	2.39	0.51
2:K:302:LEU:HD22	2:K:454:ILE:CD1	2.22	0.51
2:B:150:GLN:O	2:B:153:ILE:N	2.43	0.51
2:E:82:LEU:HB2	3:F:25:ILE:HD13	1.92	0.51
2:E:168:LEU:HD22	3:F:110:LEU:HD21	1.93	0.51
2:H:99:GLU:O	2:H:103:ASN:N	2.43	0.51
3:I:196:LYS:HG3	3:I:197:ARG:N	2.25	0.51
1:J:63:THR:CA	1:J:66:ILE:HG22	2.37	0.51
2:K:314:MET:CG	2:K:322:VAL:HG23	2.40	0.51
1:A:175:LEU:HD23	1:A:176:LYS:H	1.76	0.51
3:C:372:TRP:HZ3	3:C:379:MET:HE2	1.75	0.51
1:J:196:SER:C	1:J:197:ARG:HD3	2.31	0.51
3:L:389:PHE:CD1	3:L:389:PHE:C	2.83	0.51
2:B:360:LEU:HD22	5:O:2:HIS:CE1	2.46	0.51
1:D:63:THR:CG2	2:E:93:ILE:HD11	2.40	0.51
1:D:69:LEU:HD13	3:F:47:LEU:CD1	2.41	0.51
3:F:141:ASP:OD2	3:F:143:VAL:HG13	2.10	0.51
2:H:252:ILE:HD11	2:H:454:ILE:CD1	2.35	0.51
1:A:70:LYS:CG	2:B:100:LEU:HD11	2.40	0.51
2:B:441:LYS:HB3	2:B:445:TYR:HB3	1.92	0.51
3:C:158:ASN:C	3:C:160:GLY:H	2.12	0.51
2:H:397:GLU:HG3	2:H:431:THR:HG21	1.93	0.51
3:L:81:ALA:O	3:L:85:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.46	0.51
2:B:146:LEU:HA	2:B:149:HIS:HB3	1.93	0.51
2:B:340:ILE:HB	2:B:403:TRP:CD1	2.45	0.51
3:C:207:ASN:OD1	3:C:209:ILE:N	2.44	0.51
1:D:86:LEU:HD23	3:F:61:ILE:CD1	2.40	0.51
1:G:52:LYS:HB2	2:H:82:LEU:HD21	1.92	0.51
3:L:124:LEU:O	3:L:128:VAL:HG23	2.10	0.51
1:G:184:GLN:NE2	2:H:167:VAL:HG23	2.26	0.51
2:H:296:ASN:O	2:H:299:ILE:N	2.44	0.51
3:I:11:LEU:HD23	3:I:11:LEU:C	2.32	0.51
3:I:238:THR:OG1	3:I:238:THR:O	2.28	0.51
3:I:365:ASN:HD22	3:I:365:ASN:H	1.57	0.51
2:K:257:ASP:O	2:K:291:GLU:OE2	2.29	0.51
1:A:48:GLY:O	1:A:52:LYS:N	2.28	0.51
1:A:104:ARG:HD3	3:C:79:ILE:HG21	1.92	0.51
2:B:78:THR:HG23	1:D:43:TYR:O	2.11	0.51
2:B:364:ASN:ND2	6:U:1:NAG:C2	2.66	0.51
3:C:356:LYS:HG3	3:C:362:GLY:O	2.11	0.51
1:D:135:LEU:HD23	1:D:135:LEU:C	2.32	0.51
2:E:314:MET:HA	2:E:449:LYS:O	2.11	0.51
2:E:437:TRP:O	2:E:438:MET:C	2.49	0.51
3:I:5:ARG:CB	3:I:11:LEU:HD13	2.40	0.51
1:J:69:LEU:C	1:J:69:LEU:CD1	2.79	0.51
1:J:70:LYS:HB3	1:J:74:PHE:CZ	2.46	0.51
2:K:104:VAL:HG11	3:L:47:LEU:HB2	1.93	0.51
3:L:172:LEU:HB2	3:L:239:GLN:HB2	1.92	0.50
6:X:11:SIA:H7	6:X:11:SIA:C10	2.41	0.50
1:A:111:VAL:O	1:A:115:LEU:CD1	2.60	0.50
1:A:136:LEU:O	1:A:140:VAL:HG13	2.10	0.50
2:B:104:VAL:O	2:B:108:SER:HB3	2.11	0.50
3:C:228:LEU:CD1	3:C:232:LYS:HD2	2.41	0.50
3:C:254:ASN:N	3:C:254:ASN:ND2	2.50	0.50
1:G:64:ASN:OD1	1:G:65:ARG:N	2.44	0.50
2:K:145:GLU:HA	2:K:145:GLU:OE2	2.12	0.50
3:L:340:HIS:CE1	4:R:1:GLY:H2	2.29	0.50
2:B:171:ILE:HG22	2:B:172:LEU:N	2.26	0.50
3:C:246:LEU:HD12	3:C:386:ILE:HG22	1.93	0.50
3:I:272:ASP:OD1	3:I:275:ARG:NH1	2.45	0.50
1:J:167:ARG:HB3	2:K:192:TYR:HB3	1.92	0.50
2:K:169:ARG:HE	3:L:110:LEU:HD21	1.76	0.50
3:I:27:ASP:O	3:I:31:THR:CG2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD22	2:B:125:TRP:CZ3	2.47	0.50
2:B:223:GLU:HG2	2:B:225:TYR:CE2	2.46	0.50
3:C:69:ASN:O	3:C:71:ASP:N	2.44	0.50
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.94	0.50
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.46	0.50
1:G:147:MET:SD	3:I:121:ILE:HD11	2.52	0.50
3:I:251:GLU:HB2	3:I:257:THR:HG22	1.94	0.50
3:L:219:SER:CB	3:L:224:THR:HG21	2.42	0.50
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.92	0.50
1:D:115:LEU:HD13	3:F:86:SER:HA	1.93	0.50
3:F:224:THR:HG23	3:F:224:THR:O	2.12	0.50
1:J:108:TYR:HH	3:L:84:LEU:H	1.55	0.50
2:K:230:ASP:O	2:K:233:VAL:HG12	2.11	0.50
2:K:252:ILE:HD12	2:K:452:MET:O	2.12	0.50
2:K:257:ASP:OD1	2:K:259:SER:CB	2.60	0.50
6:X:2:NAG:C6	6:X:5:NAG:H83	2.36	0.50
1:A:48:GLY:HA2	2:B:82:LEU:HD11	1.94	0.50
2:E:360:LEU:HD13	5:P:2:HIS:ND1	2.26	0.50
2:K:257:ASP:OD1	2:K:259:SER:OG	2.23	0.50
3:L:251:GLU:CD	3:L:381:LYS:NZ	2.65	0.50
2:E:295:GLY:O	2:E:298:LYS:HB2	2.12	0.50
3:F:330:ASP:OD2	3:F:340:HIS:NE2	2.44	0.50
3:I:5:ARG:HG2	3:I:11:LEU:HB3	1.93	0.50
3:I:195:GLN:OE1	3:I:382:THR:HG22	2.11	0.50
3:I:250:LEU:N	3:I:250:LEU:CD1	2.74	0.50
2:B:284:ASN:H	2:B:284:ASN:HD22	1.59	0.50
1:D:111:VAL:HG11	3:F:87:ARG:CB	2.42	0.50
2:E:257:ASP:OD1	2:E:259:SER:OG	2.24	0.50
3:F:69:ASN:HB2	3:F:70:PRO:HD2	1.93	0.50
3:F:80:ASP:O	3:F:82:ALA:N	2.45	0.50
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.12	0.50
3:I:356:LYS:HA	3:I:359:THR:CG2	2.41	0.50
1:J:208:LYS:HB2	1:J:209:PRO:CD	2.41	0.50
1:J:210:VAL:N	1:J:211:PRO:HD2	2.27	0.50
1:A:59:ASN:ND2	2:B:86:LEU:HD23	2.20	0.49
2:B:87:LEU:HD23	2:B:87:LEU:O	2.12	0.49
3:C:262:TYR:CE2	3:C:290:PHE:HB2	2.47	0.49
1:D:63:THR:HG23	2:E:93:ILE:HD11	1.94	0.49
1:D:143:GLN:NE2	3:F:118:ASN:OD1	2.45	0.49
3:I:3:ALA:HB2	3:L:11:LEU:CD1	2.42	0.49
5:T:2:HIS:CD2	5:T:4:PRO:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ILE:HG22	2:B:172:LEU:CD1	2.42	0.49
2:H:326:TYR:CE1	2:H:353:LEU:HD12	2.48	0.49
2:K:351:ASN:ND2	2:K:354:MET:H	2.09	0.49
3:L:291:ASP:OD1	3:L:302:LYS:NZ	2.44	0.49
3:L:297:ASP:N	3:L:297:ASP:OD1	2.45	0.49
1:A:136:LEU:HD13	1:A:139:ASN:HD22	1.76	0.49
3:C:276:LEU:HD23	3:C:276:LEU:O	2.13	0.49
3:C:304:PHE:O	3:C:337:ASN:CG	2.51	0.49
3:L:194:PHE:CD1	3:L:233:ILE:HD13	2.47	0.49
3:C:289:ALA:O	3:C:292:GLY:N	2.35	0.49
2:E:314:MET:HG3	2:E:322:VAL:HG23	1.95	0.49
3:L:193:VAL:O	3:L:226:PHE:HZ	1.95	0.49
3:L:248:VAL:HG12	3:L:249:GLU:N	2.27	0.49
3:F:166:LEU:HD11	3:F:220:PRO:N	2.28	0.49
2:H:402:TRP:CE3	2:H:413:ASN:ND2	2.81	0.49
3:I:208:TRP:CE3	3:I:317:ASN:HB3	2.48	0.49
1:J:115:LEU:CD1	3:L:90:LEU:HD21	2.42	0.49
3:L:295:PHE:HE1	3:L:305:THR:HG21	1.77	0.49
3:I:281:PHE:CD2	3:I:283:GLY:HA2	2.46	0.49
1:J:93:ILE:HD12	1:J:94:LEU:HD23	1.93	0.49
2:K:215:ILE:CD1	2:K:242:MET:HB3	2.42	0.49
2:K:255:ARG:NH1	2:K:412:PRO:O	2.43	0.49
3:L:264:MET:SD	3:L:264:MET:N	2.86	0.49
3:L:379:MET:HA	3:L:379:MET:CE	2.41	0.49
2:B:385:TRP:CD1	2:B:406:ARG:HG3	2.48	0.49
1:D:86:LEU:HD21	3:F:61:ILE:HG21	1.93	0.49
2:E:108:SER:HA	2:E:111:SER:HB3	1.95	0.49
2:E:205:VAL:HG22	3:F:218:LEU:CD2	2.43	0.49
3:F:246:LEU:HD12	3:F:246:LEU:C	2.33	0.49
3:F:375:ARG:HG3	3:F:376:TRP:N	2.27	0.49
1:G:97:ASP:O	1:G:101:ALA:HB2	2.13	0.49
1:J:127:ILE:CA	1:J:130:VAL:HG12	2.39	0.49
3:L:197:ARG:O	3:L:381:LYS:HA	2.13	0.49
3:C:258:SER:HB2	3:C:286:ALA:HB2	1.94	0.49
1:D:115:LEU:HD13	3:F:86:SER:HB2	1.94	0.49
2:H:210:GLU:OE1	2:H:213:GLU:N	2.45	0.49
2:H:329:PHE:HE2	2:H:454:ILE:HG21	1.77	0.49
1:J:152:VAL:HG11	2:K:426:MET:HB3	1.95	0.49
3:L:225:GLU:O	3:L:226:PHE:HB3	2.12	0.49
1:A:133:ILE:HD11	3:C:107:ILE:CG1	2.42	0.49
1:A:200:GLN:NE2	2:B:149:HIS:NE2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:LYS:O	2:E:181:LYS:HG3	2.13	0.49
2:E:439:ASN:HD22	2:E:439:ASN:H	1.59	0.49
3:I:288:ASP:C	3:I:371:THR:HG21	2.33	0.49
1:J:129:LYS:CE	3:L:104:ASP:HB3	2.43	0.49
3:L:367:ILE:O	3:L:378:SER:HA	2.13	0.49
2:B:179:ILE:CG2	2:B:180:GLN:H	2.26	0.49
2:E:179:ILE:HD12	3:F:120:LYS:HD3	1.95	0.49
2:H:308:THR:CG2	2:H:454:ILE:HB	2.43	0.49
2:H:326:TYR:CZ	2:H:353:LEU:HD12	2.48	0.49
3:C:301:ASP:O	3:C:305:THR:OG1	2.30	0.48
1:D:149:ARG:NE	2:E:427:ALA:O	2.45	0.48
2:E:161:ILE:HG21	3:F:103:HIS:CG	2.47	0.48
2:E:330:THR:O	2:E:331:VAL:HG22	2.12	0.48
2:E:351:ASN:C	2:E:351:ASN:HD22	2.16	0.48
2:H:343:ASN:HA	2:H:354:MET:SD	2.53	0.48
2:K:410:ALA:CB	2:K:437:TRP:CE3	2.96	0.48
3:L:214:GLY:HA3	3:L:228:LEU:O	2.13	0.48
2:E:199:VAL:HG23	3:F:141:ASP:CA	2.42	0.48
3:F:166:LEU:CD2	3:F:218:LEU:HB2	2.43	0.48
3:F:191:TRP:CE3	3:F:385:LYS:CG	2.96	0.48
1:G:46:PRO:O	3:I:22:THR:HG21	2.13	0.48
1:G:116:ARG:HD3	2:H:142:TYR:OH	2.13	0.48
1:J:145:VAL:HG13	1:J:146:ASP:H	1.76	0.48
1:A:46:PRO:O	3:C:22:THR:HG21	2.13	0.48
1:D:65:ARG:O	1:D:69:LEU:HD23	2.13	0.48
3:F:352:GLY:O	3:F:354:TYR:HD2	1.95	0.48
3:I:305:THR:HB	3:I:341:ALA:HB2	1.96	0.48
3:I:355:SER:O	3:I:359:THR:HG23	2.14	0.48
2:K:122:LYS:O	2:K:125:TRP:HB3	2.13	0.48
2:E:152:TYR:O	2:E:156:THR:HG22	2.13	0.48
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.95	0.48
3:L:46:ILE:HG22	3:L:46:ILE:O	2.12	0.48
2:B:252:ILE:HD11	2:B:454:ILE:CG2	2.43	0.48
3:C:246:LEU:HD12	3:C:386:ILE:CG2	2.44	0.48
3:C:292:GLY:HA2	3:C:341:ALA:CB	2.43	0.48
3:C:340:HIS:ND1	3:C:340:HIS:C	2.67	0.48
2:E:321:LYS:O	2:E:322:VAL:HG13	2.13	0.48
3:F:169:ILE:HD11	3:F:180:VAL:CG2	2.41	0.48
6:U:2:NAG:H5	6:U:3:BMA:C2	2.43	0.48
6:V:7:SIA:O1A	6:V:7:SIA:H6	2.13	0.48
3:C:246:LEU:CD2	3:C:248:VAL:CG2	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:ILE:O	3:C:387:ILE:HG23	2.13	0.48
2:E:205:VAL:HG21	3:F:215:PHE:O	2.14	0.48
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.48	0.48
3:I:365:ASN:HD22	3:I:365:ASN:N	2.12	0.48
2:K:148:LYS:HD3	2:K:148:LYS:N	2.28	0.48
3:L:172:LEU:H	3:L:239:GLN:HE21	1.61	0.48
6:U:2:NAG:H3	6:U:3:BMA:O2	2.13	0.48
3:C:347:VAL:CG2	3:C:349:TYR:CE1	2.97	0.48
3:F:327:ALA:HB1	3:F:332:SER:O	2.13	0.48
3:I:236:ILE:HA	3:I:239:GLN:HE21	1.78	0.48
1:J:138:LYS:C	1:J:138:LYS:CD	2.82	0.48
3:L:207:ASN:C	3:L:207:ASN:OD1	2.52	0.48
3:L:259:THR:N	3:L:286:ALA:HB2	2.29	0.48
3:L:307:HIS:CE1	3:L:341:ALA:H	2.31	0.48
1:A:165:CYS:HA	2:B:196:PRO:HA	1.96	0.48
1:A:185:LEU:HD11	1:A:189:ILE:HD11	1.95	0.48
2:B:178:LYS:O	2:B:179:ILE:C	2.52	0.48
2:B:352:ALA:HB1	2:B:409:ALA:HB3	1.95	0.48
3:I:253:TRP:C	3:I:254:ASN:HD22	2.16	0.48
1:J:169:LEU:HD22	1:J:171:ARG:HG2	1.96	0.48
2:K:212:GLU:HA	2:K:215:ILE:HG22	1.95	0.48
2:K:300:SER:OG	2:K:301:GLN:N	2.46	0.48
2:B:101:ASN:CG	3:C:43:LEU:HD11	2.34	0.48
2:B:115:PHE:HE2	3:C:50:VAL:HG13	1.78	0.48
2:E:266:TRP:CD1	2:E:380:ARG:NH2	2.82	0.48
3:I:15:PHE:O	3:L:24:GLY:HA3	2.14	0.48
1:J:62:PHE:O	1:J:66:ILE:HB	2.13	0.48
2:K:353:LEU:O	2:K:369:ILE:HG23	2.14	0.48
3:L:110:LEU:HA	3:L:113:ILE:HG22	1.96	0.48
6:U:8:MAN:O5	6:U:9:NAG:H3	2.13	0.48
6:V:3:BMA:H3	6:V:4:MAN:O2	2.13	0.48
2:B:101:ASN:OD1	3:C:43:LEU:CD2	2.61	0.48
2:B:125:TRP:O	2:B:129:GLN:HB3	2.13	0.48
3:C:252:ASP:HB2	3:C:373:LYS:NZ	2.29	0.48
2:E:322:VAL:HG12	2:E:348:THR:HB	1.95	0.48
2:E:370:HIS:O	2:E:373:MET:N	2.36	0.48
2:E:424:TRP:CZ2	6:V:7:SIA:H31	2.49	0.48
1:G:123:LYS:HA	1:G:123:LYS:HE3	1.96	0.48
1:G:157:LYS:HD2	3:I:128:VAL:HG13	1.96	0.48
3:I:234:HIS:HB2	3:I:267:VAL:HG12	1.95	0.48
3:I:247:ARG:NE	3:I:261:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:VAL:HG11	3:L:87:ARG:HD2	1.95	0.48
2:K:435:VAL:HG12	2:K:435:VAL:O	2.12	0.48
3:L:154:GLN:O	3:L:157:ALA:HB3	2.14	0.48
2:B:113:SER:O	2:B:116:GLN:NE2	2.46	0.47
2:B:281:ASP:O	2:B:283:LYS:NZ	2.46	0.47
3:C:238:THR:O	3:C:238:THR:OG1	2.24	0.47
2:E:228:GLN:NE2	2:E:231:SER:HA	2.29	0.47
1:G:63:THR:O	1:G:66:ILE:HG22	2.14	0.47
3:I:169:ILE:CD1	3:I:180:VAL:HG11	2.43	0.47
1:J:194:LEU:HD12	2:K:152:TYR:CD2	2.49	0.47
1:A:135:LEU:HD22	1:A:136:LEU:HD22	1.97	0.47
2:B:295:GLY:O	2:B:299:ILE:HG13	2.13	0.47
2:K:249:TRP:HB3	2:K:453:LYS:HD3	1.96	0.47
3:C:90:LEU:O	3:C:90:LEU:HD12	2.12	0.47
3:C:215:PHE:CE2	3:C:227:TRP:CB	2.95	0.47
1:D:86:LEU:HD23	3:F:61:ILE:CG2	2.44	0.47
3:F:31:THR:HG22	3:F:35:LYS:NZ	2.28	0.47
1:G:169:LEU:HD23	1:G:170:ALA:N	2.29	0.47
2:K:199:VAL:HG23	3:L:141:ASP:CB	2.44	0.47
3:L:298:ASP:OD2	3:L:300:SER:N	2.44	0.47
6:X:2:NAG:H62	6:X:5:NAG:H81	1.95	0.47
2:B:67:HIS:CD2	2:B:69:ASP:HB3	2.50	0.47
2:B:210:GLU:OE2	2:B:210:GLU:C	2.52	0.47
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.96	0.47
2:B:409:ALA:O	2:B:438:MET:HB2	2.14	0.47
3:C:216:GLY:HA3	3:C:226:PHE:CB	2.44	0.47
2:E:351:ASN:ND2	2:E:351:ASN:C	2.68	0.47
3:F:262:TYR:OH	3:F:288:ASP:OD1	2.16	0.47
3:L:247:ARG:HG3	3:L:248:VAL:O	2.14	0.47
3:L:389:PHE:C	3:L:389:PHE:HD1	2.16	0.47
2:B:255:ARG:HA	2:B:291:GLU:HG2	1.96	0.47
2:B:342:VAL:C	2:B:343:ASN:HD22	2.17	0.47
3:C:252:ASP:OD2	3:C:256:ARG:NH1	2.47	0.47
3:F:281:PHE:HB2	3:F:288:ASP:OD2	2.14	0.47
2:H:226:LEU:HD12	2:H:236:TYR:C	2.35	0.47
2:K:112:SER:HA	2:K:115:PHE:HD2	1.79	0.47
2:K:179:ILE:O	2:K:183:GLU:HB2	2.14	0.47
2:K:257:ASP:OD1	2:K:259:SER:HB3	2.15	0.47
1:A:188:VAL:HG12	2:B:164:ASN:ND2	2.29	0.47
2:B:80:CYS:O	2:B:84:GLU:N	2.30	0.47
3:L:289:ALA:HA	3:L:371:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:CG1	1:A:59:ASN:N	2.78	0.47
3:C:27:ASP:O	3:C:31:THR:HG23	2.15	0.47
1:D:160:SER:HA	2:E:258:GLY:O	2.15	0.47
1:G:60:GLN:HE22	1:G:64:ASN:HD22	1.61	0.47
2:H:415:ARG:N	2:H:434:GLY:HA2	2.30	0.47
3:I:228:LEU:O	3:I:232:LYS:HD2	2.15	0.47
3:I:325:ASN:C	3:I:325:ASN:HD22	2.18	0.47
3:L:147:ASP:OD1	3:L:147:ASP:N	2.47	0.47
3:L:304:PHE:O	3:L:306:SER:N	2.48	0.47
5:T:4:PRO:CG	6:X:1:NAG:H62	2.45	0.47
1:A:148:LYS:O	1:A:152:VAL:HG12	2.15	0.47
1:D:59:ASN:O	1:D:63:THR:HG23	2.14	0.47
2:E:402:TRP:CZ3	2:E:412:PRO:CG	2.98	0.47
2:K:147:GLU:O	2:K:150:GLN:HG3	2.15	0.47
3:L:90:LEU:HD23	3:L:90:LEU:C	2.35	0.47
3:L:153:CYS:O	3:L:156:ILE:HB	2.15	0.47
3:C:178:PHE:CD1	3:C:232:LYS:HD3	2.50	0.47
1:D:162:ARG:HA	1:D:168:ALA:HB2	1.96	0.47
1:G:166:SER:CB	2:H:195:THR:HG1	2.28	0.47
2:H:342:VAL:CG2	2:H:354:MET:HG2	2.45	0.47
3:I:115:ASN:HD22	3:I:115:ASN:C	2.18	0.47
3:I:286:ALA:O	3:I:372:TRP:HB2	2.14	0.47
1:J:123:LYS:HA	1:J:123:LYS:HE3	1.97	0.47
2:K:172:LEU:HD11	3:L:114:TYR:HB2	1.96	0.47
3:L:219:SER:HG	3:L:224:THR:CG2	2.26	0.47
5:T:4:PRO:HG3	6:X:1:NAG:H62	1.97	0.47
2:B:163:THR:HG22	2:B:166:ARG:HH22	1.80	0.47
2:B:212:GLU:HA	2:B:215:ILE:HG22	1.96	0.47
3:C:206:LYS:HB2	3:C:211:TYR:HE1	1.78	0.47
2:E:233:VAL:HG22	2:E:234:LYS:O	2.14	0.47
2:E:402:TRP:CH2	2:E:412:PRO:CG	2.97	0.47
2:H:101:ASN:OD1	3:I:43:LEU:HD11	2.14	0.47
2:H:314:MET:HB3	2:H:314:MET:HE2	1.82	0.47
2:H:314:MET:HE2	2:H:450:MET:SD	2.55	0.47
3:L:169:ILE:HD11	3:L:180:VAL:HG11	1.97	0.47
3:L:219:SER:CB	3:L:224:THR:CG2	2.93	0.47
1:A:147:MET:O	1:A:148:LYS:C	2.53	0.46
3:C:179:LEU:CD2	3:C:180:VAL:O	2.63	0.46
1:D:134:GLN:OE1	1:D:193:LEU:HD22	2.15	0.46
2:E:410:ALA:HB2	2:E:437:TRP:CE3	2.49	0.46
3:F:51:GLU:HA	3:F:54:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:TYR:HE1	3:L:83:THR:CG2	2.28	0.46
2:B:343:ASN:HA	2:B:354:MET:SD	2.55	0.46
3:C:163:GLN:O	3:C:167:TYR:OH	2.30	0.46
3:C:183:GLU:O	3:C:191:TRP:HB2	2.16	0.46
3:C:374:THR:OG1	3:C:375:ARG:N	2.48	0.46
2:E:435:VAL:O	2:E:447:MET:HG2	2.14	0.46
2:H:200:SER:O	2:H:279:ASN:ND2	2.48	0.46
2:H:260:VAL:HG12	2:H:261:ASP:O	2.14	0.46
2:H:329:PHE:CE2	2:H:454:ILE:HG21	2.51	0.46
2:K:312:ILE:CB	2:K:324:ALA:HB3	2.41	0.46
2:B:329:PHE:HD1	2:B:342:VAL:HG12	1.79	0.46
3:C:264:MET:HB2	3:C:279:ALA:CB	2.45	0.46
3:F:211:TYR:CE1	3:F:333:GLY:HA3	2.50	0.46
3:F:332:SER:CB	3:F:343:HIS:NE2	2.78	0.46
2:H:171:ILE:HG23	2:H:172:LEU:H	1.78	0.46
2:H:420:GLY:HA2	2:H:446:SER:O	2.16	0.46
2:E:91:ARG:N	2:E:92:PRO:HD2	2.30	0.46
3:I:304:PHE:CG	3:I:338:LYS:HE3	2.51	0.46
3:L:96:TYR:O	3:L:100:ILE:HD13	2.15	0.46
1:A:41:TRP:O	1:A:42:ASN:HB2	2.15	0.46
2:B:252:ILE:CD1	2:B:454:ILE:CG2	2.91	0.46
3:C:179:LEU:HD23	3:C:180:VAL:O	2.16	0.46
3:F:122:VAL:HG13	3:F:123:ASN:ND2	2.30	0.46
1:G:135:LEU:HD23	1:G:136:LEU:HD22	1.98	0.46
2:H:140:ASN:C	2:H:140:ASN:HD22	2.19	0.46
2:H:302:LEU:HD13	2:H:454:ILE:HD11	1.98	0.46
1:J:111:VAL:HG21	3:L:87:ARG:CZ	2.45	0.46
1:J:140:VAL:CG2	1:J:141:ARG:N	2.78	0.46
2:K:172:LEU:HD22	3:L:113:ILE:CG2	2.41	0.46
2:K:340:ILE:HG21	2:K:403:TRP:CG	2.50	0.46
3:L:109:TYR:O	3:L:113:ILE:HG22	2.15	0.46
2:B:253:GLN:NE2	2:B:451:SER:HA	2.30	0.46
2:B:345:TYR:CG	2:B:346:ARG:N	2.82	0.46
3:C:113:ILE:O	3:C:117:ASN:HB2	2.15	0.46
3:F:143:VAL:O	3:F:143:VAL:HG22	2.16	0.46
3:F:334:TRP:HB3	3:F:336:MET:HE2	1.96	0.46
2:H:210:GLU:OE2	2:H:212:GLU:HB3	2.15	0.46
2:H:364:ASN:HA	2:H:367:MET:HE3	1.98	0.46
2:K:436:VAL:HG12	2:K:437:TRP:N	2.30	0.46
1:D:151:GLU:CG	1:D:173:VAL:HG11	2.45	0.46
3:I:240:SER:O	3:I:241:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:ARG:HB2	1:J:159:ARG:CZ	2.45	0.46
1:J:206:LYS:O	1:J:210:VAL:N	2.47	0.46
2:K:424:TRP:CG	2:K:425:ASP:N	2.84	0.46
3:C:21:THR:HG23	3:C:24:GLY:H	1.81	0.46
3:C:219:SER:H	3:C:224:THR:HG21	1.81	0.46
3:C:264:MET:HB2	3:C:279:ALA:HB2	1.98	0.46
3:C:290:PHE:HA	3:C:307:HIS:HD1	1.79	0.46
3:C:304:PHE:O	3:C:337:ASN:ND2	2.49	0.46
1:G:122:LEU:HD12	1:G:123:LYS:NZ	2.31	0.46
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.98	0.46
3:I:29:LEU:HD12	3:I:33:GLN:HB2	1.97	0.46
3:I:60:LEU:O	3:I:64:ILE:HD13	2.16	0.46
3:L:205:LYS:HD2	3:L:331:GLY:CA	2.46	0.46
2:B:172:LEU:CD2	3:C:110:LEU:HD22	2.46	0.46
2:B:181:LYS:HD3	2:B:182:LEU:HD12	1.97	0.46
2:B:364:ASN:ND2	6:U:1:NAG:N2	2.64	0.46
3:C:132:GLU:C	3:C:134:GLN:H	2.19	0.46
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.13	0.46
2:E:435:VAL:HG12	2:E:447:MET:CG	2.46	0.46
3:F:210:GLN:O	3:F:214:GLY:N	2.43	0.46
3:L:49:GLN:HE21	8:Y:1:NAG:C8	2.28	0.46
3:L:198:LEU:HD13	3:L:199:ASP:HB3	1.98	0.46
1:A:96:GLY:O	1:A:99:SER:N	2.44	0.46
1:A:160:SER:O	2:B:259:SER:O	2.33	0.46
2:B:345:TYR:CD2	2:B:345:TYR:C	2.90	0.46
3:C:246:LEU:CD2	3:C:248:VAL:HG23	2.45	0.46
2:E:226:LEU:HD12	2:E:236:TYR:C	2.37	0.46
2:E:376:SER:HG	2:E:382:ASN:H	1.62	0.46
3:F:254:ASN:HD22	3:F:254:ASN:N	2.15	0.46
1:G:73:LEU:HD11	2:H:103:ASN:OD1	2.16	0.46
6:U:8:MAN:H4	6:U:9:NAG:HN2	1.79	0.46
2:B:136:GLU:O	2:B:140:ASN:O	2.34	0.45
3:C:169:ILE:HD13	3:C:180:VAL:HG21	1.98	0.45
2:E:298:LYS:O	2:E:302:LEU:HB2	2.16	0.45
3:F:168:PHE:CE2	3:F:179:LEU:HD13	2.51	0.45
1:G:65:ARG:CD	3:I:40:LEU:HD23	2.47	0.45
1:G:185:LEU:CD1	1:G:189:ILE:HD11	2.44	0.45
2:H:105:GLU:OE2	3:I:46:ILE:HG21	2.16	0.45
3:I:225:GLU:O	3:I:226:PHE:HB3	2.16	0.45
2:K:259:SER:OG	2:K:291:GLU:HG3	2.16	0.45
6:V:3:BMA:H5	6:V:5:NAG:H82	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:O	1:A:152:VAL:HG13	2.16	0.45
1:A:169:LEU:H	2:B:189:GLN:HE22	1.63	0.45
1:A:188:VAL:HG12	2:B:164:ASN:HD21	1.81	0.45
2:B:134:ASP:O	2:B:138:VAL:HG12	2.16	0.45
1:D:55:ILE:HD11	3:F:25:ILE:CG2	2.46	0.45
2:H:66:LEU:HD22	1:J:35:PHE:CE1	2.51	0.45
2:H:167:VAL:HG13	2:H:168:LEU:N	2.31	0.45
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.98	0.45
3:I:148:ILE:HG22	3:I:149:THR:N	2.32	0.45
2:K:436:VAL:HG21	2:K:443:SER:O	2.16	0.45
2:B:364:ASN:ND2	6:U:1:NAG:O5	2.42	0.45
1:J:73:LEU:HD13	1:J:74:PHE:N	2.31	0.45
2:K:84:GLU:OE1	3:L:5:ARG:NH1	2.50	0.45
2:K:150:GLN:O	2:K:153:ILE:N	2.47	0.45
3:L:295:PHE:CE1	3:L:305:THR:HG21	2.50	0.45
3:L:343:HIS:O	3:L:343:HIS:CG	2.70	0.45
2:B:118:MET:HG3	3:C:57:VAL:HG13	1.99	0.45
2:B:198:THR:HG22	3:C:140:LYS:HB2	1.97	0.45
2:B:329:PHE:C	2:B:330:THR:CG2	2.85	0.45
3:C:231:GLU:OE1	3:C:274:TYR:OH	2.16	0.45
1:D:41:TRP:O	1:D:42:ASN:CB	2.65	0.45
1:D:52:LYS:HB2	2:E:82:LEU:HD21	1.97	0.45
1:G:66:ILE:HG23	1:G:70:LYS:HE2	1.98	0.45
3:I:5:ARG:HD3	3:I:5:ARG:O	2.17	0.45
3:I:108:ARG:O	3:I:111:GLN:HG2	2.16	0.45
3:L:305:THR:HB	3:L:341:ALA:HB2	1.98	0.45
1:A:73:LEU:CD2	2:B:104:VAL:HG22	2.40	0.45
3:C:216:GLY:HA3	3:C:226:PHE:HB2	1.97	0.45
2:H:367:MET:SD	2:H:406:ARG:CD	3.00	0.45
1:J:69:LEU:HD12	2:K:100:LEU:HD11	1.99	0.45
1:A:104:ARG:HH22	3:C:78:MET:CE	2.30	0.45
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.99	0.45
3:C:181:TYR:CE1	3:C:220:PRO:O	2.64	0.45
2:E:163:THR:HG23	2:E:166:ARG:HH12	1.81	0.45
2:E:300:SER:HB2	2:E:331:VAL:O	2.16	0.45
3:F:218:LEU:C	3:F:224:THR:HG21	2.37	0.45
3:F:342:GLY:O	3:F:344:LEU:N	2.48	0.45
1:G:185:LEU:O	1:G:185:LEU:HD22	2.17	0.45
3:I:21:THR:HG23	3:I:24:GLY:H	1.82	0.45
3:I:267:VAL:CG1	3:I:268:GLY:N	2.80	0.45
2:K:230:ASP:O	2:K:233:VAL:CG1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:152:ASP:OD1	3:L:152:ASP:C	2.54	0.45
1:A:94:LEU:HD22	2:B:125:TRP:HZ3	1.80	0.45
3:C:166:LEU:HD21	3:C:218:LEU:HB3	1.99	0.45
1:D:29:LYS:O	1:D:31:SER:N	2.50	0.45
3:F:251:GLU:O	3:F:380:LYS:HB3	2.17	0.45
2:K:256:GLN:O	2:K:449:LYS:NZ	2.44	0.45
2:K:326:TYR:CZ	2:K:353:LEU:HD12	2.52	0.45
5:P:4:PRO:HB3	6:V:1:NAG:H62	1.99	0.45
1:A:150:LEU:HD22	3:C:125:LYS:HE3	1.99	0.45
3:C:97:GLU:C	3:C:100:ILE:HG22	2.36	0.45
2:E:253:GLN:C	2:E:253:GLN:NE2	2.69	0.45
