Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2022 – 03:57 AM EST

PDB ID	:	1G5G
Title	:	FRAGMENT OF FUSION PROTEIN FROM NEWCASTLE DISEASE VIRUS
Authors	:	Lawrence, M.C.; Smith, B.J.
Deposited on	:	2000-11-01
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

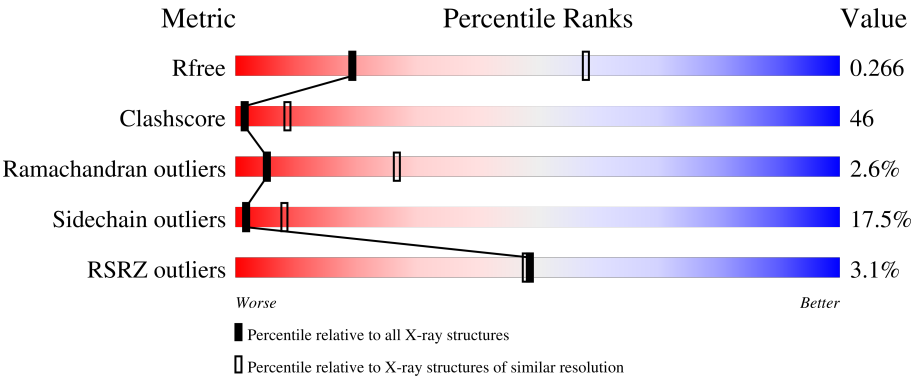
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	481	2% 27% 38% 9% 26%
1	B	481	2% 29% 35% 10% 26%
1	C	481	3% 30% 36% 9% 26%
1	D	481	3% 27% 38% 9% 26%
1	E	481	2% 30% 35% 9% 26%

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Mol	Chain	Length	Quality of chain
1	F	481	% 29% 37% 8% 26%
2	G	2	50% 50%
2	I	2	100%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	100%
2	M	2	50% 50%
2	N	2	50% 50%
3	H	3	67% 33%

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
2	NAG	J	1	-	-	-	X
2	NAG	J	2	-	-	-	X
3	NAG	H	1	-	-	-	X
3	NAG	H	2	-	-	-	X
3	BMA	H	3	-	-	-	X
4	NAG	C	4471	-	-	X	X
4	NAG	D	1911	-	-	-	X
4	NAG	E	4471	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16341 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	B	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	C	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	D	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	E	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	F	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	SER	-	expression tag	UNP A9LSB1
A	501	ARG	-	expression tag	UNP A9LSB1
A	502	GLU	-	expression tag	UNP A9LSB1
A	503	GLN	-	expression tag	UNP A9LSB1
A	504	LYS	-	expression tag	UNP A9LSB1
A	505	LEU	-	expression tag	UNP A9LSB1
A	506	ILE	-	expression tag	UNP A9LSB1
A	507	SER	-	expression tag	UNP A9LSB1
A	508	GLU	-	expression tag	UNP A9LSB1
A	509	GLU	-	expression tag	UNP A9LSB1
A	510	ASP	-	expression tag	UNP A9LSB1
A	511	LEU	-	expression tag	UNP A9LSB1
A	512	ASN	-	expression tag	UNP A9LSB1
B	500	SER	-	expression tag	UNP A9LSB1
B	501	ARG	-	expression tag	UNP A9LSB1
B	502	GLU	-	expression tag	UNP A9LSB1
B	503	GLN	-	expression tag	UNP A9LSB1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	504	LYS	-	expression tag	UNP A9LSB1
B	505	LEU	-	expression tag	UNP A9LSB1
B	506	ILE	-	expression tag	UNP A9LSB1
B	507	SER	-	expression tag	UNP A9LSB1
B	508	GLU	-	expression tag	UNP A9LSB1
B	509	GLU	-	expression tag	UNP A9LSB1
B	510	ASP	-	expression tag	UNP A9LSB1
B	511	LEU	-	expression tag	UNP A9LSB1
B	512	ASN	-	expression tag	UNP A9LSB1
C	500	SER	-	expression tag	UNP A9LSB1
C	501	ARG	-	expression tag	UNP A9LSB1
C	502	GLU	-	expression tag	UNP A9LSB1
C	503	GLN	-	expression tag	UNP A9LSB1
C	504	LYS	-	expression tag	UNP A9LSB1
C	505	LEU	-	expression tag	UNP A9LSB1
C	506	ILE	-	expression tag	UNP A9LSB1
C	507	SER	-	expression tag	UNP A9LSB1
C	508	GLU	-	expression tag	UNP A9LSB1
C	509	GLU	-	expression tag	UNP A9LSB1
C	510	ASP	-	expression tag	UNP A9LSB1
C	511	LEU	-	expression tag	UNP A9LSB1
C	512	ASN	-	expression tag	UNP A9LSB1
D	500	SER	-	expression tag	UNP A9LSB1
D	501	ARG	-	expression tag	UNP A9LSB1
D	502	GLU	-	expression tag	UNP A9LSB1
D	503	GLN	-	expression tag	UNP A9LSB1
D	504	LYS	-	expression tag	UNP A9LSB1
D	505	LEU	-	expression tag	UNP A9LSB1
D	506	ILE	-	expression tag	UNP A9LSB1
D	507	SER	-	expression tag	UNP A9LSB1
D	508	GLU	-	expression tag	UNP A9LSB1
D	509	GLU	-	expression tag	UNP A9LSB1
D	510	ASP	-	expression tag	UNP A9LSB1
D	511	LEU	-	expression tag	UNP A9LSB1
D	512	ASN	-	expression tag	UNP A9LSB1
E	500	SER	-	expression tag	UNP A9LSB1
E	501	ARG	-	expression tag	UNP A9LSB1
E	502	GLU	-	expression tag	UNP A9LSB1
E	503	GLN	-	expression tag	UNP A9LSB1
E	504	LYS	-	expression tag	UNP A9LSB1
E	505	LEU	-	expression tag	UNP A9LSB1
E	506	ILE	-	expression tag	UNP A9LSB1

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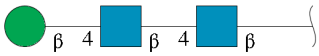
Chain	Residue	Modelled	Actual	Comment	Reference
E	507	SER	-	expression tag	UNP A9LSB1
E	508	GLU	-	expression tag	UNP A9LSB1
E	509	GLU	-	expression tag	UNP A9LSB1
E	510	ASP	-	expression tag	UNP A9LSB1
E	511	LEU	-	expression tag	UNP A9LSB1
E	512	ASN	-	expression tag	UNP A9LSB1
F	500	SER	-	expression tag	UNP A9LSB1
F	501	ARG	-	expression tag	UNP A9LSB1
F	502	GLU	-	expression tag	UNP A9LSB1
F	503	GLN	-	expression tag	UNP A9LSB1
F	504	LYS	-	expression tag	UNP A9LSB1
F	505	LEU	-	expression tag	UNP A9LSB1
F	506	ILE	-	expression tag	UNP A9LSB1
F	507	SER	-	expression tag	UNP A9LSB1
F	508	GLU	-	expression tag	UNP A9LSB1
F	509	GLU	-	expression tag	UNP A9LSB1
F	510	ASP	-	expression tag	UNP A9LSB1
F	511	LEU	-	expression tag	UNP A9LSB1
F	512	ASN	-	expression tag	UNP A9LSB1

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

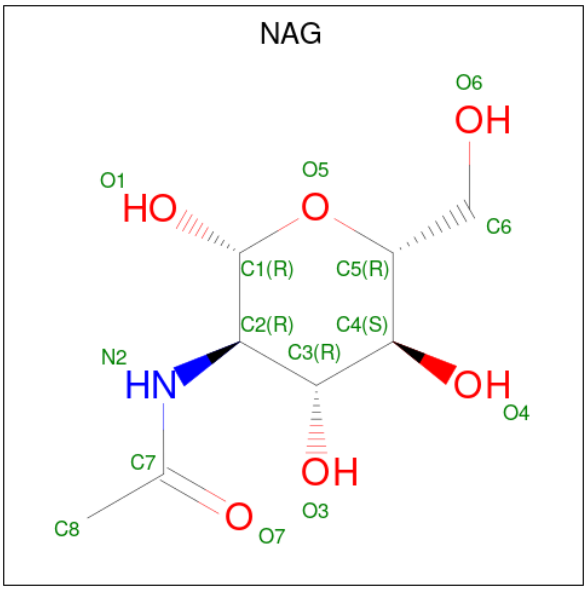
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	H	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



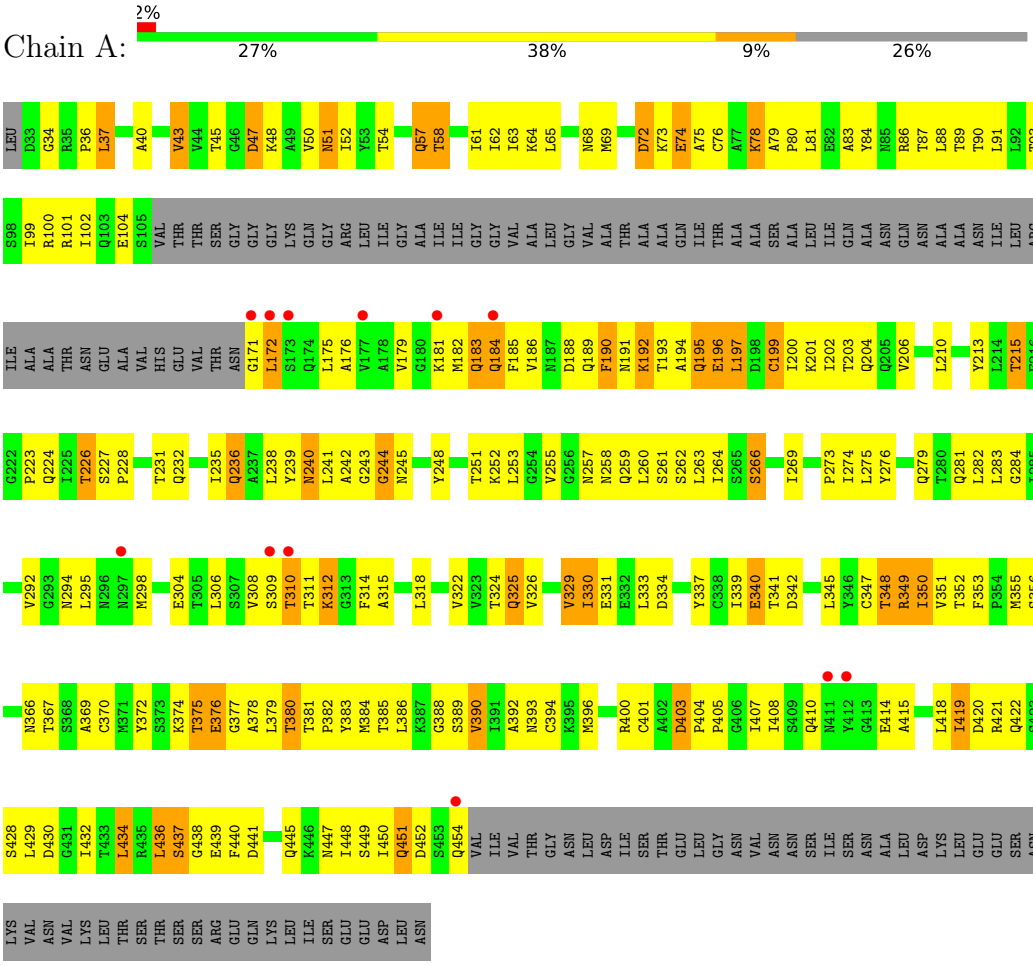
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

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

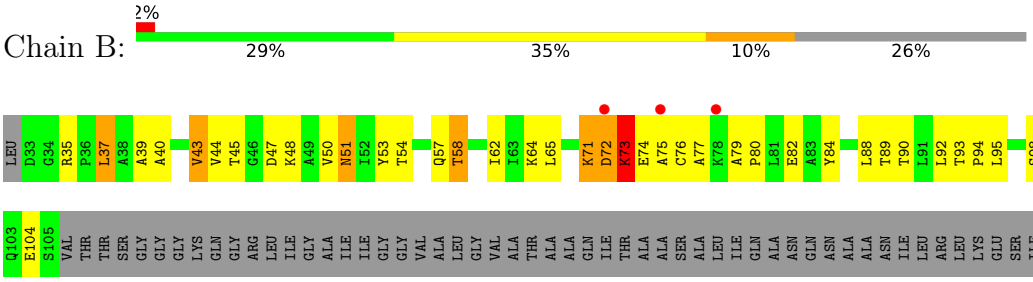
• Molecule 1: Fusion glycoprotein F0

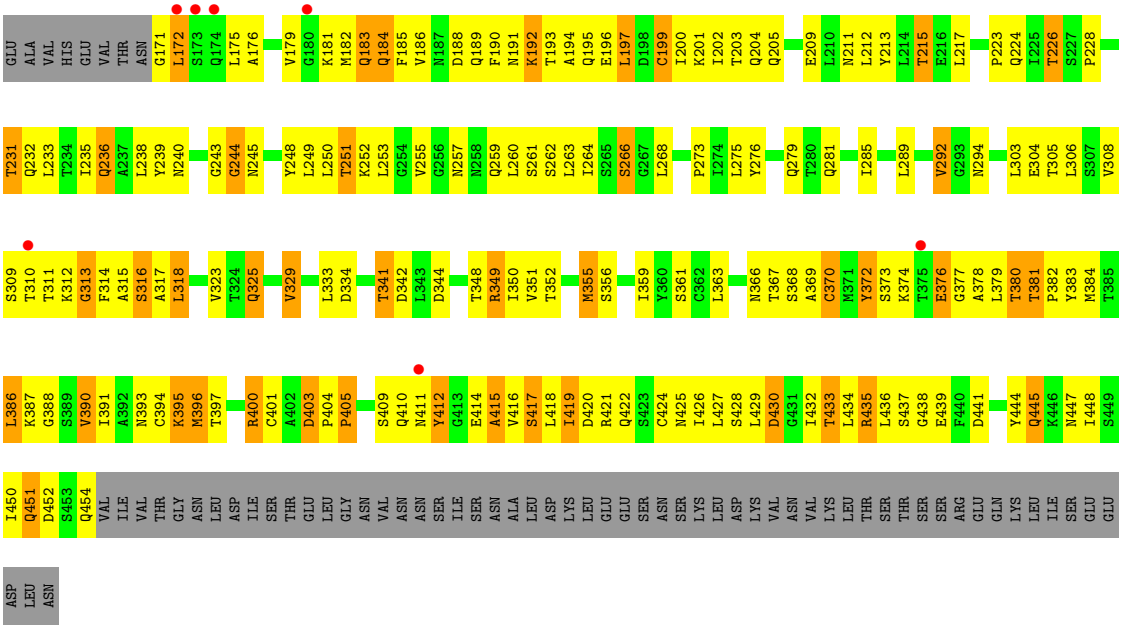
Chain A:



• Molecule 1: Fusion glycoprotein F0

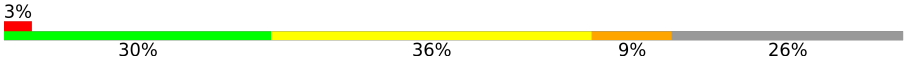
Chain B:

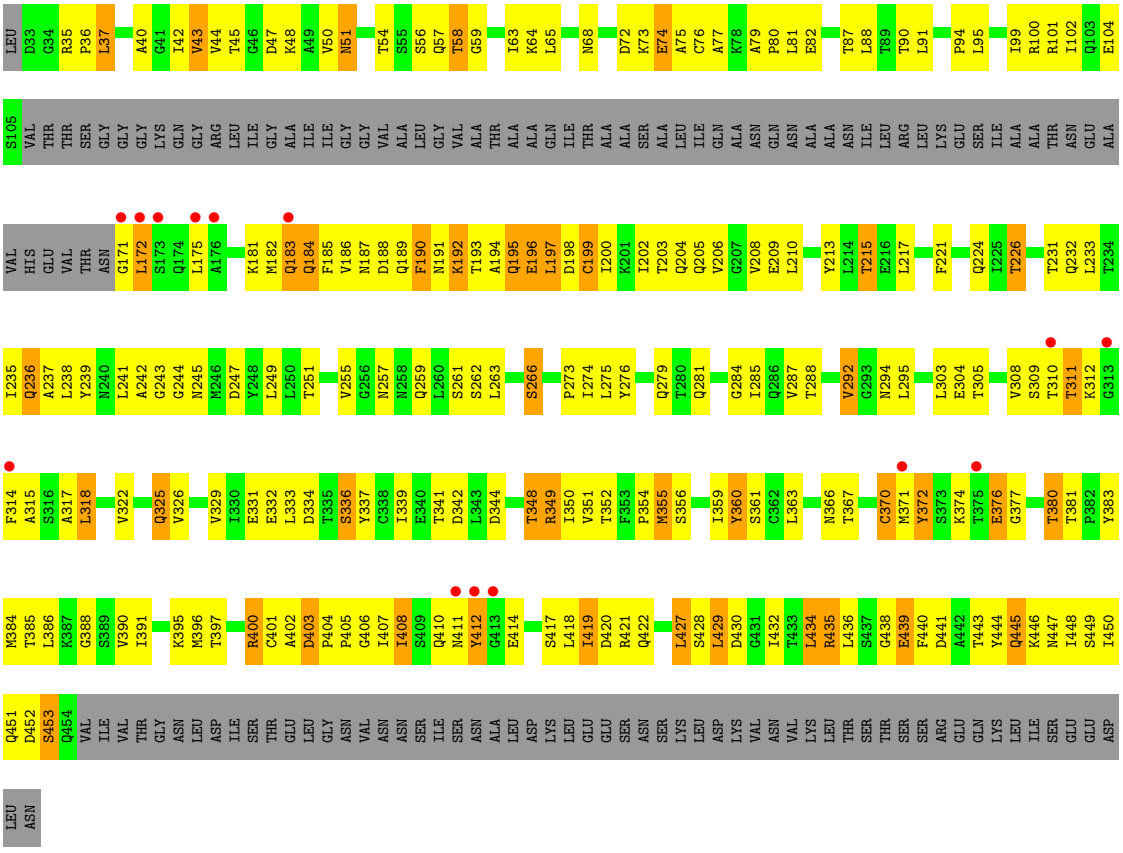




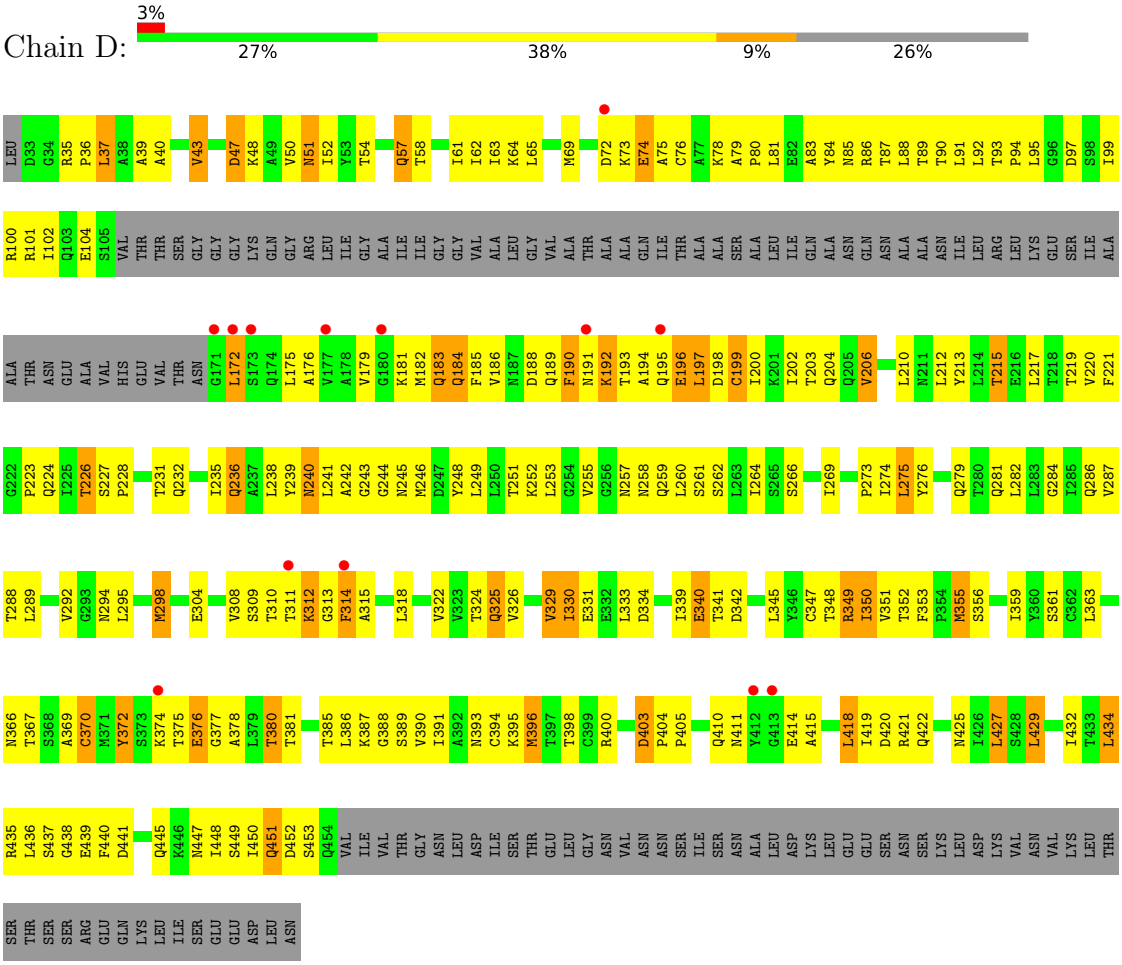
• Molecule 1: Fusion glycoprotein F0

Chain C:

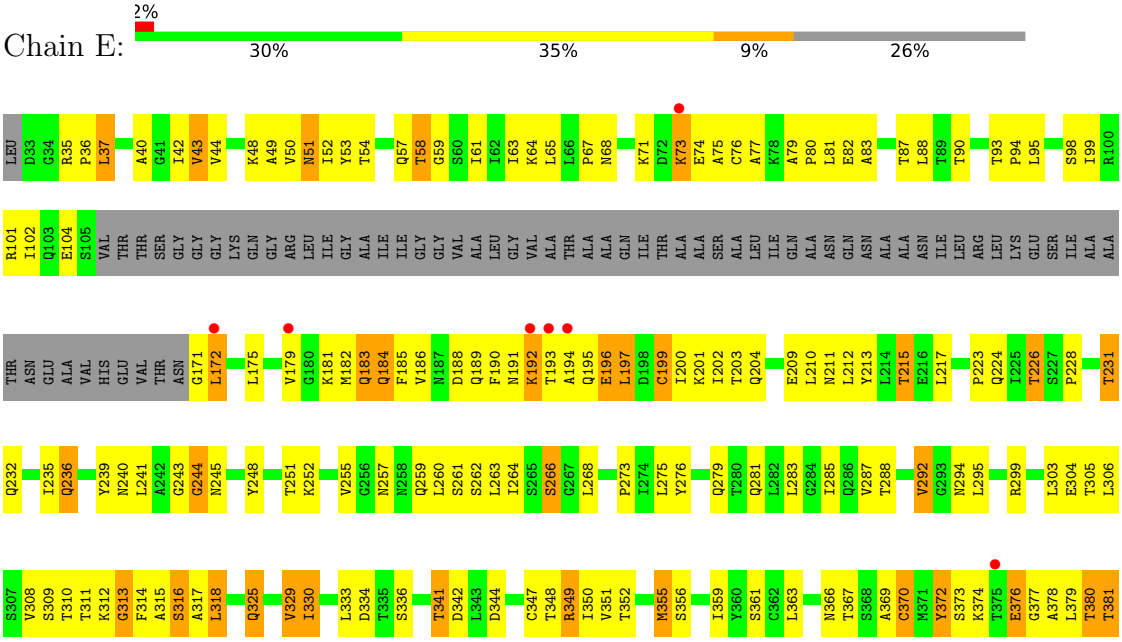


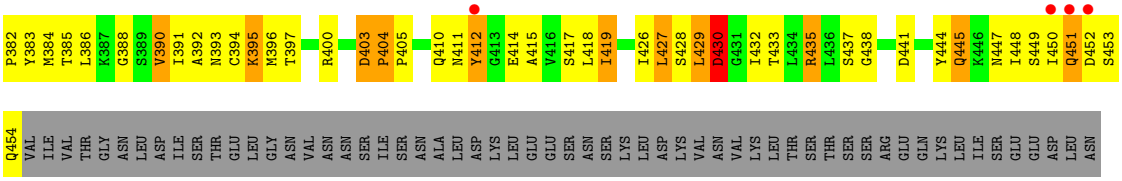


• Molecule 1: Fusion glycoprotein F0



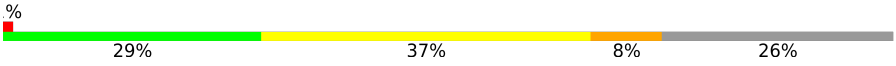
• Molecule 1: Fusion glycoprotein F0

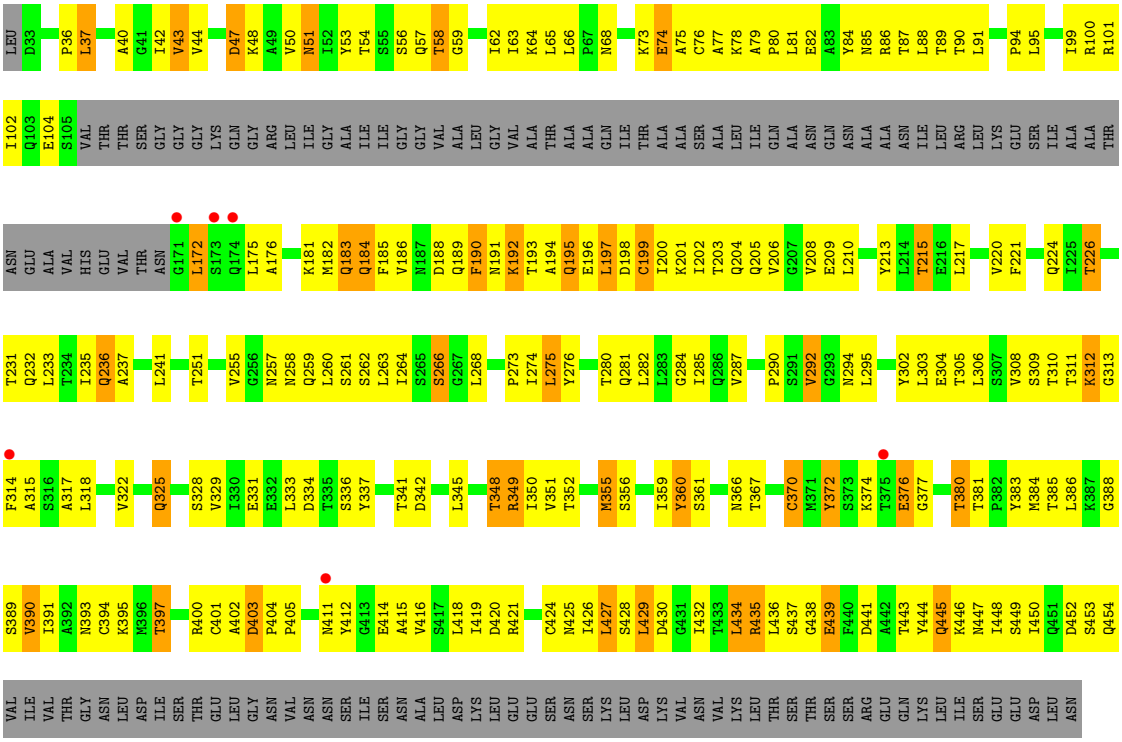




• Molecule 1: Fusion glycoprotein F0

Chain F:





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

Chain G:

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

Chain I:

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

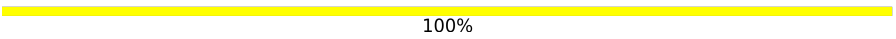
Chain J:

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

Chain K:

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

Chain L:



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

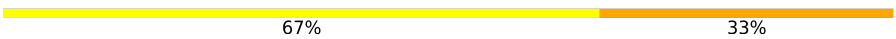
Chain M:

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

Chain N:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.39Å 308.33Å 243.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 24.84 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.30) 95.8 (24.84-3.29)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.30Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.266	Depositor DCC
R_{free} test set	3741 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	16341	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 34.87 % 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 6.3763e-04. 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/2708	0.73	1/3683 (0.0%)
1	B	0.42	0/2708	0.73	0/3683
1	C	0.42	0/2708	0.74	1/3683 (0.0%)
1	D	0.44	0/2708	0.73	1/3683 (0.0%)
1	E	0.42	0/2708	0.74	0/3683
1	F	0.43	0/2708	0.73	0/3683
All	All	0.43	0/16248	0.73	3/22098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	ILE	N-CA-C	-5.41	96.39	111.00
1	C	339	ILE	N-CA-C	-5.35	96.56	111.00
1	D	339	ILE	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2675	0	2716	311	0
1	B	2675	0	2717	313	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2675	0	2716	329	0
1	D	2675	0	2717	297	0
1	E	2675	0	2716	310	0
1	F	2675	0	2717	318	0
2	G	28	0	25	6	0
2	I	28	0	25	2	0
2	J	28	0	25	3	0
2	K	28	0	25	1	0
2	L	28	0	25	1	0
2	M	28	0	25	1	0
2	N	28	0	25	2	0
3	H	39	0	34	5	0
4	C	14	0	13	7	0
4	D	14	0	13	0	0
4	E	14	0	13	5	0
4	F	14	0	13	0	0
All	All	16341	0	16560	1521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (1521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG13	1:A:292:VAL:HG11	1.23	1.19
1:D:255:VAL:HG13	1:D:292:VAL:HG11	1.27	1.10
1:E:314:PHE:HB3	1:E:374:LYS:HD3	1.32	1.10
1:C:405:PRO:CG	1:F:64:LYS:HD2	1.81	1.10
1:A:314:PHE:HB3	1:A:374:LYS:HD3	1.31	1.09
1:D:314:PHE:HB3	1:D:374:LYS:HD3	1.30	1.08
1:F:89:THR:HG21	2:N:1:NAG:H62	1.31	1.07
1:C:405:PRO:HG3	1:F:64:LYS:HD2	1.14	1.06
1:B:314:PHE:HB3	1:B:374:LYS:HD3	1.38	1.05
1:B:451:GLN:HE21	1:B:451:GLN:HA	1.21	1.02
1:A:393:ASN:ND2	1:A:396:MET:HB2	1.73	1.01
1:F:314:PHE:HB3	1:F:374:LYS:HD3	1.38	1.00
1:A:447:ASN:O	3:H:1:NAG:H82	1.61	1.00
1:C:402:ALA:HB1	1:F:280:THR:HG21	1.40	1.00
1:E:447:ASN:H	4:E:4471:NAG:H82	1.28	0.99
1:D:101:ARG:HB3	1:E:257:ASN:HD22	1.29	0.98
1:A:101:ARG:HB3	1:B:257:ASN:HD22	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LYS:HG3	1:C:314:PHE:HB2	1.46	0.96
1:D:57:GLN:HE21	1:E:438:GLY:HA3	1.30	0.96
1:B:397:THR:HB	1:B:430:ASP:OD2	1.64	0.96
1:A:403:ASP:HB3	1:A:404:PRO:HD3	1.48	0.94
1:E:54:THR:HG22	1:F:388:GLY:HA2	1.47	0.94
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.31	0.94
1:D:350:ILE:HB	1:E:381:THR:HG22	1.48	0.94
1:B:101:ARG:HH11	1:C:257:ASN:HD21	1.07	0.93
1:D:57:GLN:NE2	1:E:438:GLY:HA3	1.83	0.92
1:E:101:ARG:HH11	1:F:257:ASN:HD21	1.17	0.91
1:A:401:CYS:SG	1:A:404:PRO:HD2	2.10	0.91
1:E:64:LYS:NZ	1:F:445:GLN:HE21	1.67	0.91
1:B:403:ASP:HB3	1:B:404:PRO:HD3	1.53	0.90
1:C:355:MET:HE1	1:C:363:LEU:HD12	1.55	0.89
1:A:57:GLN:HE21	1:B:438:GLY:HA3	1.37	0.89
1:C:405:PRO:HG3	1:F:64:LYS:CD	2.01	0.89
1:A:204:GLN:HE22	1:C:204:GLN:HA	1.36	0.89
1:E:451:GLN:HA	1:E:451:GLN:HE21	1.37	0.89
1:F:403:ASP:HB3	1:F:404:PRO:HD3	1.52	0.89
1:C:314:PHE:HB3	1:C:374:LYS:HD3	1.52	0.88
1:A:57:GLN:NE2	1:B:438:GLY:HA3	1.88	0.87
1:C:400:ARG:HG3	1:C:428:SER:HB2	1.55	0.87
1:A:350:ILE:HB	1:B:381:THR:HG22	1.56	0.87
1:B:51:ASN:HB3	1:B:294:ASN:HA	1.57	0.86
1:B:65:LEU:HD23	1:B:217:LEU:HD21	1.56	0.86
1:D:295:LEU:HD23	1:E:432:ILE:HG21	1.57	0.86
1:C:43:VAL:HG21	1:C:391:ILE:HG21	1.57	0.86
1:E:279:GLN:OE1	2:M:2:NAG:H4	1.76	0.85
1:B:410:GLN:NE2	1:B:417:SER:HA	1.91	0.85
1:E:73:LYS:HG2	1:F:450:ILE:HD11	1.57	0.85
1:C:401:CYS:SG	1:C:404:PRO:HD2	2.17	0.85
1:D:62:ILE:HD11	1:D:282:LEU:HD21	1.57	0.85
1:C:51:ASN:HB3	1:C:294:ASN:HA	1.59	0.84
1:B:35:ARG:HH22	1:B:418:LEU:HD12	1.42	0.84
1:F:401:CYS:SG	1:F:404:PRO:HD2	2.18	0.83
1:A:427:LEU:HD13	1:A:429:LEU:HD21	1.61	0.83
1:A:95:LEU:O	1:A:99:ILE:HG13	1.77	0.83
1:D:390:VAL:HG11	1:D:427:LEU:HD12	1.61	0.83
1:A:64:LYS:HB2	1:B:445:GLN:HB3	1.59	0.83
1:B:403:ASP:HB3	1:B:404:PRO:CD	2.08	0.83
1:A:215:THR:HG21	1:C:215:THR:HG22	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:THR:HG22	1:E:215:THR:HG21	1.60	0.83
1:F:51:ASN:N	1:F:51:ASN:HD22	1.76	0.83
1:A:226:THR:HA	1:B:236:GLN:NE2	1.94	0.82
1:F:312:LYS:HG3	1:F:314:PHE:HB2	1.61	0.82
1:C:400:ARG:HD3	1:F:275:LEU:HD21	1.61	0.81
1:D:101:ARG:HD3	1:E:257:ASN:ND2	1.95	0.81
1:B:279:GLN:OE1	2:I:2:NAG:H4	1.80	0.81
1:F:355:MET:HE3	1:F:359:ILE:HG22	1.63	0.81
1:D:95:LEU:O	1:D:99:ILE:HG13	1.79	0.81
1:D:451:GLN:H	1:F:205:GLN:HE22	1.28	0.81
1:F:312:LYS:O	1:F:314:PHE:N	2.13	0.81
1:E:447:ASN:N	4:E:4471:NAG:H82	1.96	0.81
1:A:204:GLN:NE2	1:C:204:GLN:HA	1.95	0.80
1:B:427:LEU:HD13	1:B:429:LEU:HD21	1.63	0.80
1:E:35:ARG:HH22	1:E:418:LEU:HD12	1.46	0.80
1:A:215:THR:HG22	1:B:215:THR:HG21	1.63	0.80
1:D:102:ILE:HD13	1:E:261:SER:HB2	1.64	0.80
1:D:341:THR:HG22	1:D:342:ASP:N	1.96	0.80
1:E:447:ASN:HB2	4:E:4471:NAG:C7	2.12	0.80
1:D:204:GLN:HE22	1:F:204:GLN:HA	1.47	0.80
1:E:419:ILE:HG21	1:E:427:LEU:HG	1.64	0.80
1:D:65:LEU:HD23	1:D:217:LEU:HD21	1.63	0.79
1:D:403:ASP:HB3	1:D:404:PRO:HD2	1.63	0.79
1:F:312:LYS:HD2	1:F:374:LYS:NZ	1.98	0.79
1:E:306:LEU:HD12	1:E:382:PRO:O	1.80	0.79
1:B:419:ILE:HG21	1:B:427:LEU:HG	1.65	0.79
1:C:403:ASP:HB3	1:C:404:PRO:HD3	1.63	0.79
1:C:95:LEU:O	1:C:99:ILE:HG13	1.83	0.78
1:A:62:ILE:HD11	1:A:282:LEU:HD21	1.65	0.78
1:E:102:ILE:HD13	1:F:261:SER:HB2	1.66	0.78
1:E:73:LYS:HG2	1:F:450:ILE:CD1	2.13	0.78
1:D:255:VAL:HG13	1:D:292:VAL:CG1	2.12	0.78
1:F:341:THR:HG22	1:F:342:ASP:N	1.99	0.77
1:A:312:LYS:HG3	1:A:314:PHE:HB2	1.66	0.77
1:A:102:ILE:HD13	1:B:261:SER:HB2	1.67	0.77
1:E:204:GLN:HA	1:F:204:GLN:HE22	1.49	0.77
1:C:419:ILE:HG21	1:C:427:LEU:HG	1.66	0.77
1:F:95:LEU:O	1:F:99:ILE:HG13	1.85	0.77
1:F:403:ASP:O	1:F:405:PRO:HD3	1.85	0.77
1:D:274:ILE:HD13	1:D:286:GLN:HB2	1.67	0.77
1:F:308:VAL:O	1:F:315:ALA:HB3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:O	1:D:264:ILE:HG12	1.85	0.77
1:E:64:LYS:HZ3	1:F:445:GLN:HE21	1.34	0.77
1:A:101:ARG:HD3	1:B:257:ASN:ND2	1.99	0.76
1:C:341:THR:HG22	1:C:342:ASP:N	2.00	0.76
1:E:40:ALA:HB2	1:E:367:THR:HG23	1.66	0.76
1:B:312:LYS:HG3	1:B:314:PHE:HB2	1.66	0.76
1:D:403:ASP:HB3	1:D:404:PRO:CD	2.14	0.76
1:B:54:THR:HG22	1:C:388:GLY:HA2	1.66	0.76
1:B:304:GLU:HG2	1:B:384:MET:CE	2.15	0.76
1:C:400:ARG:HG2	1:C:400:ARG:NH1	1.91	0.76
1:A:308:VAL:O	1:A:315:ALA:HB3	1.84	0.76
1:B:40:ALA:HB2	1:B:367:THR:HG23	1.66	0.76
1:C:308:VAL:O	1:C:315:ALA:HB3	1.85	0.76
1:D:172:LEU:HD21	1:F:172:LEU:N	2.01	0.76
1:A:295:LEU:HD23	1:B:432:ILE:HG21	1.68	0.76
1:C:279:GLN:OE1	2:K:2:NAG:H4	1.85	0.76
1:D:215:THR:HG21	1:F:215:THR:HG22	1.67	0.76
1:B:204:GLN:HA	1:C:204:GLN:NE2	2.01	0.75
1:D:204:GLN:NE2	1:F:204:GLN:HA	2.01	0.75
1:A:255:VAL:HG13	1:A:292:VAL:CG1	2.11	0.75
1:C:51:ASN:HD22	1:C:51:ASN:N	1.84	0.75
1:F:79:ALA:HB3	1:F:80:PRO:HD3	1.68	0.75
1:A:65:LEU:HD23	1:A:217:LEU:HD21	1.68	0.75
1:C:349:ARG:HD2	1:C:351:VAL:HG23	1.68	0.75
1:A:204:GLN:HA	1:B:204:GLN:NE2	2.02	0.75
1:D:308:VAL:O	1:D:315:ALA:HB3	1.86	0.75
1:E:275:LEU:HD12	1:E:276:TYR:N	2.02	0.74
1:A:37:LEU:HD23	1:A:37:LEU:H	1.51	0.74
1:D:37:LEU:H	1:D:37:LEU:HD23	1.51	0.74