2:E:435:VAL:HG12	2:E:447:MET:HG2	1.99	0.45
2:H:402:TRP:HB3	2:H:404:TYR:CD2	2.52	0.45
3:L:340:HIS:ND1	3:L:343:HIS:HB3	2.32	0.45
1:A:58:VAL:HG12	1:A:59:ASN:N	2.32	0.45
3:I:10:ILE:HG13	2:K:83:GLN:HE22	1.82	0.45
3:I:224:THR:HG23	3:I:224:THR:O	2.17	0.45
3:L:291:ASP:OD1	3:L:302:LYS:CE	2.65	0.45
3:L:372:TRP:HZ3	3:L:379:MET:HE1	1.81	0.45
1:D:45:CYS:HB3	1:D:46:PRO:HD2	1.98	0.45
1:G:116:ARG:NE	2:H:142:TYR:OH	2.50	0.45
3:I:166:LEU:HD11	3:I:220:PRO:N	2.31	0.45
1:J:115:LEU:HD11	3:L:90:LEU:HD21	1.99	0.45
1:J:151:GLU:HG2	1:J:173:VAL:HG13	1.99	0.45
2:K:128:ARG:O	2:K:132:VAL:HG22	2.17	0.45
2:K:140:ASN:O	2:K:144:SER:OG	2.22	0.45
2:K:357:ALA:HA	2:K:439:ASN:HD21	1.82	0.45
2:B:253:GLN:HE22	2:B:451:SER:HA	1.81	0.44
1:D:63:THR:O	1:D:66:ILE:HG22	2.16	0.44
1:D:150:LEU:HD11	3:F:125:LYS:NZ	2.32	0.44
2:E:415:ARG:O	2:E:434:GLY:HA2	2.17	0.44
2:K:272:GLY:HA3	2:K:295:GLY:N	2.32	0.44
3:L:221:THR:OG1	3:L:223:THR:CG2	2.64	0.44
5:S:4:PRO:HB3	7:W:1:NAG:C6	2.46	0.44
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.99	0.44
1:D:122:LEU:HD12	1:D:123:LYS:CE	2.47	0.44
2:E:104:VAL:O	2:E:104:VAL:HG12	2.17	0.44
2:E:424:TRP:CG	2:E:425:ASP:N	2.85	0.44
3:F:202:VAL:HG12	3:F:203:ASP:O	2.17	0.44
1:G:135:LEU:HD23	1:G:139:ASN:HD22	1.82	0.44
2:K:401:GLY:O	2:K:413:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:LEU:HB3	3:L:18:TYR:CZ	2.52	0.44
3:F:246:LEU:HD12	3:F:247:ARG:CA	2.46	0.44
3:I:12:ASP:CG	3:I:15:PHE:CD1	2.90	0.44
3:I:156:ILE:HD13	3:I:167:TYR:CD2	2.53	0.44
3:I:208:TRP:HB3	3:I:209:ILE:HD12	1.99	0.44
1:J:55:ILE:HG23	2:K:86:LEU:CD2	2.47	0.44
1:J:55:ILE:O	1:J:58:VAL:HG12	2.18	0.44
2:K:95:ASN:C	2:K:95:ASN:ND2	2.70	0.44
2:B:156:THR:HG22	2:B:157:VAL:HG23	2.00	0.44
1:D:69:LEU:HD13	3:F:47:LEU:HD11	2.00	0.44
2:E:63:GLY:O	2:E:77:PRO:HD3	2.18	0.44
2:E:212:GLU:O	2:E:213:GLU:C	2.56	0.44
2:H:121:LEU:HD23	2:H:124:LEU:HD23	1.99	0.44
3:I:310:MET:CE	3:I:321:LYS:NZ	2.80	0.44
1:J:66:ILE:HD11	2:K:100:LEU:HD12	1.99	0.44
3:L:173:LYS:NZ	3:L:238:THR:O	2.49	0.44
6:X:10:GAL:H4	6:X:11:SIA:H31	1.98	0.44
2:B:258:GLY:O	2:B:260:VAL:N	2.51	0.44
3:C:68:TYR:O	3:C:69:ASN:HB2	2.18	0.44
3:C:207:ASN:OD1	3:C:207:ASN:C	2.56	0.44
2:E:161:ILE:HB	2:E:162:PRO:HD3	2.00	0.44
2:H:201:CYS:HB3	2:H:224:MET:HE3	1.99	0.44
2:H:295:GLY:O	2:H:299:ILE:HG13	2.17	0.44
2:H:337:LYS:O	2:H:338:TYR:C	2.55	0.44
3:L:318:ASP:OD1	3:L:320:ASP:OD1	2.36	0.44
6:U:2:NAG:H5	6:U:3:BMA:H2	1.99	0.44
6:V:2:NAG:H5	6:V:3:BMA:C2	2.48	0.44
1:A:99:SER:HA	1:A:102:ASN:HD22	1.83	0.44
2:B:294:LEU:HD12	2:B:295:GLY:N	2.29	0.44
1:D:30:ASP:O	1:D:32:ASP:N	2.51	0.44
2:E:291:GLU:O	2:E:292:TYR:HB3	2.16	0.44
3:F:236:ILE:CG2	3:F:386:ILE:HD11	2.46	0.44
2:H:314:MET:HG3	2:H:322:VAL:CG2	2.48	0.44
3:I:251:GLU:CB	3:I:257:THR:HG22	2.48	0.44
1:J:63:THR:C	1:J:66:ILE:HG22	2.37	0.44
2:K:314:MET:HE2	2:K:314:MET:HB3	1.79	0.44
1:A:105:ASP:O	1:A:108:TYR:N	2.51	0.44
1:A:194:LEU:HG	2:B:152:TYR:CD2	2.52	0.44
3:C:275:ARG:HA	3:C:311:GLN:HA	1.99	0.44
1:D:115:LEU:HD13	3:F:86:SER:CA	2.48	0.44
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:289:ALA:CA	3:F:371:THR:HG23	2.46	0.44
1:G:166:SER:N	2:H:195:THR:O	2.40	0.44
2:H:233:VAL:HG22	2:H:234:LYS:O	2.18	0.44
3:I:10:ILE:CD1	2:K:83:GLN:HE22	2.30	0.44
1:J:69:LEU:CD1	2:K:100:LEU:HD11	2.47	0.44
1:J:201:HIS:CE1	1:J:202:LEU:HD23	2.53	0.44
3:L:193:VAL:O	3:L:226:PHE:CZ	2.71	0.44
1:D:119:ILE:HD11	3:F:93:ILE:CD1	2.40	0.44
1:D:151:GLU:HG3	1:D:173:VAL:HG11	1.98	0.44
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.99	0.44
3:F:254:ASN:N	3:F:254:ASN:ND2	2.65	0.44
3:I:151:LYS:CE	3:I:172:LEU:HD13	2.47	0.44
3:I:166:LEU:HD23	3:I:218:LEU:CB	2.47	0.44
3:L:80:ASP:N	3:L:80:ASP:OD1	2.51	0.44
3:L:248:VAL:HG12	3:L:250:LEU:HD13	2.00	0.44
6:V:2:NAG:H3	6:V:2:NAG:O7	2.17	0.44
2:B:405:ASN:CG	2:B:405:ASN:O	2.55	0.44
3:C:167:TYR:CD1	3:C:167:TYR:N	2.86	0.44
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.99	0.44
2:H:75:LEU:HD22	1:J:46:PRO:CD	2.48	0.44
2:H:135:ASN:O	2:H:139:VAL:N	2.50	0.44
3:I:240:SER:HB2	3:I:242:ILE:HG13	1.99	0.44
2:K:151:LEU:HA	2:K:154:ASP:HB3	2.00	0.44
2:K:373:MET:HG3	2:K:405:ASN:HB2	2.00	0.44
3:L:156:ILE:HG22	3:L:157:ALA:N	2.32	0.44
3:L:197:ARG:CZ	3:L:367:ILE:HD11	2.48	0.44
3:L:198:LEU:CD1	3:L:199:ASP:N	2.75	0.44
3:L:367:ILE:CG2	3:L:382:THR:HG21	2.48	0.44
3:C:197:ARG:NH2	3:C:204:PHE:CD2	2.83	0.43
3:C:288:ASP:O	3:C:289:ALA:C	2.54	0.43
1:D:115:LEU:HD13	3:F:86:SER:CB	2.48	0.43
2:E:410:ALA:HA	2:E:436:VAL:O	2.18	0.43
3:F:100:ILE:HG22	3:F:101:LEU:HD12	1.99	0.43
2:H:99:GLU:O	2:H:103:ASN:HB2	2.17	0.43
2:H:373:MET:HA	2:H:373:MET:CE	2.48	0.43
2:B:203:ILE:HD12	2:B:203:ILE:H	1.82	0.43
3:C:338:LYS:N	3:C:339:CYS:HA	2.32	0.43
2:E:241:ASP:OD2	2:E:243:ASN:N	2.42	0.43
2:E:351:ASN:ND2	2:E:354:MET:H	2.12	0.43
3:F:281:PHE:CB	3:F:288:ASP:OD2	2.66	0.43
3:L:380:LYS:HG2	3:L:381:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:THR:HG22	2:B:166:ARG:HH12	1.82	0.43
2:E:212:GLU:HA	2:E:215:ILE:HG22	2.00	0.43
2:E:302:LEU:HD22	2:E:454:ILE:HD11	1.99	0.43
3:F:50:VAL:O	3:F:54:THR:HB	2.18	0.43
3:F:193:VAL:HA	3:F:385:LYS:HB3	2.00	0.43
1:G:143:GLN:O	1:G:146:ASP:N	2.51	0.43
2:H:252:ILE:HG23	2:H:299:ILE:HD13	2.01	0.43
2:H:434:GLY:O	2:H:436:VAL:N	2.51	0.43
1:J:154:ILE:HD11	3:L:128:VAL:CG2	2.46	0.43
1:J:175:LEU:O	1:J:178:TYR:N	2.52	0.43
3:L:196:LYS:O	3:L:225:GLU:HA	2.18	0.43
3:L:207:ASN:OD1	3:L:209:ILE:N	2.51	0.43
3:L:300:SER:O	3:L:301:ASP:C	2.56	0.43
5:O:4:PRO:HG3	6:U:1:NAG:H62	2.00	0.43
2:B:105:GLU:O	2:B:109:GLN:HB2	2.18	0.43
2:B:264:ARG:HD2	2:B:273:PHE:CD2	2.54	0.43
2:B:294:LEU:HD11	2:B:298:LYS:HD3	1.99	0.43
3:C:174:ALA:CB	3:C:235:LEU:HD13	2.47	0.43
3:C:387:ILE:O	3:C:388:PRO:C	2.56	0.43
3:F:119:GLN:O	3:F:122:VAL:HG12	2.18	0.43
3:I:145:ILE:HD13	3:I:179:LEU:HD13	2.00	0.43
3:I:199:ASP:OD1	3:I:201:SER:CB	2.66	0.43
1:J:145:VAL:CG1	1:J:146:ASP:H	2.31	0.43
2:K:91:ARG:N	2:K:92:PRO:HD2	2.34	0.43
2:K:100:LEU:O	2:K:104:VAL:HG23	2.18	0.43
2:K:139:VAL:HG11	3:L:79:ILE:HG23	2.01	0.43
2:K:310:LEU:HD12	2:K:310:LEU:C	2.38	0.43
2:K:338:TYR:O	2:K:403:TRP:NE1	2.46	0.43
3:L:281:PHE:CZ	3:L:283:GLY:HA2	2.54	0.43
3:L:307:HIS:HE1	3:L:341:ALA:H	1.64	0.43
1:A:63:THR:HA	1:A:66:ILE:CG2	2.47	0.43
3:C:300:SER:O	3:C:301:ASP:C	2.56	0.43
1:G:60:GLN:NE2	1:G:64:ASN:HD22	2.16	0.43
2:H:115:PHE:CZ	3:I:54:THR:CG2	3.02	0.43
3:I:289:ALA:HA	3:I:371:THR:CG2	2.48	0.43
3:I:372:TRP:HZ3	3:I:379:MET:CE	2.32	0.43
3:L:228:LEU:CD1	3:L:232:LYS:HD2	2.48	0.43
3:C:267:VAL:HG13	3:C:268:GLY:N	2.34	0.43
3:C:295:PHE:HZ	3:C:341:ALA:HA	1.84	0.43
2:E:226:LEU:HD12	2:E:236:TYR:O	2.19	0.43
2:E:257:ASP:OD1	2:E:259:SER:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:330:THR:O	2:E:331:VAL:CG2	2.66	0.43
2:H:394:CYS:SG	2:H:406:ARG:HA	2.59	0.43
1:J:169:LEU:HD12	2:K:188:ALA:HB3	2.00	0.43
3:L:156:ILE:HD13	3:L:167:TYR:CD2	2.53	0.43
3:L:172:LEU:H	3:L:239:GLN:NE2	2.17	0.43
3:L:359:THR:HG22	3:L:365:ASN:ND2	2.33	0.43
2:B:80:CYS:HA	2:B:83:GLN:HG3	1.99	0.43
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.43
3:C:31:THR:OG1	3:C:32:TYR:N	2.52	0.43
3:C:191:TRP:CD2	3:C:385:LYS:HE3	2.54	0.43
1:D:100:SER:HB3	3:F:80:ASP:CG	2.39	0.43
1:D:156:ILE:HD13	2:E:415:ARG:NH1	2.34	0.43
3:F:90:LEU:C	3:F:90:LEU:CD2	2.85	0.43
3:F:234:HIS:CE1	3:F:238:THR:HG21	2.54	0.43
3:I:5:ARG:HA	3:I:11:LEU:CD1	2.48	0.43
3:L:211:TYR:O	3:L:230:ASN:OD1	2.36	0.43
7:W:1:NAG:O3	7:W:2:NAG:H2	2.17	0.43
2:E:330:THR:C	2:E:331:VAL:CG2	2.87	0.43
2:H:211:CYS:HB2	2:H:250:THR:OG1	2.18	0.43
3:I:5:ARG:HA	3:I:11:LEU:HD12	2.01	0.43
2:K:457:PHE:C	2:K:458:PHE:CG	2.92	0.43
3:L:387:ILE:HG23	3:L:388:PRO:O	2.19	0.43
3:C:166:LEU:CD2	3:C:218:LEU:HB3	2.49	0.43
2:E:210:GLU:OE1	2:E:213:GLU:HB2	2.18	0.43
2:E:410:ALA:CB	2:E:437:TRP:CE3	3.02	0.43
3:F:275:ARG:HA	3:F:310:MET:O	2.18	0.43
3:I:195:GLN:OE1	3:I:382:THR:CG2	2.67	0.43
3:I:326:CYS:HB2	3:I:336:MET:HG3	2.00	0.43
3:I:382:THR:CG2	3:I:383:THR:N	2.82	0.43
1:J:69:LEU:CD1	2:K:100:LEU:HD13	2.36	0.43
2:K:134:ASP:O	2:K:138:VAL:HG23	2.18	0.43
3:L:49:GLN:HE21	8:Y:1:NAG:H81	1.73	0.43
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.53	0.43
3:L:270:GLU:O	3:L:273:LYS:N	2.40	0.43
2:B:352:ALA:HB1	2:B:409:ALA:CB	2.48	0.43
3:F:168:PHE:O	3:F:169:ILE:HG23	2.19	0.43
3:F:249:GLU:O	3:F:250:LEU:HD12	2.18	0.43
1:G:67:ASN:O	1:G:71:ASN:HB2	2.19	0.43
1:G:156:ILE:O	1:G:160:SER:N	2.42	0.43
2:H:361:MET:CB	7:W:1:NAG:H81	2.47	0.43
3:I:116:SER:O	3:I:117:ASN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:SER:HB3	1:J:116:ARG:NH2	2.34	0.43
1:J:205:ILE:CG1	2:K:138:VAL:HG11	2.42	0.43
2:K:183:GLU:OE1	3:L:120:LYS:NZ	2.27	0.43
3:L:217:HIS:O	3:L:224:THR:OG1	2.33	0.43
7:W:2:NAG:H3	7:W:3:BMA:O2	2.19	0.43
2:B:160:ASN:O	2:B:163:THR:OG1	2.19	0.42
2:B:185:ASP:O	2:B:188:ALA:HB3	2.19	0.42
3:C:100:ILE:HG23	3:C:101:LEU:CD2	2.44	0.42
3:C:236:ILE:O	3:C:239:GLN:HG2	2.19	0.42
2:E:135:ASN:O	2:E:139:VAL:HG12	2.18	0.42
2:E:295:GLY:O	2:E:296:ASN:C	2.58	0.42
3:I:27:ASP:OD1	3:I:28:PHE:N	2.51	0.42
3:I:329:GLN:HA	3:I:361:ASN:HD21	1.83	0.42
2:K:137:ASN:O	2:K:141:GLU:HG2	2.19	0.42
2:K:435:VAL:HG12	2:K:447:MET:HG2	2.01	0.42
3:L:100:ILE:O	3:L:104:ASP:HB2	2.18	0.42
3:L:150:GLY:CA	3:L:155:ASP:OD1	2.66	0.42
3:C:47:LEU:HD23	3:C:47:LEU:C	2.39	0.42
1:D:73:LEU:C	1:D:73:LEU:HD13	2.40	0.42
2:E:284:ASN:C	2:E:284:ASN:HD22	2.21	0.42
2:E:303:THR:HB	2:E:330:THR:HA	2.01	0.42
2:E:355:ASP:O	2:E:369:ILE:HD11	2.19	0.42
3:F:242:ILE:H	3:F:242:ILE:HD12	1.83	0.42
1:G:42:ASN:O	2:K:78:THR:HG21	2.18	0.42
2:H:203:ILE:HG22	2:H:204:PRO:O	2.19	0.42
2:H:260:VAL:CG2	2:H:291:GLU:HB2	2.49	0.42
2:K:215:ILE:HD13	2:K:242:MET:HB3	2.01	0.42
2:K:439:ASN:N	2:K:439:ASN:ND2	2.57	0.42
3:L:361:ASN:H	3:L:361:ASN:HD22	1.68	0.42
2:B:276:VAL:HA	2:B:292:TYR:CD2	2.54	0.42
2:B:342:VAL:O	2:B:371:ASN:ND2	2.52	0.42
1:D:66:ILE:HG13	2:E:100:LEU:HD11	2.00	0.42
3:I:334:TRP:CB	3:I:336:MET:HE1	2.48	0.42
1:J:184:GLN:NE2	2:K:167:VAL:HG23	2.18	0.42
1:J:210:VAL:HG11	2:K:131:GLN:NE2	2.34	0.42
3:L:145:ILE:CD1	3:L:179:LEU:HD22	2.49	0.42
6:V:4:MAN:O3	6:V:5:NAG:C1	2.67	0.42
2:B:226:LEU:HA	2:B:226:LEU:HD12	1.71	0.42
3:C:247:ARG:HB2	3:C:261:ASP:OD2	2.19	0.42
3:C:276:LEU:C	3:C:276:LEU:CD2	2.82	0.42
2:H:139:VAL:HG11	3:I:78:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:307:HIS:CE1	3:I:341:ALA:H	2.37	0.42
1:J:144:LEU:HD23	1:J:182:GLN:HG3	2.01	0.42
2:K:293:TRP:HZ2	2:K:296:ASN:HD21	1.66	0.42
3:L:229:GLY:O	3:L:233:ILE:N	2.43	0.42
3:C:243:PRO:HG2	3:C:389:PHE:HB3	2.02	0.42
3:C:393:THR:O	3:C:394:ILE:HD13	2.20	0.42
2:E:345:TYR:CG	2:E:346:ARG:N	2.88	0.42
2:H:253:GLN:C	2:H:253:GLN:NE2	2.73	0.42
2:H:267:ASP:HB3	2:H:268:PRO:HD3	2.00	0.42
1:J:115:LEU:HD11	3:L:90:LEU:CD2	2.49	0.42
3:L:382:THR:C	3:L:383:THR:HG22	2.39	0.42
2:B:381:ASP:C	2:B:381:ASP:OD2	2.58	0.42
2:E:179:ILE:HD11	3:F:120:LYS:HG2	2.02	0.42
2:K:172:LEU:HD23	3:L:113:ILE:HD13	2.00	0.42
3:L:178:PHE:CE1	3:L:180:VAL:HG12	2.54	0.42
3:L:194:PHE:CZ	3:L:384:MET:HB3	2.55	0.42
6:U:6:GAL:H62	6:U:7:SIA:H32	1.87	0.42
2:E:356:GLY:HA2	2:E:368:THR:O	2.19	0.42
2:H:167:VAL:CG1	2:H:168:LEU:N	2.83	0.42
3:I:12:ASP:OD2	3:I:15:PHE:CE1	2.73	0.42
3:I:334:TRP:HB3	3:I:336:MET:CE	2.50	0.42
2:K:275:ASN:OD1	3:L:139:CYS:N	2.47	0.42
2:K:367:MET:SD	5:T:2:HIS:HB2	2.60	0.42
2:E:303:THR:HA	2:E:308:THR:OG1	2.19	0.42
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.20	0.42
3:F:262:TYR:HD2	3:F:278:TYR:CD1	2.37	0.42
3:F:338:LYS:N	3:F:339:CYS:HA	2.35	0.42
2:H:171:ILE:CG2	2:H:172:LEU:N	2.81	0.42
2:H:410:ALA:HA	2:H:436:VAL:O	2.19	0.42
3:I:3:ALA:CB	3:L:11:LEU:HD12	2.45	0.42
3:I:332:SER:HG	3:I:343:HIS:CE1	2.30	0.42
2:K:172:LEU:HD23	3:L:113:ILE:CD1	2.50	0.42
2:K:402:TRP:CG	2:K:403:TRP:N	2.88	0.42
3:L:367:ILE:HG21	3:L:382:THR:CG2	2.47	0.42
6:U:1:NAG:O3	6:U:2:NAG:C2	2.66	0.42
1:A:135:LEU:HD23	1:A:136:LEU:HD22	2.00	0.42
3:F:307:HIS:O	3:F:310:MET:HG2	2.19	0.42
1:G:66:ILE:HD11	2:H:100:LEU:HD12	2.02	0.42
1:G:93:ILE:HG22	1:G:94:LEU:CD1	2.42	0.42
1:G:144:LEU:HD21	1:G:182:GLN:HA	2.02	0.42
3:I:10:ILE:HD11	2:K:83:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:TYR:CE2	3:L:80:ASP:O	2.73	0.42
1:J:200:GLN:NE2	2:K:145:GLU:HB3	2.35	0.42
3:L:304:PHE:C	3:L:306:SER:H	2.23	0.42
1:A:104:ARG:HD3	3:C:79:ILE:CG2	2.49	0.42
2:B:405:ASN:O	2:B:406:ARG:CB	2.68	0.42
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.88	0.42
3:C:346:GLY:HA3	3:C:367:ILE:HG13	2.02	0.42
1:G:45:CYS:HB2	2:K:78:THR:HG22	2.02	0.42
2:H:91:ARG:N	2:H:92:PRO:HD2	2.35	0.42
2:H:109:GLN:O	2:H:113:SER:N	2.50	0.42
3:I:191:TRP:CD2	3:I:385:LYS:HD2	2.55	0.42
3:I:322:PHE:HB2	3:I:338:LYS:HG3	2.02	0.42
2:K:316:ASP:OD2	2:K:320:ASP:N	2.53	0.42
3:L:270:GLU:O	3:L:271:ALA:C	2.57	0.42
1:A:107:THR:O	1:A:111:VAL:HB	2.20	0.41
2:B:201:CYS:O	3:C:143:VAL:HG21	2.18	0.41
3:C:237:SER:OG	3:C:238:THR:HG23	2.20	0.41
3:F:193:VAL:HG13	3:F:195:GLN:O	2.19	0.41
3:F:307:HIS:O	3:F:308:ASN:C	2.56	0.41
1:G:48:GLY:HA2	2:H:82:LEU:HD11	2.02	0.41
1:G:188:VAL:HG11	2:H:164:ASN:HD21	1.85	0.41
2:H:267:ASP:O	2:H:271:GLN:HG2	2.20	0.41
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.55	0.41
1:J:210:VAL:HG21	2:K:131:GLN:CG	2.49	0.41
3:L:212:LYS:HE3	3:L:274:TYR:OH	2.20	0.41
3:L:281:PHE:CE2	3:L:283:GLY:HA2	2.55	0.41
6:U:6:GAL:H3	6:U:7:SIA:O7	2.19	0.41
2:B:223:GLU:HA	2:B:287:GLY:HA2	2.02	0.41
2:B:354:MET:O	2:B:369:ILE:CG2	2.66	0.41
2:B:415:ARG:O	2:B:434:GLY:HA2	2.20	0.41
3:C:316:ASP:OD1	3:C:316:ASP:N	2.52	0.41
3:F:90:LEU:HD22	3:F:91:GLU:CA	2.50	0.41
3:F:228:LEU:HD12	3:F:228:LEU:O	2.20	0.41
1:G:143:GLN:O	1:G:144:LEU:C	2.59	0.41
2:H:253:GLN:NE2	2:H:452:MET:HG3	2.35	0.41
1:J:54:LEU:HD23	2:K:60:PRO:HG2	2.02	0.41
2:K:226:LEU:HD12	2:K:227:ILE:H	1.84	0.41
2:K:317:TRP:CD1	2:K:420:GLY:HA3	2.55	0.41
2:B:457:PHE:O	2:B:458:PHE:HB2	2.21	0.41
2:H:125:TRP:CD1	2:H:126:GLN:N	2.88	0.41
2:H:175:LEU:O	2:H:178:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:186:VAL:CG1	2:K:187:SER:N	2.83	0.41
2:K:329:PHE:CD1	2:K:329:PHE:C	2.92	0.41
6:V:1:NAG:O3	6:V:2:NAG:N2	2.54	0.41
3:C:19:CYS:HB3	3:C:20:PRO:HD2	2.02	0.41
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.34	0.41
3:C:267:VAL:CG1	3:C:268:GLY:N	2.80	0.41
2:E:69:ASP:HB3	2:E:72:LEU:HB2	2.02	0.41
3:F:31:THR:HG22	3:F:35:LYS:HZ2	1.86	0.41
2:K:224:MET:SD	2:K:237:ARG:HB3	2.60	0.41
3:L:221:THR:O	3:L:223:THR:HG23	2.20	0.41
1:A:200:GLN:HB3	2:B:146:LEU:HD11	2.03	0.41
2:B:184:SER:O	2:B:185:ASP:C	2.58	0.41
3:C:154:GLN:O	3:C:157:ALA:HB3	2.20	0.41
1:D:185:LEU:HD22	1:D:189:ILE:HG13	2.02	0.41
1:G:139:ASN:O	1:G:142:ALA:HB3	2.21	0.41
3:L:205:LYS:HD2	3:L:331:GLY:HA2	2.01	0.41
1:A:86:LEU:HD12	1:A:89:ASN:HD22	1.85	0.41
1:A:156:ILE:HD13	2:B:415:ARG:CZ	2.50	0.41
2:B:91:ARG:HB3	2:B:92:PRO:HD3	2.03	0.41
2:E:118:MET:O	2:E:122:LYS:CB	2.68	0.41
3:F:184:ILE:HG22	3:F:185:ASP:O	2.21	0.41
3:F:246:LEU:HD12	3:F:247:ARG:C	2.40	0.41
3:I:108:ARG:O	3:I:112:GLU:HG2	2.19	0.41
3:I:340:HIS:ND1	3:I:343:HIS:HB2	2.35	0.41
1:J:148:LYS:NZ	2:K:425:ASP:OD1	2.53	0.41
2:K:205:VAL:HG12	3:L:232:LYS:HZ2	1.85	0.41
1:A:137:GLN:O	1:A:140:VAL:HG22	2.21	0.41
3:C:75:LYS:HB3	3:C:78:MET:CE	2.46	0.41
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.56	0.41
3:C:206:LYS:HB2	3:C:211:TYR:CD1	2.55	0.41
3:C:356:LYS:O	3:C:362:GLY:HA2	2.20	0.41
3:C:390:ASN:C	3:C:390:ASN:ND2	2.74	0.41
1:D:116:ARG:NH2	2:E:146:LEU:HD21	2.35	0.41
2:E:294:LEU:O	2:E:299:ILE:HD11	2.21	0.41
1:G:188:VAL:O	1:G:189:ILE:C	2.59	0.41
3:L:245:ALA:HB3	3:L:387:ILE:CG2	2.51	0.41
2:B:160:ASN:HA	2:B:163:THR:OG1	2.21	0.41
2:B:329:PHE:O	2:B:330:THR:HG22	2.21	0.41
2:B:340:ILE:CG1	2:B:341:SER:N	2.84	0.41
1:D:122:LEU:HD12	1:D:123:LYS:HZ1	1.86	0.41
2:E:118:MET:SD	3:F:60:LEU:HD23	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:THR:HG22	3:F:140:LYS:O	2.21	0.41
1:J:127:ILE:HA	1:J:130:VAL:CG1	2.46	0.41
2:K:199:VAL:HG23	3:L:141:ASP:HB2	2.02	0.41
2:K:340:ILE:HB	2:K:403:TRP:CE2	2.56	0.41
3:L:54:THR:O	3:L:58:LYS:HB2	2.21	0.41
3:L:168:PHE:CD2	3:L:179:LEU:HD13	2.56	0.41
2:B:78:THR:HG22	1:D:45:CYS:SG	2.60	0.41
2:B:103:ASN:HA	2:B:107:VAL:HG23	2.03	0.41
2:B:141:GLU:HG3	2:B:144:SER:OG	2.21	0.41
2:B:163:THR:O	2:B:167:VAL:HG12	2.21	0.41
2:B:212:GLU:O	2:B:215:ILE:N	2.53	0.41
3:C:234:HIS:O	3:C:238:THR:HG23	2.21	0.41
3:C:292:GLY:HA2	3:C:341:ALA:HB2	2.02	0.41
2:E:172:LEU:HD23	3:F:113:ILE:CG2	2.51	0.41
2:E:432:ASP:O	2:E:432:ASP:CG	2.59	0.41
1:G:133:ILE:HG21	2:H:164:ASN:OD1	2.21	0.41
2:H:405:ASN:O	2:H:406:ARG:CB	2.68	0.41
2:H:439:ASN:HD22	2:H:439:ASN:N	2.19	0.41
3:I:69:ASN:N	3:I:70:PRO:CD	2.84	0.41
3:I:207:ASN:ND2	3:I:209:ILE:HD13	2.26	0.41
3:I:372:TRP:CE3	3:I:373:LYS:HG2	2.56	0.41
1:J:210:VAL:HG21	2:K:131:GLN:CD	2.41	0.41
2:K:151:LEU:HD23	2:K:151:LEU:O	2.20	0.41
2:K:458:PHE:CD1	2:K:458:PHE:N	2.87	0.41
3:L:229:GLY:O	3:L:232:LYS:N	2.53	0.41
3:L:251:GLU:OE1	3:L:381:LYS:HE3	2.21	0.41
1:A:104:ARG:HH22	3:C:78:MET:HE2	1.86	0.41
2:B:100:LEU:O	2:B:104:VAL:HG23	2.21	0.41
3:C:294:ASP:OD2	3:C:302:LYS:HB2	2.21	0.41
1:G:165:CYS:HA	2:H:196:PRO:HA	2.02	0.41
1:J:80:ASN:OD1	1:J:80:ASN:C	2.59	0.41
3:L:115:ASN:HD22	3:L:115:ASN:HA	1.76	0.41
3:L:227:TRP:CD1	3:L:227:TRP:C	2.93	0.41
1:A:46:PRO:O	3:C:22:THR:CG2	2.70	0.40
2:B:432:ASP:OD2	2:B:432:ASP:N	2.54	0.40
3:C:124:LEU:O	3:C:128:VAL:HG12	2.21	0.40
3:C:305:THR:HB	3:C:341:ALA:HB2	2.03	0.40
3:C:365:ASN:N	3:C:365:ASN:ND2	2.66	0.40
1:D:102:ASN:OD1	1:D:103:ASN:N	2.54	0.40
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.56	0.40
1:D:141:ARG:NH1	1:D:186:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:N	1:D:193:LEU:HD23	2.36	0.40
2:E:200:SER:O	2:E:279:ASN:ND2	2.54	0.40
2:E:205:VAL:CG2	3:F:215:PHE:O	2.69	0.40
2:E:227:ILE:O	2:E:235:PRO:HA	2.21	0.40
2:E:256:GLN:NE2	2:E:289:PRO:O	2.54	0.40
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.22	0.40
2:H:349:ALA:HB1	2:H:437:TRP:NE1	2.36	0.40
3:I:194:PHE:HA	3:I:228:LEU:HB2	2.03	0.40
3:I:340:HIS:CE1	3:I:368:ILE:HD11	2.56	0.40
3:L:334:TRP:HB3	3:L:336:MET:SD	2.61	0.40
2:B:159:SER:O	2:B:163:THR:CG2	2.55	0.40
2:H:152:TYR:O	2:H:153:ILE:HD13	2.22	0.40
3:I:5:ARG:CA	3:I:11:LEU:HD13	2.51	0.40
3:I:230:ASN:HA	3:I:233:ILE:HD12	2.01	0.40
1:J:111:VAL:HG21	3:L:87:ARG:NH1	2.36	0.40
2:K:387:THR:HG22	2:K:388:SER:H	1.86	0.40
3:L:249:GLU:O	3:L:383:THR:HG23	2.20	0.40
1:A:73:LEU:HD13	1:A:73:LEU:C	2.41	0.40
1:A:184:GLN:HE21	2:B:167:VAL:HG23	1.85	0.40
2:B:266:TRP:HA	2:B:377:THR:HG21	2.02	0.40
2:B:373:MET:HA	2:B:373:MET:HE3	2.04	0.40
2:H:157:VAL:HG12	2:H:157:VAL:O	2.21	0.40
3:I:149:THR:CG2	3:I:150:GLY:N	2.84	0.40
3:I:198:LEU:O	3:I:348:TYR:OH	2.39	0.40
1:J:115:LEU:HD22	3:L:90:LEU:HD11	2.03	0.40
1:J:194:LEU:N	1:J:195:PRO:HD3	2.37	0.40
2:E:151:LEU:O	2:E:155:GLU:HB2	2.21	0.40
3:F:211:TYR:O	3:F:229:GLY:HA2	2.22	0.40
2:H:410:ALA:CB	2:H:437:TRP:CE3	3.04	0.40
1:J:45:CYS:HB3	1:J:46:PRO:HD2	2.03	0.40
3:L:168:PHE:CE2	3:L:179:LEU:HB2	2.55	0.40
1:A:76:TYR:HA	1:A:79:ASN:HB3	2.03	0.40
2:B:138:VAL:CG1	2:B:139:VAL:N	2.84	0.40
2:B:405:ASN:O	2:B:406:ARG:HB3	2.22	0.40
2:E:107:VAL:O	2:E:107:VAL:HG12	2.22	0.40
3:F:202:VAL:HG23	3:F:225:GLU:HB2	2.03	0.40
2:H:300:SER:HB2	2:H:331:VAL:O	2.21	0.40
3:I:10:ILE:C	3:I:18:TYR:OH	2.52	0.40
2:K:241:ASP:HB3	2:K:249:TRP:HB2	2.04	0.40
2:K:314:MET:HE1	2:K:450:MET:SD	2.62	0.40
2:K:340:ILE:CG2	2:K:403:TRP:CG	3.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:2:NAG:H5	7:W:3:BMA:HO2	1.87	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:GLU:OE2	1:J:84:HIS:NE2[1_455]	2.15	0.05

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	172/562 (31%)	150 (87%)	20 (12%)	2 (1%)	13 40
1	D	172/562 (31%)	158 (92%)	8 (5%)	6 (4%)	3 14
1	G	172/562 (31%)	150 (87%)	18 (10%)	4 (2%)	6 23
1	J	184/562 (33%)	164 (89%)	18 (10%)	2 (1%)	14 42
2	B	399/461 (87%)	344 (86%)	46 (12%)	9 (2%)	6 23
2	E	399/461 (87%)	337 (84%)	48 (12%)	14 (4%)	3 14
2	H	399/461 (87%)	354 (89%)	38 (10%)	7 (2%)	8 29
2	K	399/461 (87%)	348 (87%)	45 (11%)	6 (2%)	10 34
3	C	379/411 (92%)	322 (85%)	48 (13%)	9 (2%)	6 22
3	F	380/411 (92%)	320 (84%)	54 (14%)	6 (2%)	9 32
3	I	392/411 (95%)	347 (88%)	39 (10%)	6 (2%)	10 34
3	L	389/411 (95%)	338 (87%)	42 (11%)	9 (2%)	6 23
4	M	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	N	2/4 (50%)	2 (100%)	0	0	100 100
4	Q	2/4 (50%)	1 (50%)	1 (50%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	O	2/4 (50%)	2 (100%)	0	0	100	100
5	P	2/4 (50%)	2 (100%)	0	0	100	100
5	S	2/4 (50%)	2 (100%)	0	0	100	100
5	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3852/5768 (67%)	3345 (87%)	427 (11%)	80 (2%)	7	26