1:F:51:ASN:HB3	1:F:294:ASN:HA	1.67	0.74
1:E:204:GLN:HA	1:F:204:GLN:NE2	2.01	0.74
1:A:279:GLN:HB2	2:G:2:NAG:H2	1.70	0.74
1:D:226:THR:HA	1:E:236:GLN:NE2	2.02	0.74
1:A:390:VAL:HG11	1:A:427:LEU:HD12	1.68	0.74
1:E:403:ASP:HB3	1:E:404:PRO:CD	2.18	0.74
1:A:257:ASN:HD22	1:C:101:ARG:HB3	1.53	0.73
1:E:54:THR:CG2	1:F:388:GLY:HA2	2.16	0.73
1:D:64:LYS:HB2	1:E:445:GLN:HB3	1.71	0.73
1:E:419:ILE:CD1	1:E:427:LEU:HD11	2.18	0.73
1:C:405:PRO:CB	1:F:64:LYS:HD2	2.19	0.73
1:E:419:ILE:HD13	1:E:427:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD13	1:C:261:SER:HB2	1.69	0.72
1:F:181:LYS:O	1:F:184:GLN:HG3	1.88	0.72
1:B:419:ILE:H	1:B:419:ILE:HD12	1.54	0.72
1:C:65:LEU:HD23	1:C:217:LEU:HD21	1.70	0.72
1:C:419:ILE:HD12	1:C:427:LEU:HD11	1.71	0.72
1:D:438:GLY:HA3	1:F:57:GLN:NE2	2.05	0.72
1:F:349:ARG:HD2	1:F:351:VAL:HG23	1.71	0.72
1:D:419:ILE:HD13	1:D:427:LEU:HD21	1.72	0.72
1:F:255:VAL:HG13	1:F:292:VAL:HG11	1.72	0.72
1:A:377:GLY:O	1:A:380:THR:HG23	1.89	0.72
1:D:349:ARG:HD2	1:D:351:VAL:HG23	1.71	0.72
1:E:403:ASP:O	1:E:405:PRO:N	2.22	0.72
1:C:79:ALA:HB3	1:C:80:PRO:HD3	1.71	0.72
1:E:215:THR:HG22	1:F:215:THR:HG21	1.72	0.72
1:E:312:LYS:C	1:E:314:PHE:H	1.92	0.72
1:A:341:THR:HG22	1:A:342:ASP:N	2.05	0.72
1:A:381:THR:HG22	1:C:350:ILE:HB	1.70	0.72
1:B:275:LEU:HD12	1:B:276:TYR:N	2.05	0.71
1:C:435:ARG:HH11	1:C:435:ARG:HG2	1.54	0.71
1:E:43:VAL:HG21	1:E:391:ILE:HD13	1.71	0.71
1:A:403:ASP:HB3	1:A:404:PRO:CD	2.18	0.71
1:E:311:THR:OG1	1:E:315:ALA:HB2	1.89	0.71
1:D:377:GLY:O	1:D:380:THR:HG23	1.91	0.71
1:B:43:VAL:HG21	1:B:391:ILE:HD13	1.72	0.71
1:B:333:LEU:HD23	1:B:334:ASP:N	2.06	0.71
1:A:312:LYS:C	1:A:314:PHE:H	1.92	0.71
1:C:334:ASP:OD1	1:C:336:SER:HB3	1.90	0.71
1:D:275:LEU:HD12	1:D:276:TYR:N	2.06	0.71
1:E:64:LYS:HD3	1:F:445:GLN:HG2	1.73	0.71
1:D:101:ARG:HD3	1:E:257:ASN:HD21	1.54	0.71
1:D:204:GLN:HA	1:E:204:GLN:NE2	2.06	0.71
1:C:51:ASN:N	1:C:51:ASN:ND2	2.39	0.70
1:C:411:ASN:H	1:C:414:GLU:CD	1.95	0.70
1:F:51:ASN:N	1:F:51:ASN:ND2	2.37	0.70
1:A:349:ARG:HD2	1:A:351:VAL:HG23	1.73	0.70
1:F:419:ILE:HD12	1:F:427:LEU:HD11	1.72	0.70
1:A:202:ILE:HD11	1:B:450:ILE:HD12	1.74	0.70
1:B:57:GLN:NE2	1:C:438:GLY:HA3	2.06	0.70
1:E:350:ILE:HB	1:F:381:THR:HG22	1.74	0.70
1:A:427:LEU:HD13	1:A:429:LEU:CD2	2.22	0.70
1:C:255:VAL:HG13	1:C:292:VAL:HG11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ILE:HD12	1:D:434:LEU:CD1	2.22	0.70
1:E:191:ASN:O	1:E:194:ALA:HB3	1.92	0.70
1:F:435:ARG:HG2	1:F:435:ARG:HH11	1.56	0.70
1:A:388:GLY:HA2	1:C:54:THR:CG2	2.22	0.70
1:D:309:SER:O	1:D:311:THR:N	2.24	0.70
1:D:421:ARG:HH11	1:D:421:ARG:HG2	1.57	0.70
1:A:432:ILE:CG2	1:C:295:LEU:HD23	2.22	0.69
1:E:64:LYS:HB2	1:F:445:GLN:HB3	1.72	0.69
1:E:312:LYS:O	1:E:314:PHE:N	2.21	0.69
1:A:439:GLU:HA	1:C:58:THR:O	1.92	0.69
1:F:100:ARG:O	1:F:104:GLU:HG2	1.91	0.69
1:F:421:ARG:HG2	1:F:436:LEU:O	1.92	0.69
1:B:101:ARG:NH1	1:C:257:ASN:HD21	1.87	0.69
1:E:435:ARG:HG3	1:E:435:ARG:HH11	1.56	0.69
1:E:211:ASN:HD22	1:F:208:VAL:HG22	1.57	0.69
1:C:412:TYR:HE2	1:D:421:ARG:HH22	1.40	0.69
1:E:223:PRO:HB3	1:E:231:THR:HG21	1.73	0.69
1:B:57:GLN:HE22	1:C:438:GLY:HA3	1.57	0.69
1:B:226:THR:HA	1:C:236:GLN:NE2	2.07	0.69
1:E:181:LYS:O	1:E:184:GLN:HG3	1.93	0.69
3:H:2:NAG:H3	3:H:3:BMA:H2	1.73	0.69
1:B:101:ARG:HH11	1:C:257:ASN:ND2	1.87	0.69
1:A:451:GLN:H	1:C:205:GLN:HE22	1.41	0.69
1:C:447:ASN:O	4:C:4471:NAG:H82	1.92	0.68
1:D:192:LYS:HD3	1:D:193:THR:N	2.08	0.68
1:E:312:LYS:HG3	1:E:314:PHE:HB2	1.75	0.68
1:B:35:ARG:HH22	1:B:418:LEU:CD1	2.07	0.68
1:F:411:ASN:O	1:F:414:GLU:HG3	1.93	0.68
1:B:341:THR:HG22	1:B:344:ASP:H	1.57	0.68
1:D:182:MET:HG3	1:E:182:MET:HE1	1.76	0.68
1:E:377:GLY:O	1:E:380:THR:HG23	1.92	0.68
1:E:51:ASN:HB3	1:E:294:ASN:HA	1.76	0.68
1:A:419:ILE:HG21	1:A:427:LEU:HG	1.76	0.68
1:F:349:ARG:CD	1:F:351:VAL:HG23	2.24	0.68
1:F:435:ARG:HG2	1:F:435:ARG:NH1	2.08	0.68
1:B:410:GLN:HE21	1:B:417:SER:HA	1.59	0.67
1:E:226:THR:HA	1:F:236:GLN:NE2	2.08	0.67
1:F:403:ASP:HB3	1:F:404:PRO:CD	2.21	0.67
1:B:304:GLU:HG2	1:B:384:MET:HE1	1.74	0.67
1:D:333:LEU:HD23	1:D:334:ASP:N	2.09	0.67
1:A:279:GLN:OE1	2:G:2:NAG:H4	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:THR:HG22	1:F:350:ILE:HB	1.77	0.67
1:A:275:LEU:HD12	1:A:276:TYR:N	2.08	0.67
1:A:309:SER:O	1:A:311:THR:N	2.28	0.67
1:A:438:GLY:HA3	1:C:57:GLN:NE2	2.07	0.67
1:C:447:ASN:HB2	4:C:4471:NAG:N2	2.09	0.67
1:D:314:PHE:CB	1:D:374:LYS:HD3	2.19	0.67
1:E:447:ASN:H	4:E:4471:NAG:C8	2.07	0.67
1:E:182:MET:HG3	1:F:182:MET:CE	2.25	0.67
1:B:204:GLN:HA	1:C:204:GLN:HE22	1.57	0.67
1:D:390:VAL:HG11	1:D:427:LEU:CD1	2.25	0.67
1:E:429:LEU:HD22	1:E:429:LEU:H	1.60	0.67
1:A:101:ARG:HH11	1:B:257:ASN:HD21	1.43	0.67
1:D:341:THR:HG22	1:D:342:ASP:H	1.58	0.67
1:F:304:GLU:HG2	1:F:384:MET:HE1	1.76	0.67
1:A:432:ILE:HG23	1:C:295:LEU:HD23	1.77	0.66
1:E:235:ILE:HG22	1:E:236:GLN:NE2	2.10	0.66
1:A:204:GLN:HA	1:B:204:GLN:HE22	1.60	0.66
1:A:385:THR:HG23	1:C:54:THR:OG1	1.95	0.66
1:B:197:LEU:CD2	1:C:197:LEU:HD21	2.25	0.66
1:F:77:ALA:O	1:F:80:PRO:HD2	1.95	0.66
2:J:1:NAG:O6	2:J:2:NAG:H2	1.95	0.66
1:D:54:THR:HG22	1:E:388:GLY:HA2	1.76	0.66
1:F:334:ASP:OD1	1:F:336:SER:HB3	1.94	0.66
1:C:309:SER:O	1:C:311:THR:N	2.28	0.66
1:D:35:ARG:HH22	1:D:418:LEU:HD13	1.60	0.66
1:A:240:ASN:ND2	1:B:444:TYR:HD1	1.93	0.66
1:F:91:LEU:O	1:F:94:PRO:HD2	1.95	0.66
1:B:403:ASP:CB	1:B:404:PRO:HD3	2.26	0.66
1:D:381:THR:CG2	1:F:350:ILE:H	2.08	0.66
1:F:403:ASP:CB	1:F:404:PRO:HD3	2.25	0.66
1:D:439:GLU:HA	1:F:58:THR:O	1.96	0.66
1:E:240:ASN:ND2	1:F:444:TYR:HD2	1.93	0.66
1:C:349:ARG:CD	1:C:351:VAL:HG23	2.26	0.65
1:C:403:ASP:HB3	1:C:404:PRO:CD	2.26	0.65
1:E:308:VAL:O	1:E:315:ALA:HB3	1.97	0.65
1:B:104:GLU:HA	1:B:104:GLU:OE1	1.97	0.65
1:C:435:ARG:HG2	1:C:435:ARG:NH1	2.11	0.65
1:D:202:ILE:HD11	1:E:450:ILE:HD12	1.79	0.65
1:B:350:ILE:HB	1:C:381:THR:HG22	1.76	0.65
1:C:406:GLY:H	1:F:62:ILE:HD13	1.62	0.65
1:D:199:CYS:O	1:D:202:ILE:HG22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:GLN:HA	1:E:451:GLN:NE2	2.11	0.65
1:A:84:TYR:CD2	1:A:210:LEU:HG	2.32	0.65
1:B:197:LEU:HD21	1:C:197:LEU:HD21	1.79	0.65
1:B:211:ASN:HD22	1:C:208:VAL:HG22	1.62	0.65
1:B:419:ILE:H	1:B:419:ILE:CD1	2.10	0.65
1:E:395:LYS:HE2	1:E:411:ASN:OD1	1.96	0.64
1:A:257:ASN:ND2	1:C:101:ARG:HD3	2.13	0.64
1:D:341:THR:CG2	1:D:342:ASP:N	2.60	0.64
1:B:312:LYS:C	1:B:314:PHE:H	2.00	0.64
1:A:260:LEU:O	1:A:264:ILE:HG12	1.97	0.64
1:B:64:LYS:NZ	1:C:445:GLN:HE21	1.95	0.64
1:D:356:SER:HB3	1:D:359:ILE:HG12	1.79	0.64
1:D:450:ILE:CD1	1:F:202:ILE:HD11	2.27	0.64
1:E:35:ARG:HH22	1:E:418:LEU:CD1	2.11	0.64
1:E:403:ASP:HB3	1:E:404:PRO:HD3	1.79	0.64
1:A:172:LEU:HD21	1:C:172:LEU:N	2.12	0.64
1:A:281:GLN:HA	1:A:281:GLN:OE1	1.98	0.64
1:B:451:GLN:HA	1:B:451:GLN:NE2	2.02	0.64
1:C:372:TYR:CD1	1:C:372:TYR:N	2.65	0.64
1:D:54:THR:CG2	1:E:388:GLY:HA2	2.28	0.64
1:D:204:GLN:HA	1:E:204:GLN:HE22	1.63	0.64
1:A:274:ILE:HD13	1:A:286:GLN:HB2	1.80	0.64
1:B:349:ARG:HD2	1:B:351:VAL:HG23	1.80	0.64
1:A:190:PHE:CE2	1:C:189:GLN:HB3	2.33	0.64
1:E:419:ILE:HD13	1:E:427:LEU:HD21	1.80	0.63
1:E:95:LEU:HD21	1:E:273:PRO:HG3	1.79	0.63
1:A:192:LYS:HD3	1:A:193:THR:N	2.13	0.63
1:C:181:LYS:O	1:C:184:GLN:HG3	1.98	0.63
1:E:104:GLU:OE1	1:E:104:GLU:HA	1.99	0.63
1:E:171:GLY:N	1:F:172:LEU:HD11	2.13	0.63
1:F:304:GLU:HG2	1:F:384:MET:CE	2.29	0.63
1:F:314:PHE:CB	1:F:374:LYS:HD3	2.23	0.63
1:B:73:LYS:HD2	1:B:73:LYS:N	2.13	0.63
1:D:189:GLN:HB3	1:E:190:PHE:CZ	2.34	0.63
1:F:403:ASP:O	1:F:405:PRO:CD	2.46	0.63
1:A:287:VAL:HG12	1:A:288:THR:N	2.12	0.63
1:B:181:LYS:O	1:B:184:GLN:HG3	1.98	0.63
1:B:182:MET:HG3	1:C:182:MET:CE	2.28	0.63
1:B:215:THR:HG22	1:C:215:THR:HG21	1.81	0.63
1:B:419:ILE:HD12	1:B:419:ILE:N	2.13	0.63
1:D:411:ASN:O	1:D:414:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:O	1:B:315:ALA:HB3	1.99	0.63
1:C:304:GLU:HG2	1:C:384:MET:CE	2.29	0.63
1:D:450:ILE:HD12	1:F:202:ILE:HD11	1.81	0.63
1:F:191:ASN:O	1:F:194:ALA:HB3	1.98	0.63
1:F:255:VAL:HG13	1:F:292:VAL:CG1	2.28	0.63
1:B:209:GLU:HG2	1:C:448:ILE:HG23	1.81	0.63
1:C:36:PRO:HD2	1:C:37:LEU:CD2	2.29	0.63
1:D:287:VAL:HG12	1:D:288:THR:N	2.13	0.63
1:E:403:ASP:O	1:E:404:PRO:C	2.36	0.63
1:F:315:ALA:HB1	1:F:372:TYR:HD2	1.63	0.63
1:C:400:ARG:HH11	1:C:400:ARG:CG	2.08	0.62
1:E:349:ARG:HD2	1:E:351:VAL:HG23	1.78	0.62
1:D:281:GLN:OE1	1:D:281:GLN:HA	1.99	0.62
1:A:375:THR:O	1:C:354:PRO:HD3	1.98	0.62
1:A:403:ASP:CB	1:A:404:PRO:HD3	2.26	0.62
1:F:76:CYS:HB3	1:F:203:THR:CG2	2.29	0.62
1:B:367:THR:O	1:B:370:CYS:HB2	2.00	0.62
1:C:37:LEU:HD23	1:C:37:LEU:H	1.64	0.62
1:C:294:ASN:OD1	1:C:295:LEU:O	2.17	0.62
1:C:337:TYR:HB3	1:C:348:THR:CG2	2.30	0.62
1:F:386:LEU:HD23	1:F:391:ILE:HD11	1.81	0.62
1:A:350:ILE:HG22	1:A:350:ILE:O	1.98	0.62
1:B:53:TYR:O	1:C:385:THR:HG21	1.99	0.62
1:D:372:TYR:N	1:D:372:TYR:CD1	2.65	0.62
1:F:312:LYS:CG	1:F:314:PHE:HB2	2.29	0.62
1:B:306:LEU:HD12	1:B:382:PRO:O	1.99	0.62
1:A:81:LEU:HA	1:A:210:LEU:HD21	1.82	0.62
1:A:37:LEU:H	1:A:37:LEU:CD2	2.12	0.62
1:A:101:ARG:CB	1:B:257:ASN:HD22	2.09	0.62
1:C:263:LEU:O	1:C:266:SER:HB3	1.99	0.62
1:C:341:THR:CG2	1:C:342:ASP:N	2.63	0.61
1:C:304:GLU:HG2	1:C:384:MET:HE1	1.83	0.61
1:D:313:GLY:HA2	1:D:396:MET:HE1	1.82	0.61
1:E:390:VAL:HG22	1:E:390:VAL:O	2.00	0.61
1:A:95:LEU:O	1:A:95:LEU:HD22	2.00	0.61
1:F:341:THR:CG2	1:F:342:ASP:N	2.63	0.61
1:A:376:GLU:HG3	1:A:380:THR:HG21	1.82	0.61
1:D:438:GLY:HA3	1:F:57:GLN:HE22	1.64	0.61
1:E:101:ARG:HD3	1:F:257:ASN:ND2	2.15	0.61
1:F:341:THR:HG22	1:F:342:ASP:H	1.62	0.61
1:B:390:VAL:HG11	1:B:427:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:THR:HG22	1:C:342:ASP:H	1.63	0.61
1:A:171:GLY:N	1:B:172:LEU:HD11	2.16	0.61
1:B:73:LYS:HG2	1:C:450:ILE:CD1	2.31	0.61
1:E:64:LYS:HZ1	1:F:445:GLN:HE21	1.49	0.61
1:A:182:MET:CE	1:C:182:MET:HG3	2.31	0.61
1:D:181:LYS:O	1:D:184:GLN:HG3	2.00	0.61
1:D:257:ASN:HD22	1:F:101:ARG:HB3	1.64	0.61
1:B:403:ASP:OD2	1:B:425:ASN:HB2	2.01	0.61
1:D:341:THR:CG2	1:D:342:ASP:H	2.13	0.61
1:A:189:GLN:HB3	1:B:190:PHE:CZ	2.36	0.60
1:B:95:LEU:O	1:B:99:ILE:HG13	2.01	0.60
1:B:262:SER:OG	1:B:341:THR:HG21	2.01	0.60
1:D:61:ILE:HD11	1:D:241:LEU:HB2	1.83	0.60
1:B:201:LYS:HD3	1:C:453:SER:OG	2.01	0.60
1:D:84:TYR:CD2	1:D:210:LEU:HG	2.36	0.60
1:E:211:ASN:ND2	1:F:208:VAL:HG22	2.16	0.60
1:E:295:LEU:HD23	1:F:432:ILE:CG2	2.30	0.60
1:A:245:ASN:ND2	1:A:248:TYR:HB2	2.16	0.60
1:D:190:PHE:CE2	1:F:189:GLN:HB3	2.37	0.60
1:D:198:ASP:OD1	1:E:453:SER:HB3	2.01	0.60
1:D:257:ASN:ND2	1:F:101:ARG:HD3	2.17	0.60
1:D:312:LYS:C	1:D:314:PHE:H	2.04	0.60
1:D:349:ARG:CD	1:D:351:VAL:HG23	2.31	0.60
1:F:337:TYR:HB3	1:F:348:THR:CG2	2.31	0.60
1:D:380:THR:HG22	1:F:352:THR:OG1	2.01	0.60
1:D:432:ILE:HD12	1:D:434:LEU:HD13	1.84	0.60
1:F:36:PRO:HD2	1:F:37:LEU:CD2	2.32	0.60
1:D:172:LEU:HD12	1:D:172:LEU:O	2.01	0.60
1:B:182:MET:HG3	1:C:182:MET:HE1	1.83	0.60
1:D:37:LEU:H	1:D:37:LEU:CD2	2.13	0.60
1:E:95:LEU:O	1:E:99:ILE:HG13	2.01	0.60
1:D:43:VAL:HG21	1:D:391:ILE:HD13	1.83	0.60
1:D:182:MET:HE1	1:F:182:MET:HG3	1.84	0.60
1:A:191:ASN:O	1:A:194:ALA:HB3	2.02	0.60
1:C:76:CYS:HB3	1:C:203:THR:CG2	2.32	0.60
1:C:213:TYR:O	1:C:217:LEU:HB2	2.01	0.60
1:E:101:ARG:HH11	1:F:257:ASN:ND2	1.96	0.60
1:E:383:TYR:CE2	1:E:432:ILE:HD11	2.37	0.60
1:A:450:ILE:CD1	1:C:202:ILE:HD11	2.32	0.60
1:B:311:THR:OG1	1:B:315:ALA:HB2	2.02	0.59
1:B:372:TYR:CD1	1:B:372:TYR:N	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ALA:N	1:F:331:GLU:OE2	2.35	0.59
1:E:51:ASN:N	1:E:51:ASN:ND2	2.50	0.59
1:D:352:THR:OG1	1:E:380:THR:HG22	2.02	0.59
1:E:403:ASP:O	1:E:405:PRO:CD	2.50	0.59
1:A:48:LYS:HE2	1:A:342:ASP:O	2.02	0.59
1:B:192:LYS:HD3	1:B:193:THR:N	2.17	0.59
1:B:383:TYR:CE2	1:B:432:ILE:HD11	2.37	0.59
1:C:403:ASP:CB	1:C:404:PRO:HD3	2.32	0.59
1:E:333:LEU:HD23	1:E:334:ASP:N	2.17	0.59
1:F:274:ILE:HG12	1:F:284:GLY:O	2.01	0.59
1:F:372:TYR:N	1:F:372:TYR:CD1	2.71	0.59
1:A:262:SER:HA	1:A:341:THR:HG21	1.83	0.59
1:C:341:THR:CG2	1:C:342:ASP:H	2.15	0.59
1:C:405:PRO:HD3	1:F:64:LYS:HZ1	1.67	0.59
1:D:432:ILE:HD12	1:D:434:LEU:HD11	1.85	0.59
1:E:355:MET:HE3	1:E:359:ILE:HG22	1.85	0.59
1:A:181:LYS:O	1:A:184:GLN:HG3	2.03	0.59
1:A:190:PHE:CZ	1:C:189:GLN:HB3	2.37	0.59
1:D:101:ARG:HB3	1:E:257:ASN:ND2	2.11	0.59
1:E:435:ARG:HG3	1:E:435:ARG:NH1	2.17	0.59
1:A:253:LEU:HD21	1:A:289:LEU:CD2	2.33	0.59
1:A:253:LEU:HD11	1:A:289:LEU:HD23	1.83	0.59
1:C:315:ALA:HB1	1:C:372:TYR:HD2	1.67	0.59
1:E:356:SER:HB3	1:E:359:ILE:HG12	1.84	0.59
1:B:235:ILE:HG22	1:B:236:GLN:NE2	2.17	0.59
1:A:341:THR:CG2	1:A:342:ASP:N	2.66	0.59
1:A:380:THR:HG22	1:C:352:THR:OG1	2.03	0.59
1:D:372:TYR:HD1	1:D:372:TYR:H	1.51	0.59
1:E:189:GLN:HB3	1:F:190:PHE:CZ	2.37	0.59
1:F:213:TYR:O	1:F:217:LEU:HB2	2.03	0.59
1:B:403:ASP:O	1:B:405:PRO:CD	2.51	0.58
1:B:403:ASP:O	1:B:405:PRO:HD3	2.03	0.58
1:D:101:ARG:HH11	1:E:257:ASN:HD21	1.50	0.58
1:D:403:ASP:OD2	1:D:404:PRO:HD3	2.03	0.58
1:A:310:THR:HG22	1:A:311:THR:N	2.17	0.58
1:D:104:GLU:HA	1:D:104:GLU:OE1	2.03	0.58
1:C:100:ARG:O	1:C:104:GLU:HG2	2.03	0.58
1:F:312:LYS:HD2	1:F:374:LYS:HZ3	1.66	0.58
1:A:61:ILE:HD11	1:A:241:LEU:HB2	1.85	0.58
1:B:191:ASN:O	1:B:194:ALA:HB3	2.03	0.58
1:D:403:ASP:CB	1:D:404:PRO:CD	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLN:HG2	1:F:285:ILE:HD13	1.85	0.58
1:C:36:PRO:HD2	1:C:37:LEU:HD22	1.86	0.58
1:D:51:ASN:N	1:D:51:ASN:ND2	2.52	0.58
1:E:419:ILE:HG21	1:E:427:LEU:CG	2.32	0.58
1:F:37:LEU:H	1:F:37:LEU:HD23	1.68	0.58
1:F:390:VAL:HG21	1:F:429:LEU:HD21	1.84	0.58
1:B:386:LEU:HD12	1:B:387:LYS:HG3	1.85	0.58
1:C:255:VAL:HG12	1:C:259:GLN:CD	2.24	0.58
1:C:411:ASN:HB2	1:C:414:GLU:OE2	2.03	0.58
1:A:172:LEU:O	1:A:172:LEU:HD12	2.04	0.58
1:A:182:MET:SD	1:C:182:MET:HG3	2.43	0.58
1:A:306:LEU:HD21	1:A:384:MET:SD	2.43	0.58
1:A:333:LEU:HD23	1:A:334:ASP:N	2.18	0.58
1:B:211:ASN:ND2	1:C:208:VAL:HG22	2.18	0.58
1:C:410:GLN:HA	1:C:414:GLU:OE1	2.04	0.58
1:E:65:LEU:HD23	1:E:217:LEU:HD21	1.84	0.58
1:F:275:LEU:HD12	1:F:276:TYR:N	2.19	0.58
1:A:51:ASN:N	1:A:51:ASN:ND2	2.52	0.58
1:A:372:TYR:CD1	1:A:372:TYR:N	2.72	0.58
1:A:447:ASN:HB2	3:H:1:NAG:N2	2.19	0.58
1:A:450:ILE:O	1:A:450:ILE:HG13	2.04	0.58
1:B:71:LYS:O	1:B:72:ASP:HB2	2.02	0.58
1:B:252:LYS:HE2	1:C:435:ARG:HH22	1.69	0.58
1:C:40:ALA:HB2	1:C:367:THR:HG23	1.85	0.58
1:E:314:PHE:CB	1:E:374:LYS:HD3	2.22	0.58
1:A:215:THR:HG22	1:B:215:THR:CG2	2.32	0.58
1:B:95:LEU:HD21	1:B:273:PRO:HG3	1.84	0.58
1:C:77:ALA:O	1:C:80:PRO:HD2	2.04	0.58
1:D:36:PRO:HD2	1:D:37:LEU:CD2	2.33	0.58
1:B:58:THR:O	1:C:439:GLU:HA	2.04	0.58
1:C:255:VAL:HG13	1:C:292:VAL:CG1	2.34	0.58
1:F:341:THR:CG2	1:F:342:ASP:H	2.17	0.58
1:B:101:ARG:HB3	1:C:257:ASN:HD22	1.69	0.57
1:C:361:SER:O	1:C:366:ASN:HB3	2.03	0.57
1:D:215:THR:HG22	1:E:215:THR:CG2	2.32	0.57
1:D:376:GLU:HG3	1:D:380:THR:HG21	1.85	0.57
1:E:309:SER:O	1:E:311:THR:N	2.36	0.57
1:B:386:LEU:HD12	1:B:387:LYS:N	2.19	0.57
1:B:73:LYS:HG2	1:C:450:ILE:HD11	1.86	0.57
1:B:394:CYS:HB2	1:B:417:SER:OG	2.03	0.57
1:A:388:GLY:HA2	1:C:54:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:PRO:HD3	1:F:64:LYS:NZ	2.20	0.57
1:E:209:GLU:HG2	1:F:448:ILE:HG23	1.87	0.57
1:F:74:GLU:O	1:F:75:ALA:C	2.43	0.57
1:F:95:LEU:HD21	1:F:273:PRO:HG3	1.86	0.57