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	195	PRO
2	B	259	SER
3	C	70	PRO
3	C	350	GLN
3	C	357	ALA
1	D	30	ASP
2	E	265	LYS
2	E	406	ARG
1	G	31	SER
1	G	189	ILE
1	J	199	ARG
2	K	233	VAL
3	L	360	PRO
3	L	374	THR
2	B	281	ASP
2	B	351	ASN
2	B	399	GLY
3	C	198	LEU
3	C	351	GLY
1	D	42	ASN
2	E	263	GLY
2	E	339	GLN
2	E	443	SER
2	E	447	MET
3	F	198	LEU
3	F	199	ASP
2	H	362	GLY
3	I	74	SER
1	J	200	GLN

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Mol	Chain	Res	Type
2	K	316	ASP
3	L	9	CYS
3	L	305	THR
2	B	435	VAL
1	D	195	PRO
2	E	111	SER
2	E	371	ASN
2	E	386	LEU
3	F	82	ALA
3	F	360	PRO
2	H	183	GLU
2	H	206	VAL
2	H	256	GLN
3	I	241	ALA
2	K	281	ASP
3	L	23	CYS
3	L	205	LYS
3	L	365	ASN
2	B	213	GLU
3	C	159	LYS
2	E	281	ASP
2	E	344	LYS
2	E	363	GLU
2	H	435	VAL
3	I	198	LEU
2	K	357	ALA
2	B	60	PRO
2	B	185	ASP
3	C	146	HIS
1	D	31	SER
1	D	34	PRO
2	H	92	PRO
3	I	362	GLY
2	K	256	GLN
2	K	298	LYS
3	L	78	MET
3	C	122	VAL
3	C	241	ALA
3	F	343	HIS
1	G	34	PRO
2	H	280	THR
2	B	179	ILE

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Mol	Chain	Res	Type
1	G	195	PRO
3	F	143	VAL
3	I	324	GLY
1	D	194	LEU
2	E	63	GLY
3	I	76	PRO
2	E	289	PRO
3	L	171	PRO

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	164/479 (34%)	150 (92%)	14 (8%)	10 31
1	D	164/479 (34%)	150 (92%)	14 (8%)	10 31
1	G	164/479 (34%)	154 (94%)	10 (6%)	18 48
1	J	176/479 (37%)	152 (86%)	24 (14%)	3 11
2	B	350/396 (88%)	306 (87%)	44 (13%)	4 13
2	E	350/396 (88%)	312 (89%)	38 (11%)	6 19
2	H	350/396 (88%)	313 (89%)	37 (11%)	6 20
2	K	350/396 (88%)	309 (88%)	41 (12%)	5 16
3	C	328/350 (94%)	290 (88%)	38 (12%)	5 16
3	F	328/350 (94%)	284 (87%)	44 (13%)	4 11
3	I	339/350 (97%)	303 (89%)	36 (11%)	6 20
3	L	337/350 (96%)	294 (87%)	43 (13%)	4 13
4	M	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	N	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	Q	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	R	3/3 (100%)	2 (67%)	1 (33%)	0 0
5	O	3/3 (100%)	3 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	P	3/3 (100%)	3 (100%)	0	100 100
5	S	3/3 (100%)	3 (100%)	0	100 100
5	T	3/3 (100%)	3 (100%)	0	100 100
All	All	3424/4924 (70%)	3037 (89%)	387 (11%)	6 18

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	TRP
1	A	58	VAL
1	A	64	ASN
1	A	66	ILE
1	A	71	ASN
1	A	105	ASP
1	A	129	LYS
1	A	135	LEU
1	A	162	ARG
1	A	175	LEU
1	A	185	LEU
1	A	192	ASP
1	A	197	ARG
2	B	66	LEU
2	B	83	GLN
2	B	88	GLN
2	B	89	GLN
2	B	97	VAL
2	B	98	ASP
2	B	99	GLU
2	B	105	GLU
2	B	138	VAL
2	B	156	THR
2	B	158	ASN
2	B	161	ILE
2	B	165	LEU
2	B	171	ILE
2	B	179	ILE
2	B	181	LYS
2	B	184	SER
2	B	186	VAL
2	B	200	SER

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Mol	Chain	Res	Type
2	B	209	LYS
2	B	210	GLU
2	B	213	GLU
2	B	227	ILE
2	B	234	LYS
2	B	237	ARG
2	B	253	GLN
2	B	280	THR
2	B	283	LYS
2	B	284	ASN
2	B	297	ASP
2	B	318	LYS
2	B	320	ASP
2	B	321	LYS
2	B	330	THR
2	B	343	ASN
2	B	345	TYR
2	B	351	ASN
2	B	359	GLN
2	B	376	SER
2	B	380	ARG
2	B	381	ASP
2	B	387	THR
2	B	426	MET
2	B	438	MET
3	C	22	THR
3	C	32	TYR
3	C	33	GLN
3	C	37	ASP
3	C	41	GLN
3	C	58	LYS
3	C	75	LYS
3	C	86	SER
3	C	100	ILE
3	C	131	LEU
3	C	140	LYS
3	C	147	ASP
3	C	151	LYS
3	C	177	GLN
3	C	179	LEU
3	C	195	GLN
3	C	198	LEU

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Mol	Chain	Res	Type
3	C	221	THR
3	C	239	GLN
3	C	254	ASN
3	C	259	THR
3	C	267	VAL
3	C	276	LEU
3	C	277	THR
3	C	306	SER
3	C	317	ASN
3	C	318	ASP
3	C	325	ASN
3	C	340	HIS
3	C	354	TYR
3	C	356	LYS
3	C	358	SER
3	C	359	THR
3	C	365	ASN
3	C	383	THR
3	C	390	ASN
3	C	392	LEU
3	C	393	THR
1	D	37	SER
1	D	47	SER
1	D	64	ASN
1	D	68	LYS
1	D	123	LYS
1	D	131	GLN
1	D	136	LEU
1	D	138	LYS
1	D	153	ASP
1	D	171	ARG
1	D	174	ASP
1	D	185	LEU
1	D	191	LYS
1	D	200	GLN
2	E	71	ASP
2	E	90	GLU
2	E	118	MET
2	E	135	ASN
2	E	136	GLU
2	E	138	VAL
2	E	141	GLU

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Mol	Chain	Res	Type
2	E	158	ASN
2	E	171	ILE
2	E	179	ILE
2	E	180	GLN
2	E	181	LYS
2	E	187	SER
2	E	191	GLU
2	E	199	VAL
2	E	206	VAL
2	E	209	LYS
2	E	238	VAL
2	E	253	GLN
2	E	270	LYS
2	E	280	THR
2	E	284	ASN
2	E	294	LEU
2	E	301	GLN
2	E	302	LEU
2	E	321	LYS
2	E	323	LYS
2	E	330	THR
2	E	339	GLN
2	E	342	VAL
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	380	ARG
2	E	406	ARG
2	E	415	ARG
2	E	421	GLN
2	E	438	MET
3	F	35	LYS
3	F	72	GLU
3	F	73	SER
3	F	85	LYS
3	F	90	LEU
3	F	100	ILE
3	F	104	ASP
3	F	114	TYR
3	F	117	ASN
3	F	119	GLN
3	F	126	GLU

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Mol	Chain	Res	Type
3	F	130	GLN
3	F	140	LYS
3	F	143	VAL
3	F	147	ASP
3	F	151	LYS
3	F	152	ASP
3	F	156	ILE
3	F	162	LYS
3	F	175	ASN
3	F	178	PHE
3	F	218	LEU
3	F	246	LEU
3	F	249	GLU
3	F	254	ASN
3	F	259	THR
3	F	264	MET
3	F	285	ASP
3	F	297	ASP
3	F	306	SER
3	F	313	SER
3	F	317	ASN
3	F	325	ASN
3	F	350	GLN
3	F	356	LYS
3	F	358	SER
3	F	361	ASN
3	F	365	ASN
3	F	376	TRP
3	F	379	MET
3	F	383	THR
3	F	385	LYS
3	F	386	ILE
3	F	392	LEU
1	G	41	TRP
1	G	58	VAL
1	G	71	ASN
1	G	73	LEU
1	G	122	LEU
1	G	123	LYS
1	G	138	LYS
1	G	143	GLN
1	G	160	SER

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Mol	Chain	Res	Type
1	G	185	LEU
2	H	61	ASP
2	H	83	GLN
2	H	99	GLU
2	H	103	ASN
2	H	109	GLN
2	H	111	SER
2	H	115	PHE
2	H	116	GLN
2	H	117	TYR
2	H	122	LYS
2	H	123	ASP
2	H	125	TRP
2	H	128	ARG
2	H	138	VAL
2	H	140	ASN
2	H	179	ILE
2	H	181	LYS
2	H	182	LEU
2	H	191	GLU
2	H	206	VAL
2	H	209	LYS
2	H	213	GLU
2	H	232	SER
2	H	238	VAL
2	H	253	GLN
2	H	284	ASN
2	H	296	ASN
2	H	320	ASP
2	H	321	LYS
2	H	323	LYS
2	H	330	THR
2	H	351	ASN
2	H	359	GLN
2	H	380	ARG
2	H	385	TRP
2	H	387	THR
2	H	415	ARG
3	I	4	THR
3	I	5	ARG
3	I	7	ASN
3	I	8	CYS

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Mol	Chain	Res	Type
3	I	32	TYR
3	I	52	ASN
3	I	78	MET
3	I	103	HIS
3	I	111	GLN
3	I	115	ASN
3	I	117	ASN
3	I	128	VAL
3	I	166	LEU
3	I	195	GLN
3	I	196	LYS
3	I	198	LEU
3	I	207	ASN
3	I	223	THR
3	I	237	SER
3	I	240	SER
3	I	250	LEU
3	I	258	SER
3	I	266	LYS
3	I	277	THR
3	I	285	ASP
3	I	294	ASP
3	I	325	ASN
3	I	356	LYS
3	I	365	ASN
3	I	376	TRP
3	I	383	THR
3	I	385	LYS
3	I	386	ILE
3	I	390	ASN
3	I	391	ARG
3	I	392	LEU
1	J	28	CYS
1	J	39	GLU
1	J	41	TRP
1	J	58	VAL
1	J	67	ASN
1	J	68	LYS
1	J	69	LEU
1	J	71	ASN
1	J	73	LEU
1	J	80	ASN

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Mol	Chain	Res	Type
1	J	82	ASP
1	J	106	ASN
1	J	108	TYR
1	J	109	ASN
1	J	114	ASP
1	J	123	LYS
1	J	138	LYS
1	J	150	LEU
1	J	156	ILE
1	J	169	LEU
1	J	172	GLU
1	J	181	GLN
1	J	201	HIS
1	J	204	LEU
2	K	66	LEU
2	K	84	GLU
2	K	95	ASN
2	K	96	SER
2	K	128	ARG
2	K	140	ASN
2	K	145	GLU
2	K	149	HIS
2	K	150	GLN
2	K	152	TYR
2	K	158	ASN
2	K	172	LEU
2	K	174	ASN
2	K	179	ILE
2	K	186	VAL
2	K	199	VAL
2	K	209	LYS
2	K	226	LEU
2	K	238	VAL
2	K	252	ILE
2	K	253	GLN
2	K	257	ASP
2	K	280	THR
2	K	297	ASP
2	K	302	LEU
2	K	310	LEU
2	K	312	ILE
2	K	321	LYS

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Mol	Chain	Res	Type
2	K	323	LYS
2	K	325	HIS
2	K	330	THR
2	K	346	ARG
2	K	351	ASN
2	K	359	GLN
2	K	377	THR
2	K	387	THR
2	K	415	ARG
2	K	439	ASN
2	K	443	SER
2	K	457	PHE
2	K	458	PHE
3	L	8	CYS
3	L	22	THR
3	L	27	ASP
3	L	40	LEU
3	L	78	MET
3	L	90	LEU
3	L	97	GLU
3	L	108	ARG
3	L	110	LEU
3	L	111	GLN
3	L	117	ASN
3	L	122	VAL
3	L	147	ASP
3	L	149	THR
3	L	151	LYS
3	L	163	GLN
3	L	170	LYS
3	L	175	ASN
3	L	176	GLN
3	L	184	ILE
3	L	185	ASP
3	L	198	LEU
3	L	199	ASP
3	L	233	ILE
3	L	242	ILE
3	L	249	GLU
3	L	250	LEU
3	L	259	THR
3	L	261	ASP

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Mol	Chain	Res	Type
3	L	264	MET
3	L	276	LEU
3	L	297	ASP
3	L	306	SER
3	L	314	THR
3	L	344	LEU
3	L	353	THR
3	L	361	ASN
3	L	365	ASN
3	L	374	THR
3	L	376	TRP
3	L	380	LYS
3	L	383	THR
3	L	389	PHE
4	M	3	ARG
4	N	3	ARG
4	Q	3	ARG
4	R	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	71	ASN
1	A	79	ASN
1	A	80	ASN
1	A	84	HIS
1	A	89	ASN
1	A	103	ASN
1	A	134	GLN
1	A	139	ASN
1	A	181	GLN
1	A	184	GLN
1	A	200	GLN
2	B	67	HIS
2	B	88	GLN
2	B	89	GLN
2	B	129	GLN
2	B	150	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN

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Mol	Chain	Res	Type
2	B	180	GLN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	284	ASN
2	B	296	ASN
2	B	343	ASN
2	B	351	ASN
2	B	393	GLN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	69	ASN
3	C	117	ASN
3	C	144	GLN
3	C	146	HIS
3	C	189	ASN
3	C	230	ASN
3	C	254	ASN
3	C	307	HIS
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	365	ASN
3	C	390	ASN
1	D	64	ASN
1	D	131	GLN
1	D	137	GLN
1	D	143	GLN
1	D	200	GLN
2	E	67	HIS
2	E	149	HIS
2	E	158	ASN
2	E	253	GLN
2	E	256	GLN
2	E	284	ASN
2	E	296	ASN
2	E	351	ASN
2	E	405	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN

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Mol	Chain	Res	Type
3	F	33	GLN
3	F	118	ASN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	158	ASN
3	F	189	ASN
3	F	210	GLN
3	F	230	ASN
3	F	254	ASN
3	F	317	ASN
3	F	350	GLN
3	F	365	ASN
1	G	59	ASN
1	G	60	GLN
1	G	71	ASN
1	G	131	GLN
1	G	134	GLN
1	G	143	GLN
1	G	181	GLN
1	G	184	GLN
2	H	89	GLN
2	H	95	ASN
2	H	102	ASN
2	H	140	ASN
2	H	150	GLN
2	H	158	ASN
2	H	160	ASN
2	H	180	GLN
2	H	253	GLN
2	H	256	GLN
2	H	284	ASN
2	H	296	ASN
2	H	301	GLN
2	H	325	HIS
2	H	351	ASN
2	H	413	ASN
2	H	421	GLN
2	H	439	ASN
3	I	59	GLN
3	I	115	ASN
3	I	117	ASN

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Mol	Chain	Res	Type
3	I	119	GLN
3	I	144	GLN
3	I	207	ASN
3	I	230	ASN
3	I	239	GLN
3	I	254	ASN
3	I	319	ASN
3	I	325	ASN
3	I	365	ASN
3	I	390	ASN
1	J	59	ASN
1	J	67	ASN
1	J	106	ASN
1	J	131	GLN
1	J	181	GLN
1	J	182	GLN
1	J	184	GLN
2	K	83	GLN
2	K	89	GLN
2	K	95	ASN
2	K	135	ASN
2	K	158	ASN
2	K	160	ASN
2	K	189	GLN
2	K	253	GLN
2	K	256	GLN
2	K	296	ASN
2	K	301	GLN
2	K	351	ASN
2	K	364	ASN
2	K	421	GLN
2	K	439	ASN
3	L	33	GLN
3	L	49	GLN
3	L	52	ASN
3	L	115	ASN
3	L	117	ASN
3	L	144	GLN
3	L	177	GLN
3	L	189	ASN
3	L	239	GLN
3	L	317	ASN

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Mol	Chain	Res	Type
3	L	325	ASN
3	L	361	ASN
3	L	365	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)

40 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	$\#\|Z\| > 2$
6	NAG	U	1	6	14,14,15	0.94	0	17,19,21	1.44	1 (5%)
6	GAL	U	10	6	11,11,12	0.98	0	15,15,17	0.76	0
6	SIA	U	11	6	20,20,21	1.73	3 (15%)	24,28,31	1.42	2 (8%)
6	NAG	U	2	6	14,14,15	0.79	0	17,19,21	1.02	1 (5%)
6	BMA	U	3	6	11,11,12	1.09	1 (9%)	15,15,17	1.20	1 (6%)
6	MAN	U	4	6	11,11,12	1.17	0	15,15,17	0.93	1 (6%)
6	NAG	U	5	6	14,14,15	1.10	1 (7%)	17,19,21	1.03	1 (5%)
6	GAL	U	6	6	11,11,12	0.62	0	15,15,17	0.55	0
6	SIA	U	7	6	20,20,21	1.89	7 (35%)	24,28,31	1.10	1 (4%)
6	MAN	U	8	6	11,11,12	1.65	3 (27%)	15,15,17	1.36	1 (6%)
6	NAG	U	9	6	14,14,15	1.07	1 (7%)	17,19,21	0.87	0
6	NAG	V	1	6,2	14,14,15	0.78	0	17,19,21	1.18	3 (17%)
6	GAL	V	10	6	11,11,12	1.00	1 (9%)	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SIA	V	11	6	20,20,21	1.46	2 (10%)	24,28,31	0.94	1 (4%)
6	NAG	V	2	6	14,14,15	0.91	1 (7%)	17,19,21	0.94	0
6	BMA	V	3	6	11,11,12	1.12	1 (9%)	15,15,17	1.38	1 (6%)
6	MAN	V	4	6	11,11,12	1.45	2 (18%)	15,15,17	1.19	3 (20%)
6	NAG	V	5	6	14,14,15	1.24	2 (14%)	17,19,21	0.84	0
6	GAL	V	6	6	11,11,12	1.18	0	15,15,17	0.74	0
6	SIA	V	7	6	20,20,21	0.99	1 (5%)	24,28,31	1.26	2 (8%)
6	MAN	V	8	6	11,11,12	0.97	0	15,15,17	1.64	3 (20%)
6	NAG	V	9	6	14,14,15	1.10	1 (7%)	17,19,21	0.94	0
7	NAG	W	1	7,2	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
7	NAG	W	2	7	14,14,15	0.78	1 (7%)	17,19,21	1.00	1 (5%)
7	BMA	W	3	7	11,11,12	0.76	0	15,15,17	1.18	1 (6%)
7	MAN	W	4	7	11,11,12	1.20	2 (18%)	15,15,17	1.16	1 (6%)
7	MAN	W	5	7	11,11,12	0.65	0	15,15,17	0.69	0
6	NAG	X	1	6	14,14,15	0.99	0	17,19,21	1.29	3 (17%)
6	GAL	X	10	6	11,11,12	1.28	1 (9%)	15,15,17	0.75	0
6	SIA	X	11	6	20,20,21	1.40	1 (5%)	24,28,31	1.08	2 (8%)
6	NAG	X	2	6	14,14,15	1.24	2 (14%)	17,19,21	1.01	0
6	BMA	X	3	6	11,11,12	1.29	1 (9%)	15,15,17	1.04	2 (13%)
6	MAN	X	4	6	11,11,12	1.06	0	15,15,17	1.31	2 (13%)
6	NAG	X	5	6	14,14,15	1.07	1 (7%)	17,19,21	0.92	0
6	GAL	X	6	6	11,11,12	1.03	0	15,15,17	0.98	2 (13%)
6	SIA	X	7	6	20,20,21	1.36	3 (15%)	24,28,31	1.60	4 (16%)
6	MAN	X	8	6	11,11,12	1.15	2 (18%)	15,15,17	1.39	3 (20%)
6	NAG	X	9	6	14,14,15	1.11	1 (7%)	17,19,21	1.11	2 (11%)
8	NAG	Y	1	8	14,14,15	1.00	0	17,19,21	1.04	1 (5%)
8	NAG	Y	2	8	14,14,15	1.18	2 (14%)	17,19,21	0.87	1 (5%)