1:F:206:VAL:O	1:F:210:LEU:HB2	2.04	0.57
1:F:312:LYS:HD2	1:F:374:LYS:HZ1	1.69	0.57
1:A:385:THR:HG22	1:A:386:LEU:N	2.19	0.57
1:D:312:LYS:HG3	1:D:314:PHE:HB2	1.85	0.57
1:A:393:ASN:HD22	1:A:396:MET:HB2	1.67	0.57
1:C:311:THR:OG1	1:C:312:LYS:HG2	2.05	0.57
1:D:175:LEU:C	1:D:175:LEU:HD23	2.25	0.57
1:E:366:ASN:OD1	1:E:367:THR:N	2.38	0.57
1:A:172:LEU:HD21	1:C:171:GLY:CA	2.35	0.57
1:A:206:VAL:O	1:A:210:LEU:HB2	2.04	0.57
1:A:356:SER:HB3	1:A:359:ILE:HG12	1.87	0.57
1:A:390:VAL:O	1:A:418:LEU:O	2.23	0.57
1:B:263:LEU:O	1:B:266:SER:HB3	2.04	0.57
1:D:69:MET:SD	1:E:448:ILE:HD12	2.45	0.57
1:D:325:GLN:CB	1:D:330:ILE:HG12	2.35	0.57
1:A:101:ARG:HD3	1:B:257:ASN:HD21	1.70	0.57
1:B:76:CYS:O	1:B:203:THR:HG22	2.05	0.57
1:C:407:ILE:HG22	1:C:407:ILE:O	2.04	0.57
1:D:182:MET:HG3	1:E:182:MET:CE	2.33	0.57
1:E:260:LEU:O	1:E:264:ILE:HG12	2.05	0.57
2:G:2:NAG:O7	2:G:2:NAG:H3	2.04	0.57
1:A:314:PHE:CB	1:A:374:LYS:HD3	2.21	0.57
1:A:378:ALA:N	1:C:331:GLU:OE2	2.36	0.57
1:D:350:ILE:HG22	1:D:350:ILE:O	2.03	0.57
1:E:213:TYR:O	1:E:217:LEU:HB2	2.05	0.57
1:F:40:ALA:HB2	1:F:367:THR:HG23	1.86	0.57
1:F:199:CYS:O	1:F:203:THR:HG23	2.05	0.57
1:F:233:LEU:HG	1:F:237:ALA:HB3	1.86	0.57
1:B:102:ILE:HD12	1:B:228:PRO:HB2	1.87	0.56
1:B:304:GLU:HG2	1:B:384:MET:HE3	1.85	0.56
1:C:199:CYS:O	1:C:203:THR:HG23	2.05	0.56
1:C:447:ASN:H	4:C:4471:NAG:H82	1.70	0.56
1:E:102:ILE:HD12	1:E:228:PRO:HB2	1.86	0.56
1:E:182:MET:HG3	1:F:182:MET:HE1	1.86	0.56
1:E:403:ASP:CB	1:E:404:PRO:HD3	2.34	0.56
1:C:377:GLY:O	1:C:380:THR:HG23	2.05	0.56
1:A:312:LYS:O	1:A:314:PHE:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ILE:HG23	1:C:209:GLU:HG2	1.88	0.56
1:B:51:ASN:N	1:B:51:ASN:ND2	2.52	0.56
1:B:64:LYS:HB2	1:C:445:GLN:HB2	1.87	0.56
1:C:104:GLU:OE1	1:C:104:GLU:HA	2.04	0.56
1:D:325:GLN:HB3	1:D:330:ILE:HG12	1.88	0.56
1:E:175:LEU:C	1:E:175:LEU:HD23	2.25	0.56
1:E:182:MET:HG3	1:F:182:MET:SD	2.44	0.56
1:E:192:LYS:HD3	1:E:193:THR:N	2.20	0.56
1:E:312:LYS:C	1:E:314:PHE:N	2.59	0.56
1:F:63:ILE:HD11	1:F:221:PHE:CD2	2.40	0.56
1:A:73:LYS:HD3	1:B:450:ILE:HD11	1.87	0.56
1:C:189:GLN:OE1	1:C:189:GLN:HA	2.05	0.56
1:A:253:LEU:HD21	1:A:289:LEU:HD22	1.88	0.56
1:B:44:VAL:HG12	1:B:44:VAL:O	2.05	0.56
1:C:376:GLU:HG3	1:C:380:THR:HG21	1.86	0.56
1:A:199:CYS:O	1:A:202:ILE:HG22	2.05	0.56
1:A:324:THR:HB	1:A:333:LEU:HD12	1.88	0.56
1:A:381:THR:CG2	1:C:350:ILE:H	2.19	0.56
1:E:57:GLN:HE22	1:F:438:GLY:HA3	1.70	0.56
1:E:224:GLN:HG2	1:E:285:ILE:CD1	2.36	0.56
1:F:65:LEU:HD23	1:F:217:LEU:HD21	1.87	0.56
1:D:200:ILE:HD11	1:E:201:LYS:HG3	1.87	0.56
1:D:453:SER:CB	1:F:201:LYS:HD3	2.36	0.56
1:F:235:ILE:HG22	1:F:236:GLN:NE2	2.19	0.56
1:A:182:MET:HG3	1:B:182:MET:HE1	1.88	0.56
1:B:427:LEU:HD13	1:B:429:LEU:CD2	2.35	0.56
1:D:91:LEU:O	1:D:94:PRO:HD2	2.05	0.56
1:E:37:LEU:CD2	1:E:37:LEU:H	2.19	0.56
1:C:239:TYR:CE1	1:C:244:GLY:HA2	2.40	0.56
1:D:206:VAL:O	1:D:210:LEU:HB2	2.04	0.56
1:A:40:ALA:HB2	1:A:367:THR:HG23	1.88	0.55
1:A:104:GLU:OE1	1:A:104:GLU:HA	2.05	0.55
1:A:226:THR:HA	1:B:236:GLN:HE22	1.66	0.55
1:A:295:LEU:CD2	1:B:432:ILE:HG21	2.35	0.55
1:B:43:VAL:CG2	1:B:391:ILE:HD13	2.34	0.55
1:C:309:SER:HA	1:C:312:LYS:O	2.05	0.55
1:F:50:VAL:C	1:F:51:ASN:ND2	2.60	0.55
1:A:172:LEU:HD21	1:C:171:GLY:N	2.22	0.55
1:B:390:VAL:HG22	1:B:390:VAL:O	2.05	0.55
1:C:95:LEU:HD21	1:C:273:PRO:HG3	1.88	0.55
1:E:57:GLN:NE2	1:F:438:GLY:HA3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:ND2	1:C:444:TYR:HD2	2.05	0.55
1:C:206:VAL:O	1:C:210:LEU:HB2	2.06	0.55
1:E:43:VAL:CG2	1:E:391:ILE:HD13	2.36	0.55
1:F:309:SER:O	1:F:311:THR:N	2.40	0.55
1:B:377:GLY:O	1:B:380:THR:HG23	2.06	0.55
1:C:191:ASN:O	1:C:194:ALA:HB3	2.06	0.55
1:C:287:VAL:HG12	1:C:288:THR:N	2.22	0.55
1:C:421:ARG:HG2	1:C:436:LEU:O	2.05	0.55
1:D:240:ASN:ND2	1:E:444:TYR:HD1	2.04	0.55
1:E:37:LEU:H	1:E:37:LEU:HD23	1.71	0.55
1:E:53:TYR:O	1:F:385:THR:HG21	2.06	0.55
1:E:403:ASP:CB	1:E:404:PRO:CD	2.84	0.55
1:B:175:LEU:HD23	1:B:175:LEU:C	2.27	0.55
1:B:403:ASP:CB	1:B:404:PRO:CD	2.83	0.55
1:C:325:GLN:O	1:C:325:GLN:HG3	2.07	0.55
1:F:314:PHE:HB3	1:F:374:LYS:CD	2.26	0.55
1:C:274:ILE:HG12	1:C:284:GLY:O	2.06	0.55
1:C:403:ASP:OD1	1:C:404:PRO:HD3	2.06	0.55
1:D:245:ASN:ND2	1:D:248:TYR:HB2	2.21	0.55
1:E:197:LEU:CD2	1:F:197:LEU:HD21	2.37	0.55
1:A:182:MET:HG3	1:B:182:MET:CE	2.37	0.55
1:A:220:VAL:HG22	1:A:236:GLN:HG3	1.87	0.55
1:F:311:THR:OG1	1:F:315:ALA:HB2	2.06	0.55
1:B:35:ARG:NH2	1:B:418:LEU:HD12	2.17	0.55
1:A:421:ARG:HG2	1:A:437:SER:OG	2.07	0.55
1:B:73:LYS:N	1:B:73:LYS:CD	2.69	0.55
1:B:403:ASP:O	1:B:405:PRO:N	2.40	0.55
1:C:312:LYS:HG3	1:C:314:PHE:CB	2.29	0.55
1:D:261:SER:HB3	1:F:102:ILE:CD1	2.37	0.55
1:D:350:ILE:HB	1:E:381:THR:CG2	2.28	0.55
1:A:172:LEU:N	1:B:172:LEU:HD21	2.22	0.54
1:A:309:SER:HA	1:A:312:LYS:O	2.06	0.54
1:B:309:SER:OG	1:B:313:GLY:HA2	2.06	0.54
1:C:224:GLN:HG2	1:C:285:ILE:HD13	1.88	0.54
1:D:81:LEU:HA	1:D:210:LEU:HD21	1.89	0.54
1:E:224:GLN:HG2	1:E:285:ILE:HD13	1.89	0.54
1:B:393:ASN:OD1	1:B:395:LYS:HB3	2.07	0.54
1:B:394:CYS:CB	1:B:417:SER:HG	2.21	0.54
1:D:448:ILE:HG23	1:F:209:GLU:HG2	1.89	0.54
1:F:81:LEU:HA	1:F:210:LEU:HD21	1.89	0.54
1:A:388:GLY:HA2	1:C:54:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:H	1:C:381:THR:CG2	2.20	0.54
1:D:51:ASN:HB3	1:D:294:ASN:HA	1.88	0.54
1:D:330:ILE:O	1:D:330:ILE:HG22	2.07	0.54
1:E:223:PRO:HB3	1:E:231:THR:CG2	2.36	0.54
1:E:308:VAL:HG11	1:E:372:TYR:HE2	1.73	0.54
1:B:37:LEU:CD2	1:B:37:LEU:H	2.20	0.54
1:E:65:LEU:HB3	1:E:88:LEU:HD11	1.89	0.54
1:E:304:GLU:HG2	1:E:384:MET:CE	2.38	0.54
1:F:432:ILE:HD12	1:F:434:LEU:HD13	1.88	0.54
2:J:1:NAG:H4	2:J:2:NAG:C7	2.37	0.54
1:A:175:LEU:C	1:A:175:LEU:HD23	2.28	0.54
1:D:331:GLU:OE2	1:E:378:ALA:N	2.40	0.54
1:D:432:ILE:CG2	1:F:295:LEU:HD23	2.38	0.54
1:F:104:GLU:OE1	1:F:104:GLU:HA	2.06	0.54
1:F:377:GLY:O	1:F:380:THR:HG23	2.07	0.54
1:F:421:ARG:NH1	1:F:421:ARG:HB2	2.22	0.54
1:D:65:LEU:HB3	1:D:88:LEU:HD11	1.89	0.54
1:D:102:ILE:CD1	1:E:261:SER:HB2	2.34	0.54
1:E:372:TYR:N	1:E:372:TYR:CD1	2.73	0.54
1:E:377:GLY:H	1:E:380:THR:CG2	2.21	0.54
1:F:255:VAL:HB	1:F:259:GLN:HB3	1.88	0.54
1:F:421:ARG:HB2	1:F:421:ARG:HH11	1.72	0.54
1:A:236:GLN:NE2	1:C:226:THR:HA	2.23	0.54
1:C:405:PRO:CD	1:F:64:LYS:NZ	2.71	0.54
1:E:262:SER:OG	1:E:341:THR:HG21	2.06	0.54
1:F:175:LEU:C	1:F:175:LEU:HD23	2.28	0.54
1:F:315:ALA:HB1	1:F:372:TYR:CD2	2.40	0.54
1:D:414:GLU:O	1:D:415:ALA:HB3	2.07	0.54
1:B:37:LEU:H	1:B:37:LEU:HD23	1.73	0.54
1:E:76:CYS:HB3	1:E:203:THR:CG2	2.38	0.54
1:E:341:THR:CG2	1:E:342:ASP:N	2.71	0.54
1:E:428:SER:OG	1:E:433:THR:HG22	2.07	0.54
1:B:44:VAL:HG22	1:B:303:LEU:CD2	2.39	0.53
1:B:201:LYS:HD3	1:C:453:SER:CB	2.37	0.53
1:C:403:ASP:O	1:C:405:PRO:CD	2.56	0.53
1:C:411:ASN:N	1:C:414:GLU:CD	2.60	0.53
1:D:295:LEU:CD2	1:E:432:ILE:HG21	2.31	0.53
1:D:325:GLN:HB2	1:D:329:VAL:O	2.09	0.53
1:F:312:LYS:HG3	1:F:314:PHE:CB	2.37	0.53
1:D:40:ALA:HB2	1:D:367:THR:HG23	1.90	0.53
1:E:367:THR:O	1:E:370:CYS:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:PRO:HD2	1:F:37:LEU:HD22	1.90	0.53
1:A:312:LYS:C	1:A:314:PHE:N	2.60	0.53
1:C:447:ASN:HB2	4:C:4471:NAG:C7	2.38	0.53
1:E:101:ARG:HD3	1:F:257:ASN:HD21	1.72	0.53
1:F:350:ILE:HG22	1:F:350:ILE:O	2.08	0.53
1:A:432:ILE:HG21	1:C:295:LEU:HD23	1.91	0.53
1:B:179:VAL:O	1:B:183:GLN:HB3	2.08	0.53
1:B:366:ASN:OD1	1:B:367:THR:N	2.41	0.53
1:C:447:ASN:H	4:C:4471:NAG:C8	2.21	0.53
1:D:420:ASP:C	1:D:420:ASP:OD1	2.46	0.53
1:F:255:VAL:HG12	1:F:259:GLN:CD	2.28	0.53
1:A:325:GLN:CB	1:A:330:ILE:HG12	2.39	0.53
1:A:440:PHE:HB2	1:C:241:LEU:HD11	1.90	0.53
1:E:252:LYS:HE2	1:F:435:ARG:HH22	1.73	0.53
1:E:341:THR:HG22	1:E:344:ASP:H	1.73	0.53
1:F:48:LYS:HE2	1:F:342:ASP:O	2.08	0.53
1:A:257:ASN:C	1:A:259:GLN:H	2.12	0.53
1:B:252:LYS:CE	1:C:435:ARG:HH22	2.22	0.53
1:B:281:GLN:OE1	1:B:281:GLN:HA	2.09	0.53
1:D:48:LYS:HE2	1:D:342:ASP:O	2.09	0.53
1:E:309:SER:HA	1:E:313:GLY:HA2	1.91	0.53
1:A:349:ARG:CD	1:A:351:VAL:HG23	2.38	0.53
1:A:440:PHE:CB	1:C:241:LEU:HD11	2.38	0.53
1:B:239:TYR:CE1	1:B:244:GLY:HA2	2.43	0.53
1:B:341:THR:CG2	1:B:342:ASP:N	2.71	0.53
1:A:36:PRO:HD2	1:A:37:LEU:CD2	2.39	0.53
1:A:51:ASN:N	1:A:51:ASN:HD22	2.07	0.53
1:B:74:GLU:O	1:B:75:ALA:C	2.45	0.53
1:D:95:LEU:HD21	1:D:273:PRO:HG3	1.91	0.53
1:D:246:MET:HB3	1:F:101:ARG:NH2	2.24	0.53
1:B:74:GLU:O	1:B:77:ALA:N	2.41	0.53
1:B:260:LEU:O	1:B:264:ILE:HG12	2.09	0.53
1:E:240:ASN:ND2	1:F:444:TYR:CD2	2.75	0.53
1:F:189:GLN:HA	1:F:189:GLN:OE1	2.09	0.53
1:B:414:GLU:O	1:B:415:ALA:HB3	2.08	0.53
1:F:383:TYR:CE2	1:F:429:LEU:HB3	2.44	0.53
1:A:325:GLN:HB3	1:A:330:ILE:HG12	1.91	0.52
1:B:356:SER:HB3	1:B:359:ILE:HG12	1.89	0.52
1:B:420:ASP:CG	1:B:421:ARG:H	2.13	0.52
1:C:411:ASN:N	1:C:414:GLU:OE2	2.42	0.52
1:F:43:VAL:HG21	1:F:391:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:HG21	1:C:54:THR:HA	1.89	0.52
1:B:65:LEU:HB3	1:B:88:LEU:HD11	1.91	0.52
1:D:393:ASN:C	1:D:395:LYS:H	2.12	0.52
1:E:403:ASP:CG	1:E:404:PRO:HD3	2.29	0.52
1:F:312:LYS:HG3	1:F:314:PHE:CD1	2.43	0.52
1:D:63:ILE:HD11	1:D:221:PHE:CD1	2.44	0.52
1:D:253:LEU:HD11	1:D:289:LEU:HD23	1.90	0.52
1:F:233:LEU:HD22	1:F:287:VAL:HG13	1.91	0.52
1:B:76:CYS:C	1:B:203:THR:HG22	2.30	0.52
1:B:171:GLY:N	1:C:172:LEU:HD11	2.24	0.52
1:C:372:TYR:N	1:C:372:TYR:HD1	2.05	0.52
1:C:403:ASP:O	1:C:405:PRO:HD3	2.09	0.52
1:D:298:MET:HG3	1:D:326:VAL:HG22	1.91	0.52
1:D:440:PHE:CB	1:F:241:LEU:HD11	2.39	0.52
1:E:35:ARG:NH2	1:E:418:LEU:HD12	2.19	0.52
1:E:76:CYS:O	1:E:203:THR:HG22	2.10	0.52
1:A:93:THR:HB	1:A:94:PRO:HD3	1.91	0.52
1:A:182:MET:HE1	1:C:182:MET:HG3	1.91	0.52
1:A:197:LEU:CD2	1:B:197:LEU:HD21	2.39	0.52
1:A:403:ASP:O	1:A:405:PRO:HD3	2.10	0.52
1:A:421:ARG:HG3	1:A:436:LEU:O	2.09	0.52
1:D:192:LYS:HD3	1:D:193:THR:H	1.74	0.52
1:B:50:VAL:HG11	1:B:350:ILE:HD11	1.91	0.52
1:D:182:MET:CE	1:F:182:MET:HG3	2.39	0.52
1:D:419:ILE:HG21	1:D:427:LEU:HG	1.91	0.52
1:F:213:TYR:CE1	1:F:217:LEU:HD13	2.45	0.52
1:F:260:LEU:O	1:F:264:ILE:HG12	2.09	0.52
1:F:367:THR:O	1:F:370:CYS:HB2	2.09	0.52
1:D:257:ASN:C	1:D:259:GLN:H	2.13	0.52
1:E:196:GLU:HB3	1:F:197:LEU:CD1	2.40	0.52
1:E:334:ASP:OD1	1:E:336:SER:HB3	2.10	0.52
1:F:202:ILE:CG2	1:F:203:THR:N	2.73	0.52
1:A:76:CYS:C	1:A:203:THR:HG22	2.30	0.52
1:B:410:GLN:HE21	1:B:417:SER:CA	2.23	0.52
1:D:393:ASN:O	1:D:395:LYS:N	2.41	0.52
1:E:376:GLU:HG3	1:E:380:THR:HG21	1.92	0.52
1:A:341:THR:HG22	1:A:342:ASP:H	1.74	0.52
1:A:403:ASP:CB	1:A:404:PRO:CD	2.87	0.52
1:C:76:CYS:C	1:C:203:THR:HG22	2.30	0.52
1:C:235:ILE:HG22	1:C:236:GLN:NE2	2.25	0.52
1:C:372:TYR:HD1	1:C:372:TYR:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:ILE:HD12	1:F:197:LEU:HD22	1.92	0.52
1:E:427:LEU:HD13	1:E:429:LEU:HD21	1.92	0.52
1:A:238:LEU:O	1:A:241:LEU:HB3	2.10	0.51
1:B:309:SER:O	1:B:311:THR:N	2.43	0.51
1:D:199:CYS:O	1:D:203:THR:HG23	2.11	0.51
1:D:451:GLN:H	1:F:205:GLN:NE2	2.04	0.51
1:B:51:ASN:CB	1:B:294:ASN:HA	2.34	0.51
1:C:367:THR:O	1:C:370:CYS:HB2	2.10	0.51
1:A:172:LEU:CD2	1:C:172:LEU:N	2.73	0.51
1:A:261:SER:HB3	1:C:102:ILE:CD1	2.40	0.51
1:C:74:GLU:O	1:C:75:ALA:C	2.47	0.51
1:D:196:GLU:OE1	1:D:196:GLU:HA	2.09	0.51
1:E:50:VAL:HG11	1:E:350:ILE:HD11	1.92	0.51
1:E:101:ARG:NH1	1:F:257:ASN:HD21	1.98	0.51
1:E:200:ILE:HD13	1:F:200:ILE:CG2	2.40	0.51
1:E:314:PHE:O	1:E:374:LYS:HB3	2.10	0.51
1:E:453:SER:OG	1:E:454:GLN:N	2.43	0.51
1:B:43:VAL:HG21	1:B:391:ILE:HG21	1.93	0.51
1:D:100:ARG:O	1:D:104:GLU:HG2	2.11	0.51
1:D:398:THR:HG21	1:D:400:ARG:CZ	2.41	0.51
1:E:76:CYS:C	1:E:203:THR:HG22	2.31	0.51
1:F:306:LEU:HD21	1:F:384:MET:SD	2.51	0.51
1:F:402:ALA:HB3	1:F:426:ILE:HB	1.93	0.51
2:J:1:NAG:H4	2:J:2:NAG:N2	2.24	0.51
1:A:69:MET:SD	1:B:448:ILE:HD12	2.50	0.51
1:A:261:SER:HB3	1:C:102:ILE:HD13	1.93	0.51
1:B:226:THR:HA	1:C:236:GLN:HE21	1.74	0.51
1:B:315:ALA:HB1	1:B:372:TYR:HD2	1.76	0.51
1:B:318:LEU:HD21	1:B:373:SER:HB3	1.92	0.51
1:C:312:LYS:O	1:C:314:PHE:N	2.33	0.51
1:D:223:PRO:HB2	1:D:224:GLN:NE2	2.25	0.51
1:A:84:TYR:CD1	1:A:84:TYR:C	2.84	0.51
1:B:372:TYR:N	1:B:372:TYR:HD1	2.08	0.51
1:C:235:ILE:HG23	1:C:236:GLN:N	2.25	0.51
1:D:89:THR:HG22	1:D:281:GLN:HE22	1.76	0.51
1:A:68:ASN:HB2	1:B:447:ASN:OD1	2.11	0.51
1:A:102:ILE:CD1	1:B:261:SER:HB2	2.38	0.51
1:C:37:LEU:CD2	1:C:37:LEU:H	2.24	0.51
1:D:202:ILE:HD11	1:E:450:ILE:CD1	2.41	0.51
1:D:400:ARG:HG3	1:D:400:ARG:HH11	1.76	0.51
1:E:76:CYS:HB3	1:E:203:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:GLN:HB3	1:F:190:PHE:CE2	2.46	0.51
1:A:438:GLY:HA3	1:C:57:GLN:HE22	1.74	0.51
1:B:309:SER:HA	1:B:313:GLY:HA2	1.92	0.51
1:C:199:CYS:O	1:C:202:ILE:HG22	2.11	0.51
1:C:412:TYR:CE2	1:D:421:ARG:NH2	2.68	0.51
1:C:412:TYR:N	1:C:412:TYR:CD1	2.78	0.51
1:D:253:LEU:HD21	1:D:289:LEU:CD2	2.41	0.51
1:E:392:ALA:O	1:E:417:SER:N	2.39	0.51
1:F:432:ILE:HD12	1:F:434:LEU:CD1	2.41	0.51
1:A:197:LEU:HD21	1:B:197:LEU:HD21	1.92	0.51
1:A:341:THR:CG2	1:A:342:ASP:H	2.23	0.51
1:C:202:ILE:CG2	1:C:203:THR:N	2.74	0.51
1:C:403:ASP:OD1	1:C:404:PRO:CD	2.59	0.51
1:D:47:ASP:OD1	1:D:47:ASP:C	2.49	0.51
1:D:312:LYS:C	1:D:314:PHE:N	2.65	0.51
1:A:83:ALA:HA	1:A:86:ARG:NH2	2.26	0.51
1:A:239:TYR:CZ	1:A:244:GLY:HA2	2.46	0.51
1:A:383:TYR:HB2	1:A:392:ALA:HB2	1.93	0.51
1:B:39:ALA:O	1:B:415:ALA:HB2	2.11	0.51
1:B:308:VAL:HG11	1:B:372:TYR:HE2	1.76	0.51
1:A:100:ARG:O	1:A:104:GLU:HG2	2.11	0.50
1:B:390:VAL:CG1	1:B:427:LEU:HD12	2.41	0.50
1:B:410:GLN:HB3	1:B:414:GLU:OE1	2.11	0.50
1:A:410:GLN:HA	1:A:414:GLU:OE1	2.11	0.50
1:B:262:SER:OG	1:B:344:ASP:HB2	2.11	0.50
1:C:91:LEU:O	1:C:94:PRO:HD2	2.11	0.50
1:D:242:ALA:HB2	1:D:249:LEU:HD22	1.93	0.50
1:D:333:LEU:HD23	1:D:333:LEU:C	2.31	0.50
1:D:421:ARG:HH11	1:D:421:ARG:CG	2.21	0.50
1:E:252:LYS:HD2	1:F:435:ARG:HH22	1.77	0.50
1:E:304:GLU:HG2	1:E:384:MET:HE1	1.93	0.50
1:A:252:LYS:NZ	1:A:252:LYS:HB3	2.26	0.50
1:C:255:VAL:HB	1:C:259:GLN:CB	2.42	0.50
1:D:326:VAL:HG23	1:E:379:LEU:CD1	2.41	0.50
1:E:81:LEU:HA	1:E:210:LEU:HD21	1.93	0.50
1:A:43:VAL:HG12	1:A:304:GLU:HB3	1.93	0.50
1:F:333:LEU:HD23	1:F:334:ASP:N	2.27	0.50
1:A:37:LEU:HD23	1:A:37:LEU:N	2.23	0.50
1:B:62:ILE:O	1:C:443:THR:HG23	2.11	0.50
1:B:312:LYS:C	1:B:314:PHE:N	2.65	0.50
1:B:394:CYS:HB2	1:B:417:SER:HG	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HD12	1:C:42:ILE:N	2.27	0.50
1:E:93:THR:HB	1:E:94:PRO:HD3	1.93	0.50
1:E:252:LYS:CE	1:F:435:ARG:HH22	2.23	0.50
1:A:89:THR:HG21	2:G:1:NAG:H61	1.94	0.50
1:B:312:LYS:O	1:B:314:PHE:N	2.44	0.50
1:A:76:CYS:HB3	1:A:203:THR:CG2	2.41	0.50
1:A:213:TYR:CZ	1:A:217:LEU:HD13	2.46	0.50
1:A:257:ASN:HD21	1:C:101:ARG:HH11	1.59	0.50
1:B:51:ASN:HB3	1:B:294:ASN:CA	2.36	0.50
1:B:315:ALA:HB1	1:B:372:TYR:CD2	2.47	0.50
1:D:191:ASN:O	1:D:194:ALA:HB3	2.11	0.50
1:D:197:LEU:CD2	1:E:197:LEU:HD21	2.42	0.50
1:E:67:PRO:HG3	1:E:213:TYR:CD2	2.47	0.50
1:E:88:LEU:HB3	1:E:281:GLN:NE2	2.27	0.50
1:A:47:ASP:OD1	1:A:47:ASP:C	2.50	0.50
1:D:50:VAL:HG11	1:D:350:ILE:HD11	1.92	0.50
1:D:179:VAL:O	1:D:183:GLN:HB3	2.12	0.50
1:E:197:LEU:HD21	1:F:197:LEU:HD21	1.94	0.50
1:F:309:SER:O	1:F:310:THR:C	2.50	0.50
1:A:197:LEU:HD21	1:C:197:LEU:CD2	2.41	0.50
1:C:192:LYS:HD3	1:C:193:THR:N	2.26	0.50
1:D:101:ARG:CB	1:E:257:ASN:HD22	2.12	0.50
1:D:403:ASP:O	1:D:405:PRO:CD	2.60	0.50
1:A:274:ILE:HG12	1:A:284:GLY:O	2.12	0.49