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	U	1	6	-	2/6/23/26	0/1/1/1
6	GAL	U	10	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	U	11	6	-	2/18/34/38	0/1/1/1
6	NAG	U	2	6	1/1/5/7	5/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	0/1/1/1
6	NAG	U	5	6	1/1/5/7	3/6/23/26	0/1/1/1
6	GAL	U	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	U	7	6	-	11/18/34/38	0/1/1/1
6	MAN	U	8	6	-	1/2/19/22	0/1/1/1
6	NAG	U	9	6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	V	1	6,2	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	V	10	6	-	1/2/19/22	0/1/1/1
6	SIA	V	11	6	-	6/18/34/38	0/1/1/1
6	NAG	V	2	6	1/1/5/7	6/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1
6	MAN	V	4	6	-	1/2/19/22	0/1/1/1
6	NAG	V	5	6	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	V	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	V	7	6	-	11/18/34/38	0/1/1/1
6	MAN	V	8	6	-	2/2/19/22	0/1/1/1
6	NAG	V	9	6	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	W	1	7,2	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	W	2	7	1/1/5/7	4/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	1/2/19/22	0/1/1/1
7	MAN	W	5	7	-	2/2/19/22	0/1/1/1
6	NAG	X	1	6	-	4/6/23/26	0/1/1/1
6	GAL	X	10	6	-	2/2/19/22	0/1/1/1
6	SIA	X	11	6	-	11/18/34/38	0/1/1/1
6	NAG	X	2	6	1/1/5/7	3/6/23/26	0/1/1/1
6	BMA	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	NAG	X	5	6	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	X	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	X	7	6	-	12/18/34/38	0/1/1/1
6	MAN	X	8	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	9	6	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	Y	1	8	-	5/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	6/6/23/26	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	7	SIA	C2-C1	4.51	1.56	1.52
6	U	11	SIA	C3-C2	4.51	1.60	1.52
6	X	11	SIA	C2-C1	4.50	1.56	1.52
6	V	11	SIA	C2-C1	4.13	1.56	1.52
6	U	11	SIA	C2-C1	4.12	1.56	1.52
6	U	8	MAN	C2-C3	4.07	1.58	1.52
6	X	7	SIA	C4-C5	3.70	1.56	1.53
6	U	7	SIA	C4-C5	3.46	1.56	1.53
6	V	3	BMA	C2-C3	3.24	1.57	1.52
6	U	7	SIA	O6-C2	2.96	1.47	1.43
8	Y	2	NAG	C1-C2	2.96	1.56	1.52
6	V	4	MAN	C4-C5	2.93	1.59	1.53
6	V	9	NAG	C1-C2	2.68	1.56	1.52
7	W	4	MAN	C4-C3	2.68	1.59	1.52
6	V	2	NAG	C1-C2	2.55	1.56	1.52
6	V	10	GAL	C1-C2	2.53	1.58	1.52
6	V	11	SIA	C4-C5	2.50	1.55	1.53
6	U	7	SIA	C7-C6	2.47	1.56	1.53
6	X	2	NAG	C1-C2	2.46	1.56	1.52
7	W	4	MAN	C4-C5	2.45	1.58	1.53
6	U	5	NAG	C1-C2	2.44	1.56	1.52
6	V	5	NAG	O5-C5	2.43	1.48	1.43
6	V	4	MAN	C2-C3	2.41	1.56	1.52
6	X	7	SIA	C3-C4	2.40	1.56	1.52
6	X	5	NAG	C1-C2	2.40	1.55	1.52
6	X	2	NAG	O5-C5	2.39	1.48	1.43
6	U	7	SIA	C3-C2	2.35	1.56	1.52
6	X	8	MAN	C1-C2	2.28	1.57	1.52
6	X	7	SIA	C3-C2	2.25	1.56	1.52
6	X	10	GAL	C1-C2	2.24	1.57	1.52
6	V	7	SIA	C4-C5	2.23	1.55	1.53
6	X	8	MAN	C2-C3	2.23	1.55	1.52
6	U	8	MAN	O2-C2	2.22	1.48	1.43
6	X	9	NAG	C1-C2	2.19	1.55	1.52
7	W	2	NAG	C1-C2	2.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	9	NAG	C1-C2	2.13	1.55	1.52
6	U	3	BMA	O3-C3	2.11	1.47	1.43
6	U	8	MAN	C1-C2	2.10	1.57	1.52
6	X	3	BMA	C2-C3	2.08	1.55	1.52
6	U	11	SIA	O6-C6	2.07	1.47	1.44
8	Y	2	NAG	O5-C5	2.06	1.47	1.43
6	U	7	SIA	C6-C5	2.05	1.56	1.53
6	V	5	NAG	C4-C5	2.03	1.57	1.53
6	U	7	SIA	O6-C6	2.03	1.47	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	11	SIA	C4-C3-C2	5.13	119.01	109.81
6	U	1	NAG	C2-N2-C7	-5.10	115.64	122.90
6	V	8	MAN	C1-C2-C3	4.63	115.36	109.67
6	V	3	BMA	C1-C2-C3	-4.19	104.52	109.67
6	U	8	MAN	C1-C2-C3	3.98	114.56	109.67
6	X	7	SIA	C4-C3-C2	3.97	116.93	109.81
7	W	3	BMA	C1-C2-C3	-3.95	104.81	109.67
6	X	4	MAN	C3-C4-C5	3.64	116.73	110.24
6	X	7	SIA	C3-C4-C5	3.61	115.82	111.46
6	V	7	SIA	C3-C4-C5	3.49	115.67	111.46
6	X	8	MAN	C1-C2-C3	3.46	113.92	109.67
7	W	4	MAN	C3-C4-C5	3.46	116.41	110.24
7	W	1	NAG	C2-N2-C7	-3.06	118.55	122.90
6	X	9	NAG	C2-N2-C7	-3.06	118.55	122.90
6	X	4	MAN	C2-C3-C4	2.93	115.97	110.89
6	X	1	NAG	C2-N2-C7	-2.91	118.76	122.90
6	V	1	NAG	C1-O5-C5	2.85	116.06	112.19
6	U	7	SIA	C4-C3-C2	2.84	114.90	109.81
6	U	3	BMA	C3-C4-C5	2.84	115.30	110.24
6	V	10	GAL	C1-C2-C3	2.76	113.05	109.67
8	Y	1	NAG	C4-C3-C2	2.74	115.04	111.02
6	X	8	MAN	C6-C5-C4	2.70	119.34	113.00
6	X	7	SIA	C8-C7-C6	-2.68	107.95	113.03
6	V	8	MAN	O2-C2-C1	2.68	114.63	109.15
6	X	11	SIA	C4-C3-C2	2.62	114.51	109.81
6	X	1	NAG	C1-O5-C5	2.56	115.67	112.19
6	V	1	NAG	C4-C3-C2	-2.56	107.27	111.02
6	U	5	NAG	C3-C4-C5	2.52	114.73	110.24
6	V	7	SIA	C4-C3-C2	2.52	114.32	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	2	NAG	C2-N2-C7	-2.50	119.35	122.90
8	Y	2	NAG	C1-O5-C5	2.44	115.50	112.19
6	V	8	MAN	C2-C3-C4	2.38	115.02	110.89
6	U	4	MAN	C2-C3-C4	2.36	114.97	110.89
6	X	3	BMA	C1-C2-C3	-2.34	106.79	109.67
6	X	7	SIA	C5-N5-C10	-2.33	117.52	123.18
6	V	1	NAG	C2-N2-C7	-2.31	119.61	122.90
6	X	3	BMA	C2-C3-C4	-2.31	106.90	110.89
6	X	11	SIA	O1B-C1-C2	2.28	119.55	113.03
6	X	8	MAN	O2-C2-C1	2.28	113.82	109.15
6	U	2	NAG	C2-N2-C7	-2.28	119.66	122.90
6	V	4	MAN	C1-O5-C5	2.27	115.26	112.19
6	X	1	NAG	C6-C5-C4	2.24	118.25	113.00
6	X	6	GAL	O2-C2-C1	2.19	113.63	109.15
6	U	11	SIA	O1B-C1-C2	2.17	119.22	113.03
6	V	11	SIA	O1B-C1-C2	2.13	119.12	113.03
6	X	9	NAG	C6-C5-C4	2.12	117.98	113.00
6	V	4	MAN	C1-C2-C3	-2.06	107.13	109.67
6	V	4	MAN	O2-C2-C1	2.06	113.37	109.15
6	X	6	GAL	C1-C2-C3	2.01	112.13	109.67

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	U	2	NAG	C1
6	U	5	NAG	C1
6	U	6	GAL	C1
6	U	9	NAG	C1
6	V	1	NAG	C1
6	V	2	NAG	C1
6	V	5	NAG	C1
6	V	6	GAL	C1
6	V	9	NAG	C1
6	X	2	NAG	C1
6	X	5	NAG	C1
6	X	6	GAL	C1
6	X	9	NAG	C1
7	W	1	NAG	C1
7	W	2	NAG	C1

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	U	5	NAG	C8-C7-N2-C2
6	U	5	NAG	O7-C7-N2-C2
6	U	7	SIA	C5-C6-C7-C8
6	U	7	SIA	C5-C6-C7-O7
6	U	7	SIA	O6-C6-C7-C8
6	U	7	SIA	O6-C6-C7-O7
6	U	7	SIA	C11-C10-N5-C5
6	U	7	SIA	O10-C10-N5-C5
6	U	9	NAG	C8-C7-N2-C2
6	U	9	NAG	O7-C7-N2-C2
6	U	11	SIA	C11-C10-N5-C5
6	U	11	SIA	O10-C10-N5-C5
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	V	7	SIA	C5-C6-C7-O7
6	V	7	SIA	O6-C6-C7-O7
6	V	7	SIA	C6-C7-C8-C9
6	V	7	SIA	C6-C7-C8-O8
6	V	7	SIA	O7-C7-C8-C9
6	V	7	SIA	O7-C7-C8-O8
6	V	7	SIA	C11-C10-N5-C5
6	V	7	SIA	O10-C10-N5-C5
6	V	9	NAG	C8-C7-N2-C2
6	V	9	NAG	O7-C7-N2-C2
6	V	11	SIA	C5-C6-C7-C8
6	V	11	SIA	C5-C6-C7-O7
6	V	11	SIA	O6-C6-C7-C8
6	V	11	SIA	O6-C6-C7-O7
6	V	11	SIA	C7-C8-C9-O9
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	X	2	NAG	C8-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
6	X	5	NAG	C8-C7-N2-C2
6	X	5	NAG	O7-C7-N2-C2
6	X	7	SIA	O1A-C1-C2-O6
6	X	7	SIA	C5-C6-C7-O7
6	X	7	SIA	O6-C6-C7-O7
6	X	7	SIA	C11-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
6	X	7	SIA	O10-C10-N5-C5
6	X	9	NAG	C8-C7-N2-C2
6	X	9	NAG	O7-C7-N2-C2
6	X	11	SIA	O1A-C1-C2-O6
6	X	11	SIA	C5-C6-C7-C8
6	X	11	SIA	C5-C6-C7-O7
6	X	11	SIA	O6-C6-C7-C8
6	X	11	SIA	O6-C6-C7-O7
6	X	11	SIA	O8-C8-C9-O9
6	X	11	SIA	C11-C10-N5-C5
6	X	11	SIA	O10-C10-N5-C5
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
7	W	2	NAG	C8-C7-N2-C2
7	W	2	NAG	O7-C7-N2-C2
6	V	2	NAG	O5-C5-C6-O6
6	X	4	MAN	C4-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
8	Y	2	NAG	C1-C2-N2-C7
6	V	11	SIA	O8-C8-C9-O9
6	U	9	NAG	C4-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
6	X	11	SIA	C7-C8-C9-O9
6	V	2	NAG	C8-C7-N2-C2
6	U	3	BMA	O5-C5-C6-O6
6	V	6	GAL	O5-C5-C6-O6
6	V	6	GAL	C4-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
6	X	10	GAL	O5-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
6	U	9	NAG	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	U	6	GAL	O5-C5-C6-O6
6	U	10	GAL	C4-C5-C6-O6
6	X	5	NAG	O5-C5-C6-O6
6	X	6	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	X	8	MAN	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	V	2	NAG	O7-C7-N2-C2
6	V	5	NAG	C8-C7-N2-C2
6	V	5	NAG	O7-C7-N2-C2
6	X	5	NAG	C4-C5-C6-O6
6	X	10	GAL	C4-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
6	U	6	GAL	C4-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
6	U	10	GAL	O5-C5-C6-O6
6	V	8	MAN	O5-C5-C6-O6
6	U	2	NAG	C1-C2-N2-C7
6	X	2	NAG	C1-C2-N2-C7
6	X	6	GAL	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	X	8	MAN	O5-C5-C6-O6
6	U	4	MAN	C4-C5-C6-O6
6	X	3	BMA	C4-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6
6	U	7	SIA	C6-C7-C8-O8
6	U	7	SIA	O7-C7-C8-O8
7	W	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
6	V	10	GAL	O5-C5-C6-O6
6	X	7	SIA	O7-C7-C8-C9
6	V	9	NAG	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
7	W	5	MAN	C4-C5-C6-O6
6	V	5	NAG	C4-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
6	U	8	MAN	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
6	U	7	SIA	C6-C7-C8-C9
6	V	7	SIA	O1A-C1-C2-O6
8	Y	2	NAG	C3-C2-N2-C7
6	X	7	SIA	C6-C7-C8-C9
6	X	7	SIA	O7-C7-C8-O8
6	X	7	SIA	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
6	X	11	SIA	O1A-C1-C2-C3
6	X	11	SIA	O1B-C1-C2-C3
6	V	7	SIA	C5-C6-C7-C8
6	V	7	SIA	O6-C6-C7-C8
6	X	7	SIA	C5-C6-C7-C8
6	X	7	SIA	O6-C6-C7-C8
7	W	5	MAN	O5-C5-C6-O6
6	U	5	NAG	C1-C2-N2-C7
6	U	7	SIA	O1A-C1-C2-O6
6	X	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C3-C2-N2-C7
8	Y	1	NAG	C3-C2-N2-C7
6	U	7	SIA	O7-C7-C8-C9
6	X	7	SIA	O1B-C1-C2-O6
6	V	8	MAN	C4-C5-C6-O6
6	V	2	NAG	C3-C2-N2-C7
6	V	5	NAG	C1-C2-N2-C7
6	V	4	MAN	O5-C5-C6-O6
6	V	2	NAG	C1-C2-N2-C7

There are no ring outliers.

36 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	3	BMA	2	0
6	U	11	SIA	1	0
6	V	5	NAG	3	0
6	V	8	MAN	1	0
6	V	9	NAG	1	0
6	V	7	SIA	5	0
6	U	8	MAN	4	0
6	U	7	SIA	5	0
7	W	3	BMA	2	0
6	V	11	SIA	1	0
6	V	1	NAG	2	0
6	X	6	GAL	1	0
6	X	2	NAG	7	0
6	X	11	SIA	3	0
6	X	10	GAL	1	0
6	U	6	GAL	4	0
8	Y	2	NAG	1	0
6	V	4	MAN	2	0

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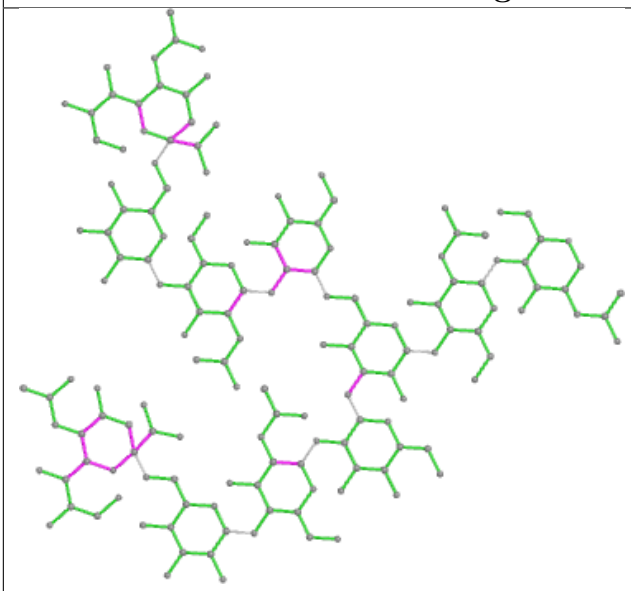
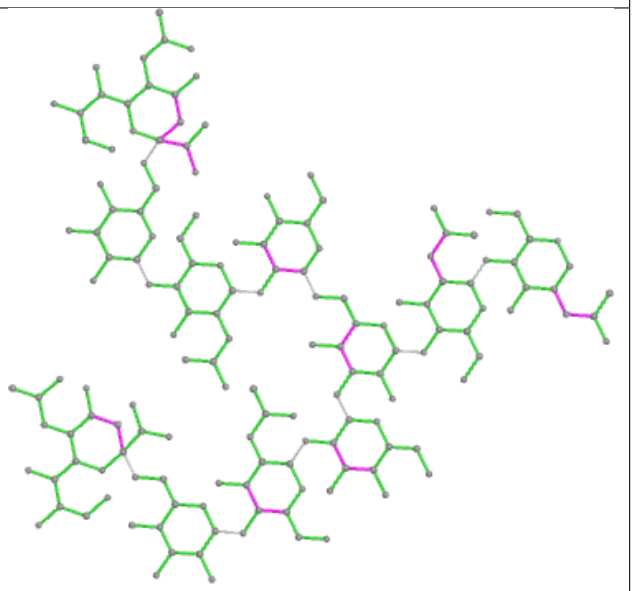
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	9	NAG	2	0
8	Y	1	NAG	12	0
7	W	1	NAG	5	0
6	U	10	GAL	1	0
6	X	5	NAG	4	0
6	V	2	NAG	4	0
6	U	2	NAG	6	0
6	V	10	GAL	1	0
6	U	1	NAG	9	0
6	X	8	MAN	2	0
6	U	9	NAG	4	0
6	X	1	NAG	7	0
6	U	3	BMA	3	0
6	X	7	SIA	1	0
7	W	2	NAG	4	0
6	U	5	NAG	2	0
6	V	3	BMA	4	0
6	V	6	GAL	2	0

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

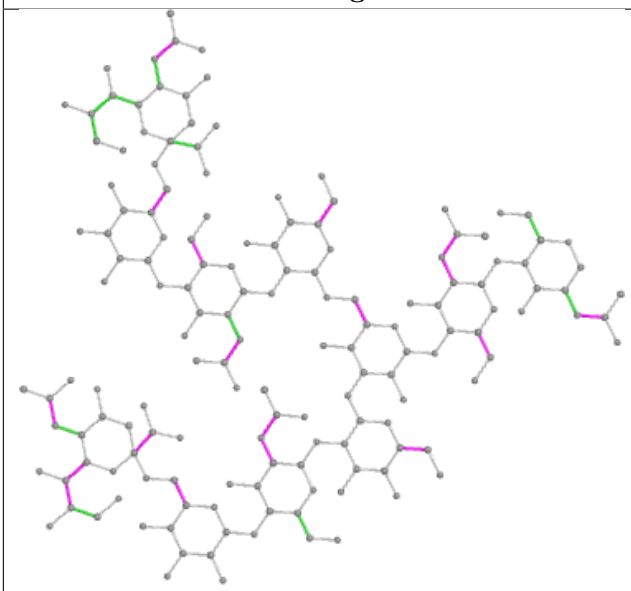
Oligosaccharide Chain U



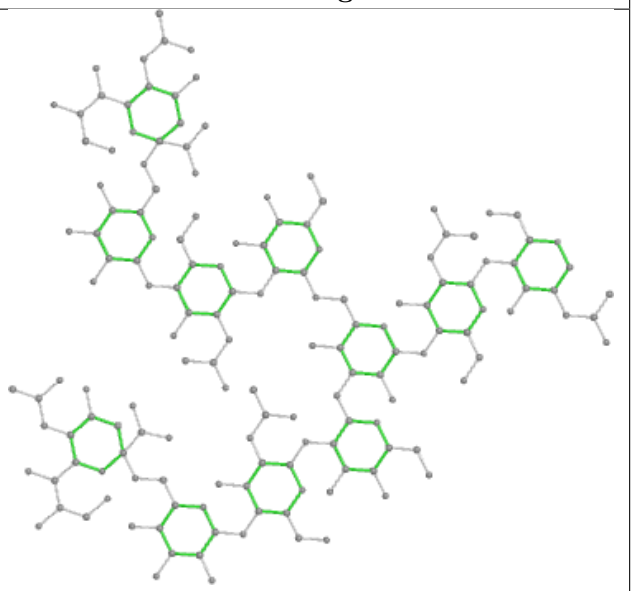
Bond lengths



Bond angles

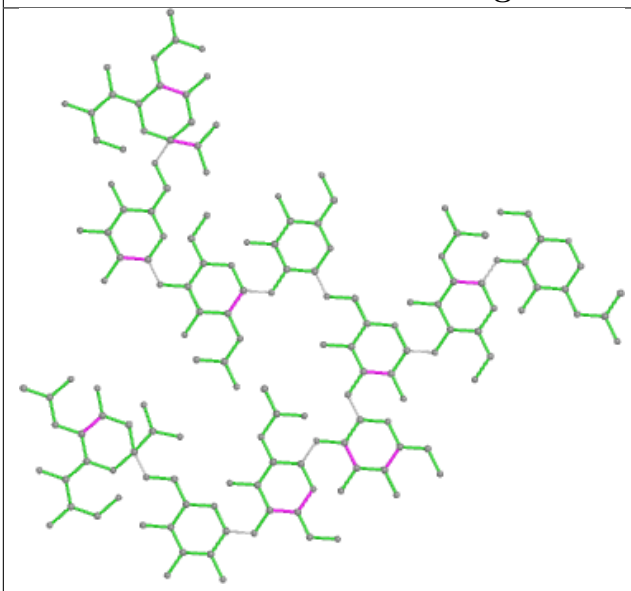


Torsions

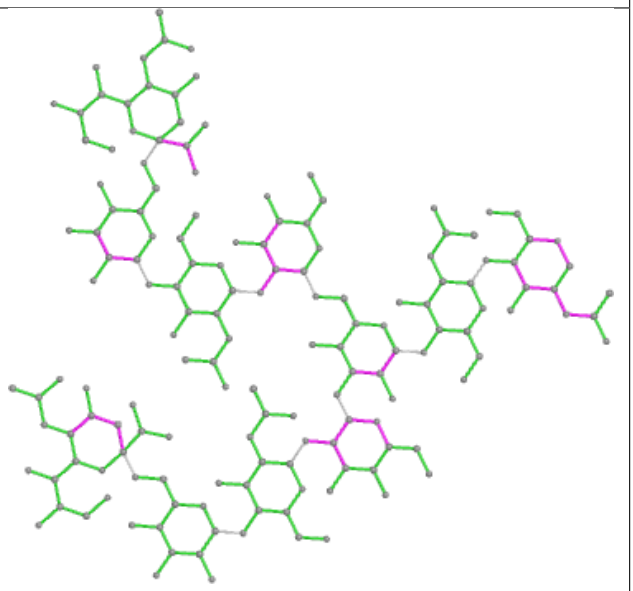


Rings

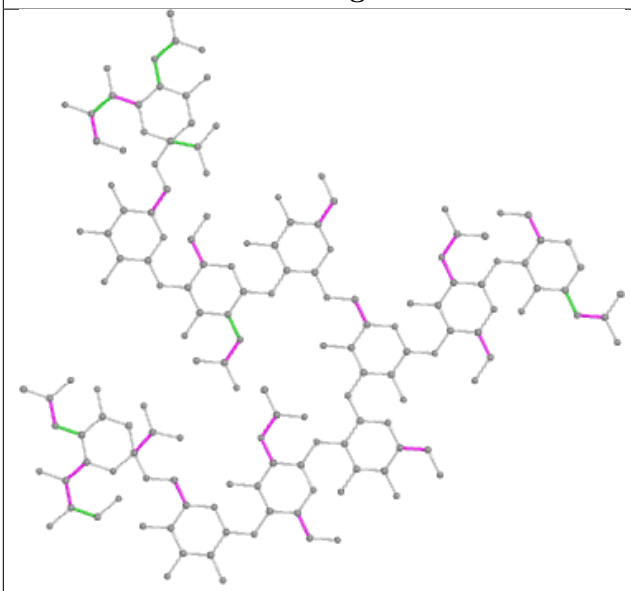
Oligosaccharide Chain V



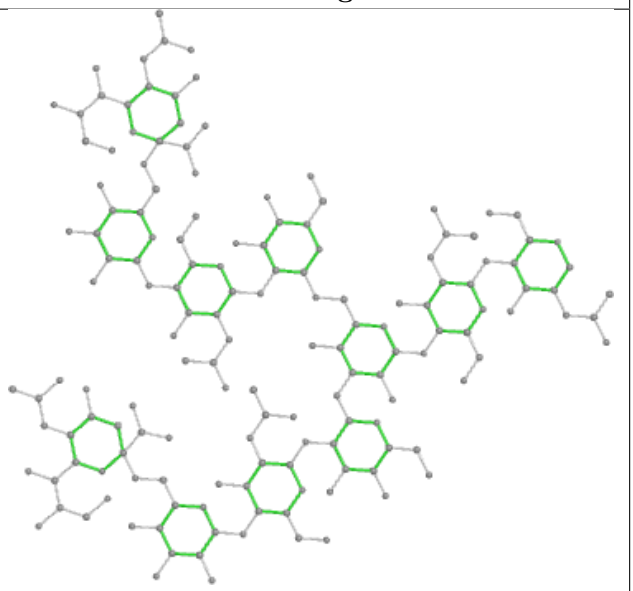
Bond lengths



Bond angles

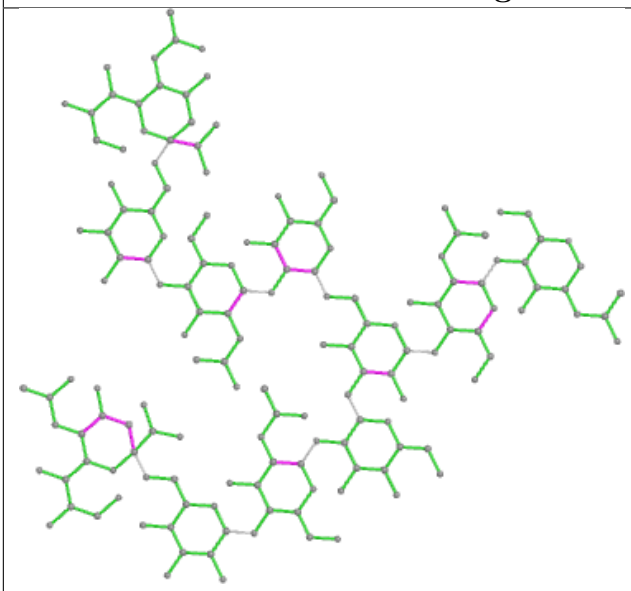


Torsions

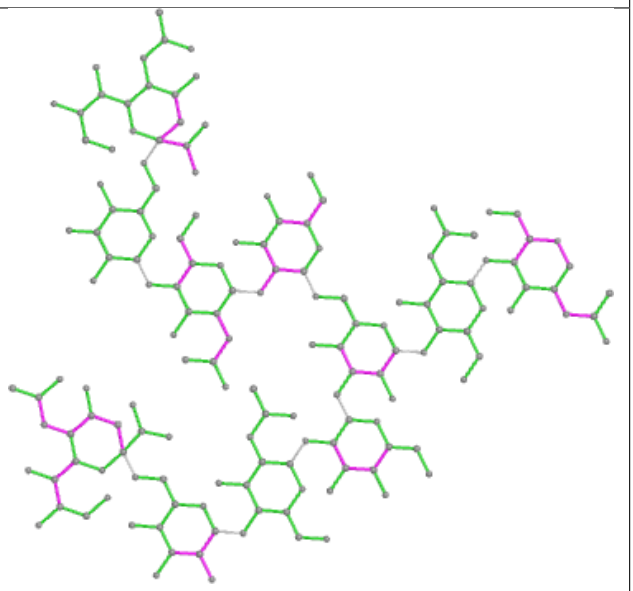


Rings

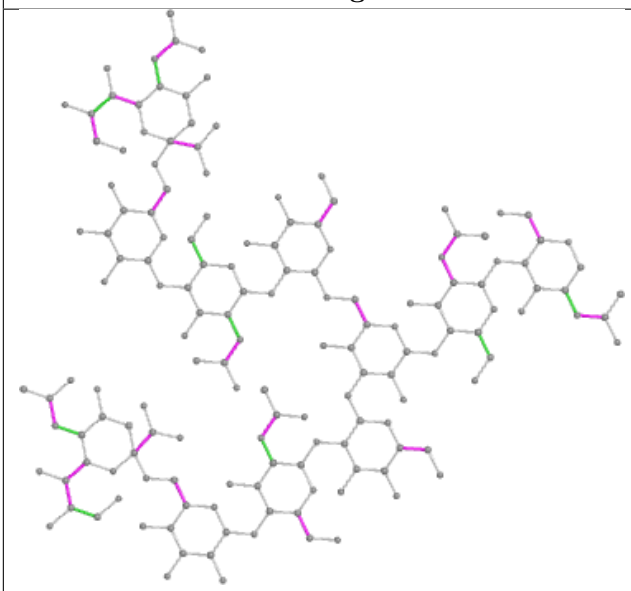
Oligosaccharide Chain X



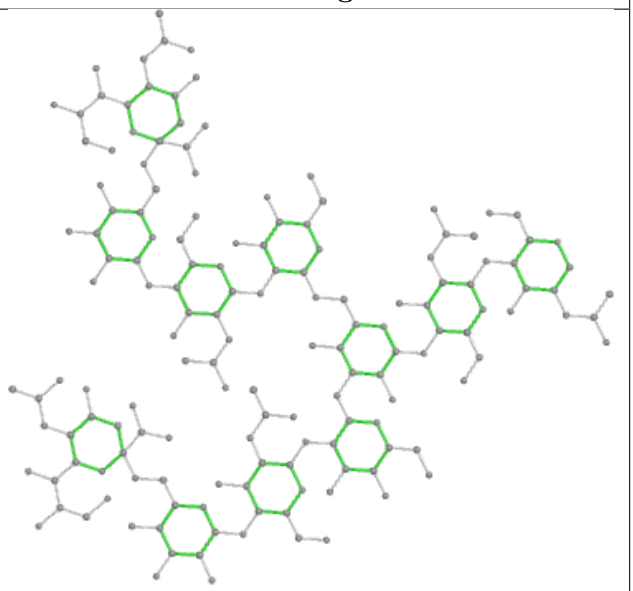
Bond lengths



Bond angles

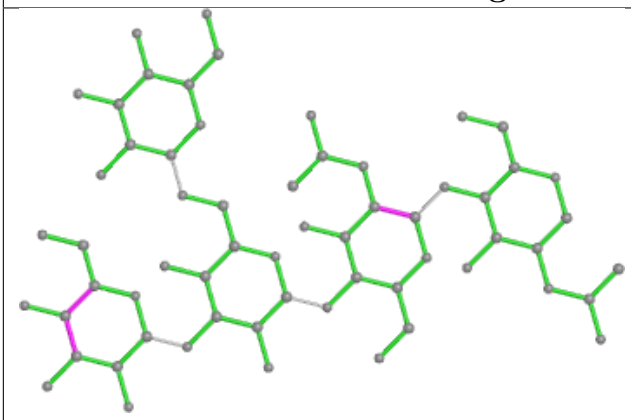


Torsions

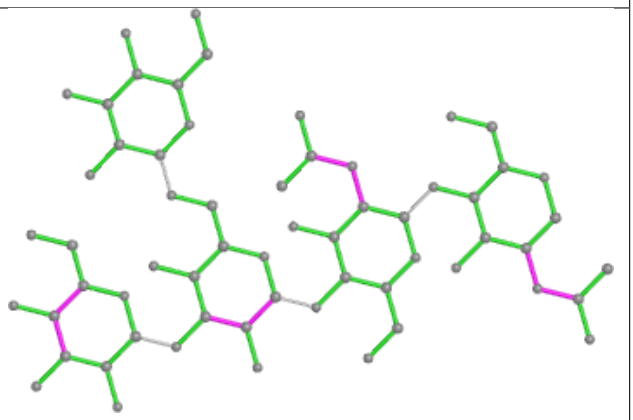


Rings

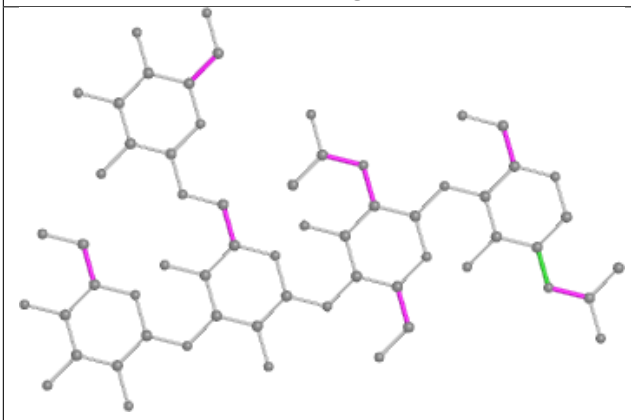
Oligosaccharide Chain W



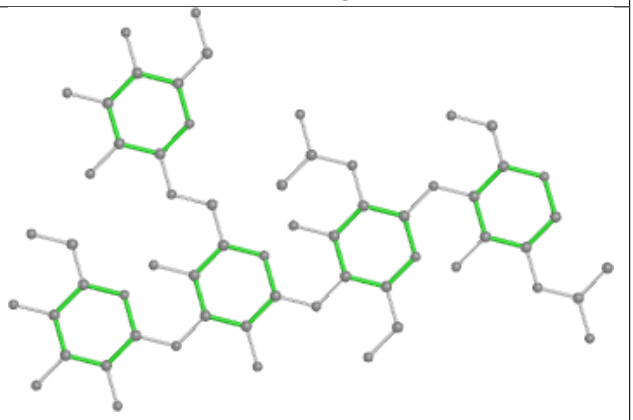
Bond lengths



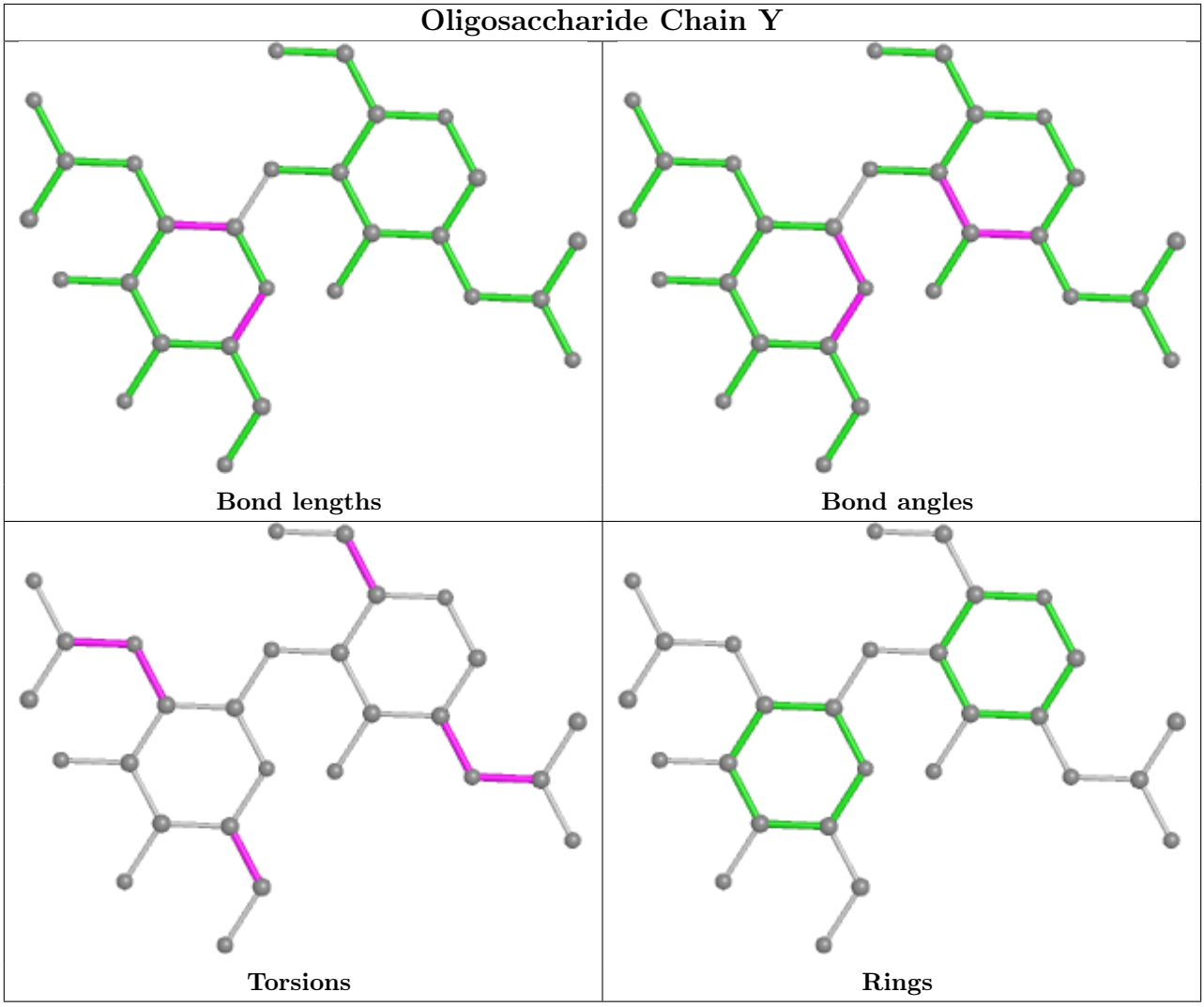
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	174/562 (30%)	0.06	8 (4%) 32 29	21, 106, 173, 187	0
1	D	174/562 (30%)	0.83	33 (18%) 1 0	62, 137, 231, 238	0
1	G	174/562 (30%)	0.11	10 (5%) 23 19	51, 120, 163, 173	0
1	J	186/562 (33%)	0.45	23 (12%) 4 3	64, 135, 224, 246	0
2	B	401/461 (86%)	-0.32	5 (1%) 79 79	21, 53, 151, 184	0
2	E	401/461 (86%)	0.07	35 (8%) 10 7	40, 64, 211, 226	0
2	H	401/461 (86%)	-0.14	15 (3%) 41 37	30, 62, 168, 195	0
2	K	401/461 (86%)	-0.25	6 (1%) 73 73	40, 64, 156, 164	0
3	C	381/411 (92%)	-0.46	15 (3%) 39 35	8, 39, 189, 232	0
3	F	382/411 (92%)	0.13	23 (6%) 21 18	52, 89, 208, 221	0
3	I	394/411 (95%)	-0.17	19 (4%) 30 27	29, 69, 179, 207	0
3	L	391/411 (95%)	-0.10	22 (5%) 24 20	35, 70, 177, 203	0
4	M	4/4 (100%)	0.37	0 100 100	63, 64, 103, 108	0
4	N	4/4 (100%)	0.15	0 100 100	119, 131, 149, 154	0
4	Q	4/4 (100%)	-0.59	0 100 100	78, 89, 90, 115	0
4	R	4/4 (100%)	0.35	0 100 100	92, 105, 106, 118	0
5	O	4/4 (100%)	-0.54	0 100 100	66, 68, 73, 93	0
5	P	4/4 (100%)	-0.21	0 100 100	90, 99, 106, 113	0
5	S	4/4 (100%)	-0.97	0 100 100	58, 69, 75, 95	0
5	T	4/4 (100%)	-0.09	0 100 100	75, 91, 98, 108	0
All	All	3892/5768 (67%)	-0.06	214 (5%) 25 21	8, 75, 189, 246	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	73	GLY	8.6
1	J	206	LYS	7.8
3	I	9	CYS	7.5
2	H	107	VAL	7.5
1	D	117	SER	7.2
1	J	28	CYS	6.2
1	J	27	ALA	6.1
1	D	118	ARG	6.1
3	L	8	CYS	6.0
1	J	29	LYS	6.0
1	D	116	ARG	6.0
3	F	394	ILE	5.9
3	F	68	TYR	5.8
3	L	5	ARG	5.8
3	F	53	LYS	5.8
3	L	6	ASP	5.7
1	A	28	CYS	5.6
3	C	66	LEU	5.5
3	F	52	ASN	5.4
3	L	76	PRO	5.4
1	D	96	GLY	5.4
2	E	116	GLN	5.3
3	C	68	TYR	5.2
1	D	195	PRO	5.1
3	L	66	LEU	5.0
1	D	85	SER	5.0
3	I	395	GLY	5.0
3	L	63	ALA	5.0
3	F	59	GLN	4.9
1	G	28	CYS	4.8
3	I	8	CYS	4.7
2	E	147	GLU	4.7
1	D	88	THR	4.6
3	F	66	LEU	4.6
1	J	41	TRP	4.6
1	J	210	VAL	4.5
3	F	67	THR	4.5
3	L	67	THR	4.5
3	I	70	PRO	4.4
1	J	201	HIS	4.4
1	D	102	ASN	4.4
1	A	29	LYS	4.2
1	G	200	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	27	ALA	4.2
3	F	65	GLN	4.2
3	F	63	ALA	4.2
1	D	98	PHE	4.1
1	D	196	SER	4.1
3	F	76	PRO	4.0
1	D	27	ALA	4.0
1	G	31	SER	4.0
1	J	76	TYR	3.9
3	F	49	GLN	3.9
2	E	153	ILE	3.9
1	D	95	ARG	3.9
1	A	82	ASP	3.9
3	F	70	PRO	3.9
3	C	76	PRO	3.9
3	C	67	THR	3.9
2	E	139	VAL	3.9
3	I	14	ARG	3.9
1	D	101	ALA	3.8
2	E	218	GLY	3.7
3	I	13	GLU	3.7
1	A	83	SER	3.7
1	D	83	SER	3.7
2	E	119	TYR	3.7
2	E	152	TYR	3.7
1	G	29	LYS	3.5
1	D	110	ARG	3.5
3	I	393	THR	3.5
2	E	142	TYR	3.5
1	D	91	MET	3.5
1	G	99	SER	3.4
1	D	28	CYS	3.4
1	J	199	ARG	3.4
1	G	95	ARG	3.3
1	A	93	ILE	3.3
3	C	71	ASP	3.3
3	L	77	ASN	3.3
2	H	68	ALA	3.2
3	C	18	TYR	3.2
1	D	74	PHE	3.2
2	H	108	SER	3.2
3	C	74	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	I	7	ASN	3.2
3	F	78	MET	3.1
3	L	7	ASN	3.1
2	E	151	LEU	3.1
1	D	97	ASP	3.1
1	D	106	ASN	3.1
2	E	117	TYR	3.1
2	B	112	SER	3.1
3	F	61	ILE	3.1
3	L	11	LEU	3.0
2	H	149	HIS	3.0
1	D	114	ASP	3.0
2	E	131	GLN	3.0
1	G	104	ARG	3.0
1	A	84	HIS	3.0
3	I	19	CYS	3.0
1	D	162	ARG	3.0
2	E	64	GLY	3.0
3	I	16	GLY	2.9
1	D	107	THR	2.9
3	F	55	SER	2.9
2	E	120	LEU	2.9
2	B	119	TYR	2.9
2	K	130	LYS	2.9
3	I	17	SER	2.9
1	J	83	SER	2.9
2	E	141	GLU	2.9
3	L	13	GLU	2.9
1	D	81	LYS	2.9
2	E	123	ASP	2.9
2	K	107	VAL	2.8
2	B	142	TYR	2.8
1	D	194	LEU	2.8
2	E	112	SER	2.8
2	B	115	PHE	2.8
2	E	219	GLY	2.8
1	D	82	ASP	2.8
2	K	458	PHE	2.7
3	I	394	ILE	2.7
3	L	71	ASP	2.7
2	E	138	VAL	2.7
3	C	63	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	82	ALA	2.7
2	E	59	ALA	2.7
1	D	127	ILE	2.7
3	L	69	ASN	2.7
2	K	120	LEU	2.7
1	J	81	LYS	2.7
2	E	154	ASP	2.7
3	L	12	ASP	2.7
1	J	80	ASN	2.6
2	H	81	GLN	2.6
1	A	81	LYS	2.6
2	E	143	SER	2.6
3	C	65	GLN	2.6
3	F	79	ILE	2.6
3	F	56	GLU	2.6
3	C	69	ASN	2.6
2	E	144	SER	2.6
2	H	74	VAL	2.6
3	F	18	TYR	2.6
2	H	119	TYR	2.6
3	C	73	SER	2.5
3	I	10	ILE	2.5
1	D	80	ASN	2.5
1	J	205	ILE	2.5
1	A	76	TYR	2.5
2	H	59	ALA	2.5
3	L	68	TYR	2.5
3	I	69	ASN	2.5
3	I	68	TYR	2.5
2	E	114	SER	2.4
2	H	132	VAL	2.4
3	F	190	GLY	2.4
2	E	74	VAL	2.4
1	G	30	ASP	2.4
2	H	72	LEU	2.4
1	J	203	PRO	2.4
1	J	209	PRO	2.4
2	B	116	GLN	2.4
1	J	82	ASP	2.4
2	E	140	ASN	2.4
3	C	70	PRO	2.4
2	E	155	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	81	ALA	2.3
3	I	66	LEU	2.3
1	D	41	TRP	2.3
2	H	147	GLU	2.3
2	E	58	LYS	2.3
3	I	63	ALA	2.3
3	F	393	THR	2.3
2	E	105	GLU	2.3
2	E	149	HIS	2.3
3	L	18	TYR	2.3
1	J	38	ASP	2.2
1	D	92	GLU	2.2
1	D	113	GLU	2.2
2	E	104	VAL	2.2
1	J	202	LEU	2.2
1	J	195	PRO	2.2
2	E	162	PRO	2.2
1	J	208	LYS	2.2
3	C	45	ASP	2.2
1	J	68	LYS	2.2
2	H	120	LEU	2.2
2	K	162	PRO	2.2
3	F	109	TYR	2.2
3	L	395	GLY	2.2
3	F	74	SER	2.1
2	H	219	GLY	2.1
3	F	346	GLY	2.1
3	I	71	ASP	2.1
1	D	76	TYR	2.1
2	H	152	TYR	2.1
2	K	125	TRP	2.1
3	L	74	SER	2.1
3	C	64	ILE	2.1
2	E	148	LYS	2.1
3	I	6	ASP	2.1
2	E	150	GLN	2.1
3	L	64	ILE	2.1
1	J	77	GLN	2.1
2	E	62	ALA	2.1
1	G	96	GLY	2.1
2	E	458	PHE	2.0
3	C	84	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	14	ARG	2.0
1	J	211	PRO	2.0
1	D	79	ASN	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MAN	W	4	11/12	0.34	0.50	100,103,105,107	0
6	SIA	X	11	20/21	0.45	0.69	105,113,116,116	0
6	SIA	U	7	20/21	0.46	0.52	99,104,108,108	0
6	MAN	V	4	11/12	0.55	0.56	106,108,109,112	0
6	GAL	X	10	11/12	0.55	0.94	113,116,117,117	0
6	SIA	U	11	20/21	0.57	0.60	97,103,109,111	0
6	GAL	U	10	11/12	0.59	0.62	106,107,108,112	0
6	SIA	V	11	20/21	0.59	0.67	109,114,119,125	0
6	BMA	X	3	11/12	0.59	0.44	101,104,107,107	0
6	GAL	V	6	11/12	0.62	0.49	109,112,115,116	0
6	NAG	X	2	14/15	0.62	0.47	97,100,102,104	0
6	SIA	X	7	20/21	0.63	0.42	102,107,109,109	0
6	GAL	X	6	11/12	0.66	0.59	105,110,111,111	0
7	MAN	W	5	11/12	0.67	0.69	104,108,110,110	0
6	MAN	V	8	11/12	0.68	0.76	99,104,107,107	0
8	NAG	Y	2	14/15	0.68	0.73	105,108,109,109	0
6	MAN	X	4	11/12	0.69	0.43	93,103,105,105	0
8	NAG	Y	1	14/15	0.69	0.60	106,109,110,111	0
6	MAN	U	4	11/12	0.69	0.51	109,111,112,113	0
6	BMA	V	3	11/12	0.71	0.35	98,103,106,108	0
6	NAG	V	5	14/15	0.72	0.57	103,110,115,117	0
6	GAL	V	10	11/12	0.73	0.48	115,118,118,119	0
7	BMA	W	3	11/12	0.73	0.32	100,104,108,110	0
6	NAG	X	5	14/15	0.74	0.55	97,105,107,109	0

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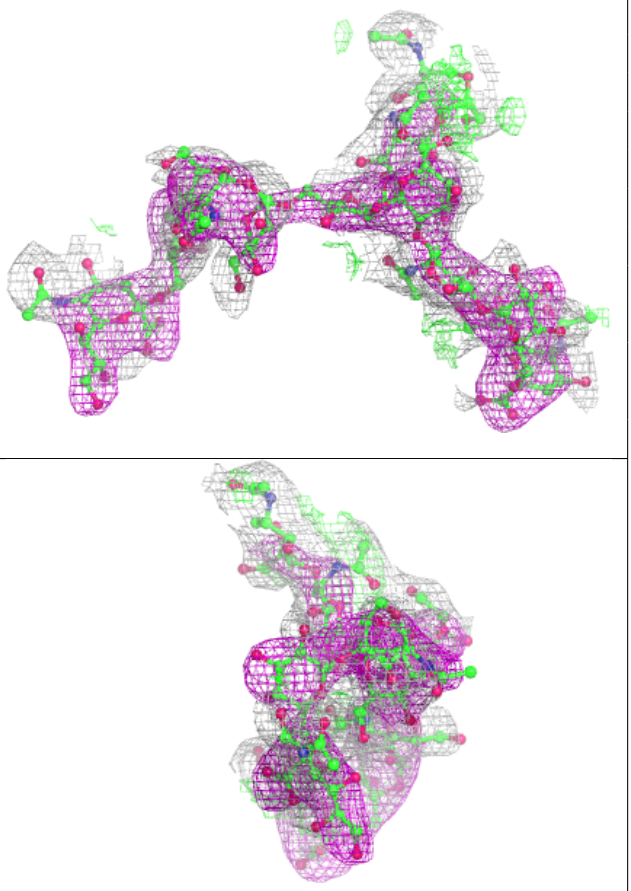
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	X	9	14/15	0.74	0.45	106,111,112,115	0
6	NAG	V	9	14/15	0.74	0.62	105,109,111,115	0
6	NAG	U	5	14/15	0.75	0.47	104,111,112,113	0
6	NAG	U	9	14/15	0.75	0.55	104,107,109,110	0
6	MAN	U	8	11/12	0.76	0.48	104,108,109,109	0
6	MAN	X	8	11/12	0.80	0.33	99,101,106,108	0
6	SIA	V	7	20/21	0.81	0.46	103,107,111,112	0
6	NAG	U	2	14/15	0.81	0.31	96,98,101,102	0
7	NAG	W	1	14/15	0.82	0.20	83,87,91,93	0
6	BMA	U	3	11/12	0.82	0.47	99,105,108,109	0
6	NAG	X	1	14/15	0.82	0.18	83,87,92,96	0
7	NAG	W	2	14/15	0.83	0.28	94,97,102,103	0
6	NAG	V	1	14/15	0.84	0.15	80,85,89,92	0
6	GAL	U	6	11/12	0.84	0.50	98,104,107,108	0
6	NAG	U	1	14/15	0.85	0.18	83,89,92,95	0
6	NAG	V	2	14/15	0.87	0.28	95,97,101,101	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.

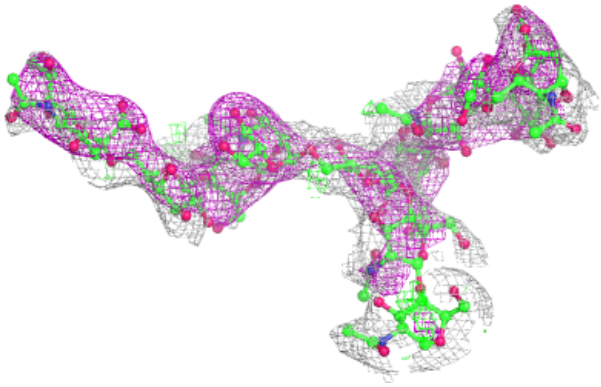
Electron density around Chain U:

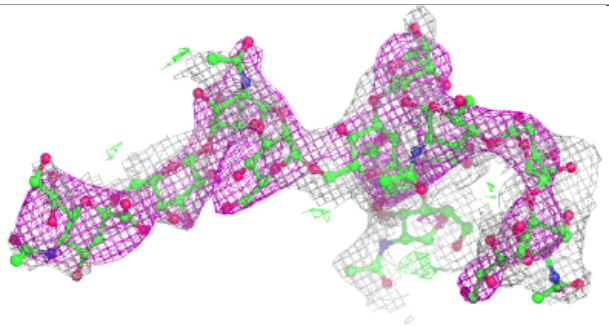
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

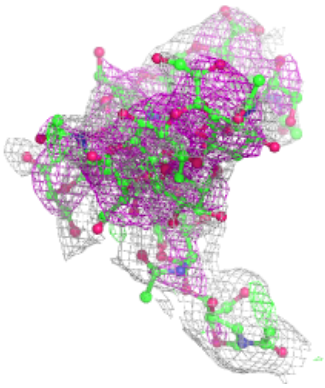


Electron density around Chain V:

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

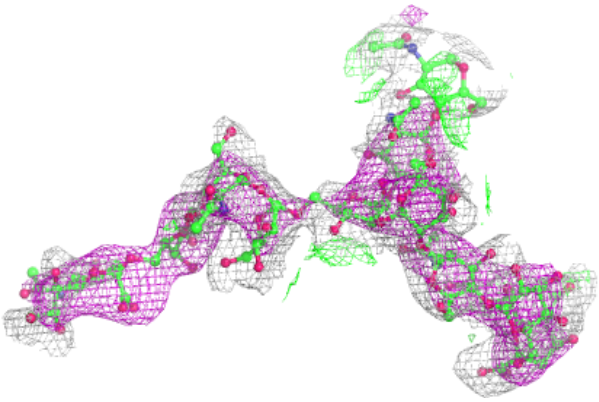


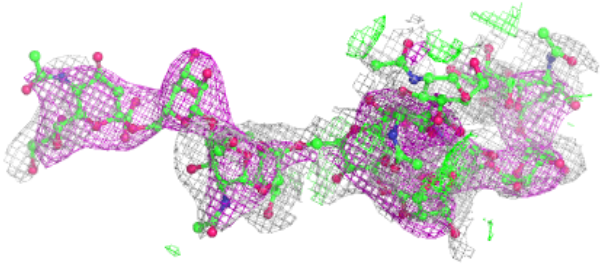


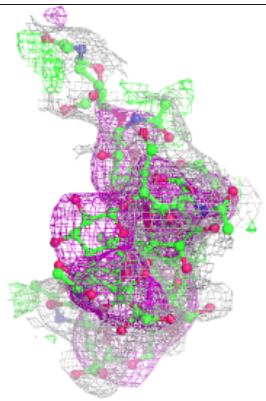


Electron density around Chain X:

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

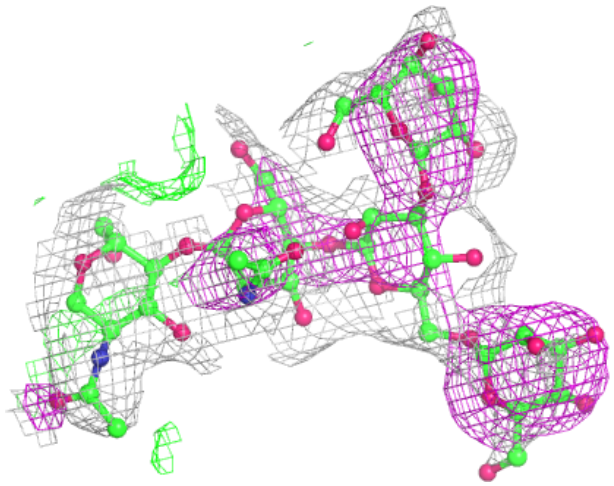


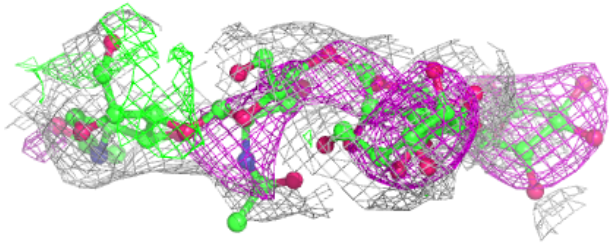


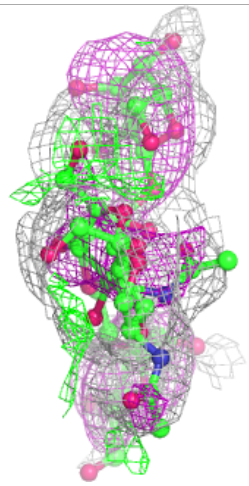


Electron density around Chain W:

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

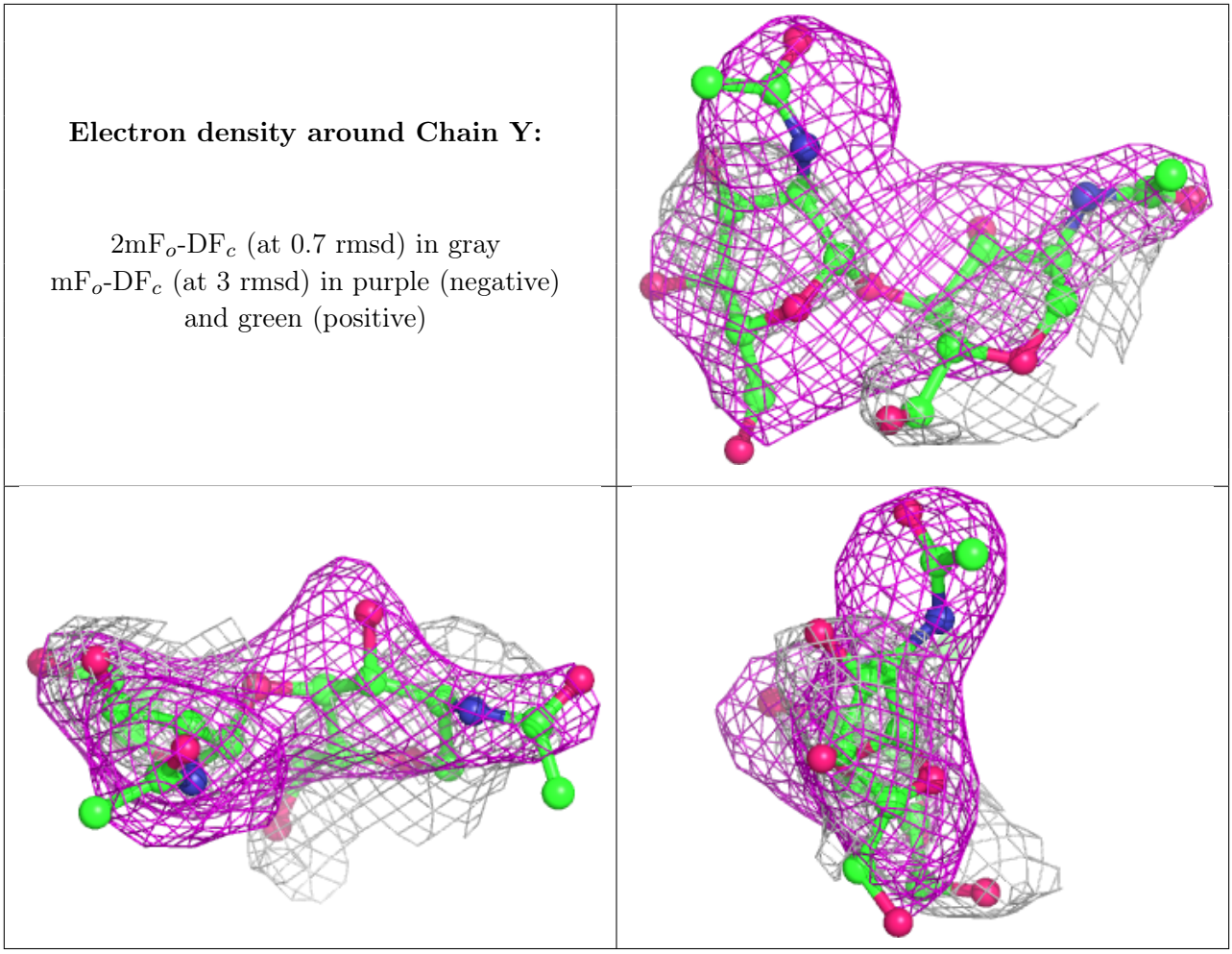






Electron density around Chain Y:

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



6.4 Ligands

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, 95^{th} 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
9	CA	K	501	1/1	0.91	0.07	68,68,68,68	0
9	CA	E	501	1/1	0.94	0.09	47,47,47,47	0
9	CA	L	601	1/1	0.96	0.07	51,51,51,51	0
9	CA	I	601	1/1	0.97	0.05	56,56,56,56	0
9	CA	F	601	1/1	0.98	0.05	49,49,49,49	0
9	CA	C	601	1/1	0.98	0.06	31,31,31,31	0
9	CA	H	501	1/1	0.99	0.05	51,51,51,51	0
9	CA	B	501	1/1	0.99	0.08	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.