1:A:287:VAL:CG1	1:A:288:THR:N	2.74	0.49
1:B:64:LYS:HZ3	1:C:445:GLN:HE21	1.60	0.49
1:B:65:LEU:O	1:B:84:TYR:OH	2.23	0.49
1:B:383:TYR:O	1:B:383:TYR:CD2	2.65	0.49
1:E:315:ALA:HB1	1:E:372:TYR:CD2	2.46	0.49
1:A:294:ASN:OD1	1:A:295:LEU:O	2.30	0.49
1:A:350:ILE:O	1:B:380:THR:HA	2.13	0.49
1:A:372:TYR:HD1	1:A:372:TYR:H	1.59	0.49
1:B:35:ARG:HA	1:B:37:LEU:HD23	1.94	0.49
1:B:53:TYR:CE2	1:B:268:LEU:HD21	2.47	0.49
1:B:255:VAL:HG13	1:B:292:VAL:CG1	2.42	0.49
1:D:257:ASN:HD21	1:F:101:ARG:HH11	1.58	0.49
1:E:235:ILE:HG23	1:E:236:GLN:N	2.27	0.49
1:E:361:SER:HB3	1:E:369:ALA:CB	2.41	0.49
1:F:400:ARG:NH1	1:F:400:ARG:HB2	2.27	0.49
1:A:383:TYR:HA	1:A:392:ALA:HA	1.94	0.49
1:A:450:ILE:HD13	1:C:202:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLU:HG3	1:B:380:THR:HG21	1.94	0.49
1:C:405:PRO:CD	1:F:64:LYS:HZ1	2.24	0.49
1:D:37:LEU:HD23	1:D:37:LEU:N	2.24	0.49
1:D:315:ALA:HB1	1:D:372:TYR:CD2	2.47	0.49
1:D:403:ASP:O	1:D:405:PRO:HD3	2.11	0.49
1:E:226:THR:HA	1:F:236:GLN:HE21	1.77	0.49
1:A:450:ILE:HD12	1:C:202:ILE:HD11	1.93	0.49
1:B:200:ILE:HD12	1:C:197:LEU:HD22	1.95	0.49
1:C:400:ARG:CG	1:C:428:SER:HB2	2.36	0.49
1:D:76:CYS:C	1:D:203:THR:HG22	2.33	0.49
1:D:440:PHE:HB2	1:F:241:LEU:HD11	1.95	0.49
1:E:190:PHE:O	1:E:194:ALA:N	2.45	0.49
1:A:383:TYR:HB3	1:A:392:ALA:CB	2.41	0.49
1:B:255:VAL:HG13	1:B:292:VAL:HG11	1.93	0.49
1:C:59:GLY:O	1:C:287:VAL:N	2.45	0.49
1:D:57:GLN:HE21	1:E:438:GLY:CA	2.14	0.49
1:D:450:ILE:HG13	1:D:450:ILE:O	2.11	0.49
1:E:101:ARG:HB3	1:F:257:ASN:HD22	1.78	0.49
1:C:48:LYS:HE2	1:C:342:ASP:O	2.12	0.49
1:C:383:TYR:CG	1:C:429:LEU:HD23	2.47	0.49
1:C:421:ARG:HB2	1:C:421:ARG:NH1	2.28	0.49
1:E:58:THR:O	1:F:439:GLU:HA	2.11	0.49
1:E:255:VAL:HG12	1:E:259:GLN:CD	2.33	0.49
1:E:316:SER:H	1:E:372:TYR:HB3	1.76	0.49
1:E:419:ILE:HG21	1:E:427:LEU:CD1	2.43	0.49
1:B:45:THR:HG22	1:B:386:LEU:HD22	1.94	0.49
1:B:240:ASN:ND2	1:C:444:TYR:CD2	2.81	0.49
1:D:239:TYR:CZ	1:D:244:GLY:HA2	2.48	0.49
1:E:350:ILE:H	1:F:381:THR:CG2	2.24	0.49
1:F:302:TYR:OH	1:F:345:LEU:HD11	2.12	0.49
1:A:84:TYR:HE1	1:A:88:LEU:CD1	2.26	0.49
1:A:91:LEU:O	1:A:94:PRO:HD2	2.12	0.49
1:D:84:TYR:CD1	1:D:84:TYR:C	2.86	0.49
1:D:220:VAL:HG22	1:D:236:GLN:HG3	1.93	0.49
1:D:388:GLY:HA2	1:F:54:THR:CG2	2.43	0.49
1:D:435:ARG:HB2	1:D:435:ARG:NH1	2.28	0.49
1:F:37:LEU:CD2	1:F:37:LEU:H	2.26	0.49
1:A:199:CYS:O	1:A:203:THR:HG23	2.13	0.49
1:C:427:LEU:HD22	1:C:428:SER:H	1.77	0.49
1:D:261:SER:HB3	1:F:102:ILE:HD13	1.95	0.49
1:E:98:SER:O	1:E:102:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:LYS:HB2	1:E:314:PHE:HD1	1.77	0.49
1:E:411:ASN:HB3	1:E:412:TYR:CD2	2.48	0.49
1:E:418:LEU:HD23	1:E:418:LEU:O	2.12	0.49
1:B:252:LYS:CD	1:C:435:ARG:HH22	2.25	0.49
1:C:50:VAL:C	1:C:51:ASN:ND2	2.66	0.49
1:C:175:LEU:C	1:C:175:LEU:HD23	2.33	0.49
1:D:224:GLN:CD	1:D:224:GLN:H	2.16	0.49
1:E:372:TYR:N	1:E:372:TYR:HD1	2.11	0.49
1:F:76:CYS:C	1:F:203:THR:HG22	2.33	0.49
1:B:377:GLY:H	1:B:380:THR:CG2	2.25	0.48
1:C:35:ARG:HH22	1:C:418:LEU:CD1	2.26	0.48
1:E:432:ILE:HG13	1:E:432:ILE:O	2.13	0.48
1:A:226:THR:HA	1:B:236:GLN:HE21	1.77	0.48
1:B:185:PHE:CD1	1:B:186:VAL:N	2.81	0.48
1:B:355:MET:CE	1:B:363:LEU:HD12	2.42	0.48
1:A:189:GLN:HA	1:A:189:GLN:OE1	2.12	0.48
1:A:309:SER:HA	1:A:312:LYS:C	2.34	0.48
1:A:445:GLN:HB3	1:C:64:LYS:HB2	1.95	0.48
1:B:205:GLN:HE22	1:C:451:GLN:H	1.60	0.48
1:B:245:ASN:ND2	1:B:248:TYR:HB2	2.28	0.48
1:F:312:LYS:C	1:F:314:PHE:N	2.66	0.48
1:C:81:LEU:HA	1:C:210:LEU:HD21	1.94	0.48
1:D:52:ILE:HD11	1:D:350:ILE:HG13	1.95	0.48
1:B:202:ILE:HD11	1:C:450:ILE:CD1	2.43	0.48
1:D:172:LEU:HD21	1:F:172:LEU:H	1.73	0.48
1:D:421:ARG:HB3	1:D:421:ARG:CZ	2.43	0.48
1:E:74:GLU:O	1:E:75:ALA:C	2.49	0.48
1:F:185:PHE:CD2	1:F:186:VAL:N	2.81	0.48
1:F:263:LEU:O	1:F:266:SER:HB3	2.13	0.48
1:F:427:LEU:HD22	1:F:428:SER:H	1.77	0.48
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.48
1:B:314:PHE:CB	1:B:374:LYS:HD3	2.26	0.48
1:C:54:THR:O	1:C:56:SER:N	2.42	0.48
1:C:312:LYS:HG3	1:C:314:PHE:CD2	2.49	0.48
1:E:252:LYS:CD	1:F:435:ARG:HH22	2.26	0.48
1:E:255:VAL:HG13	1:E:292:VAL:CG1	2.43	0.48
1:E:377:GLY:H	1:E:380:THR:HG21	1.79	0.48
1:A:367:THR:O	1:A:370:CYS:HB2	2.13	0.48
1:C:406:GLY:N	1:F:62:ILE:HD13	2.28	0.48
1:D:236:GLN:NE2	1:F:226:THR:HA	2.28	0.48
1:F:255:VAL:HB	1:F:259:GLN:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:GLN:O	1:F:325:GLN:HG3	2.14	0.48
1:A:54:THR:HG21	1:B:388:GLY:O	2.13	0.48
1:C:88:LEU:HB3	1:C:281:GLN:NE2	2.28	0.48
1:C:255:VAL:HB	1:C:259:GLN:HB3	1.94	0.48
1:A:330:ILE:HG22	1:A:355:MET:HE1	1.96	0.48
1:B:190:PHE:O	1:B:194:ALA:N	2.46	0.48
1:C:333:LEU:HD23	1:C:334:ASP:N	2.29	0.48
1:D:262:SER:HA	1:D:341:THR:HG21	1.95	0.48
1:E:35:ARG:HA	1:E:37:LEU:HD23	1.96	0.48
1:E:172:LEU:HA	1:F:172:LEU:HD21	1.96	0.48
1:E:400:ARG:HH11	1:E:400:ARG:CB	2.26	0.48
1:A:63:ILE:HB	1:A:283:LEU:HB3	1.96	0.48
1:A:182:MET:HG3	1:B:182:MET:SD	2.53	0.48
1:B:223:PRO:HB3	1:B:231:THR:HG21	1.95	0.48
1:B:252:LYS:HD2	1:C:435:ARG:HH22	1.79	0.48
1:C:312:LYS:C	1:C:314:PHE:H	2.15	0.48
1:D:366:ASN:OD1	1:D:367:THR:N	2.46	0.48
1:D:403:ASP:O	1:D:405:PRO:N	2.46	0.48
1:F:257:ASN:C	1:F:259:GLN:H	2.17	0.48
1:A:385:THR:CG2	1:C:54:THR:OG1	2.61	0.47
1:B:314:PHE:O	1:B:374:LYS:HB3	2.14	0.47
1:D:450:ILE:HD13	1:F:202:ILE:HD11	1.96	0.47
1:E:200:ILE:HG21	1:F:200:ILE:HG21	1.95	0.47
1:E:262:SER:OG	1:E:344:ASP:HB2	2.14	0.47
1:F:199:CYS:O	1:F:202:ILE:HG22	2.14	0.47
1:F:355:MET:HE3	1:F:359:ILE:CG2	2.40	0.47
1:A:72:ASP:C	1:A:74:GLU:H	2.16	0.47
1:B:205:GLN:NE2	1:C:451:GLN:H	2.12	0.47
1:C:242:ALA:HB2	1:C:249:LEU:HD22	1.95	0.47
1:C:315:ALA:HB1	1:C:372:TYR:CD2	2.47	0.47
1:D:76:CYS:HB3	1:D:203:THR:CG2	2.43	0.47
1:D:287:VAL:CG1	1:D:288:THR:N	2.76	0.47
1:D:309:SER:HA	1:D:312:LYS:O	2.15	0.47
1:D:331:GLU:HB3	1:D:353:PHE:O	2.14	0.47
1:D:410:GLN:HA	1:D:414:GLU:OE1	2.15	0.47
1:E:83:ALA:O	1:E:87:THR:HG23	2.14	0.47
1:E:400:ARG:HB2	1:E:400:ARG:NH1	2.29	0.47
1:A:101:ARG:NH1	1:B:257:ASN:HD21	2.08	0.47
1:A:331:GLU:OE2	1:B:378:ALA:N	2.45	0.47
1:B:76:CYS:HB3	1:B:203:THR:CG2	2.44	0.47
1:C:360:TYR:HD1	1:C:360:TYR:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:HA	1:D:347:CYS:O	2.13	0.47
1:D:97:ASP:O	1:D:100:ARG:HB3	2.14	0.47
1:D:385:THR:HG21	1:F:53:TYR:O	2.13	0.47
1:E:88:LEU:HB3	1:E:281:GLN:HE22	1.79	0.47
1:F:372:TYR:N	1:F:372:TYR:HD1	2.12	0.47
1:F:425:ASN:O	1:F:436:LEU:HB2	2.14	0.47
1:A:63:ILE:HD11	1:A:221:PHE:CD1	2.48	0.47
1:B:410:GLN:HA	1:B:414:GLU:OE1	2.14	0.47
1:C:190:PHE:O	1:C:194:ALA:N	2.44	0.47
1:C:235:ILE:CG2	1:C:236:GLN:N	2.76	0.47
1:D:391:ILE:HG12	1:D:418:LEU:HD12	1.96	0.47
1:D:419:ILE:CD1	1:D:427:LEU:HD21	2.42	0.47
1:D:421:ARG:CG	1:D:421:ARG:NH1	2.76	0.47
1:A:89:THR:HG22	1:A:281:GLN:HE22	1.80	0.47
1:B:420:ASP:CG	1:B:421:ARG:N	2.68	0.47
1:C:185:PHE:CD2	1:C:186:VAL:N	2.83	0.47
1:C:395:LYS:NZ	1:C:412:TYR:OH	2.48	0.47
1:C:405:PRO:HD3	1:F:64:LYS:CE	2.45	0.47
1:D:311:THR:OG1	1:D:315:ALA:HB2	2.14	0.47
1:E:223:PRO:O	1:E:226:THR:HG22	2.15	0.47
1:E:341:THR:HB	1:E:344:ASP:O	2.14	0.47
1:B:350:ILE:HB	1:C:381:THR:CG2	2.44	0.47
1:C:202:ILE:HG23	1:C:203:THR:N	2.30	0.47
1:D:255:VAL:HG12	1:D:259:GLN:CD	2.35	0.47
1:E:64:LYS:NZ	1:F:445:GLN:NE2	2.48	0.47
1:E:199:CYS:O	1:E:202:ILE:HG22	2.15	0.47
1:F:190:PHE:O	1:F:194:ALA:N	2.45	0.47
1:A:101:ARG:HB3	1:B:257:ASN:ND2	2.13	0.47
1:A:179:VAL:O	1:A:183:GLN:HB3	2.15	0.47
1:A:421:ARG:NH1	1:A:437:SER:OG	2.46	0.47
1:B:239:TYR:CZ	1:B:244:GLY:HA2	2.49	0.47
1:B:249:LEU:O	1:B:252:LYS:N	2.47	0.47
1:B:333:LEU:HD23	1:B:334:ASP:H	1.79	0.47
1:B:421:ARG:HG3	1:B:422:GLN:N	2.28	0.47
1:C:337:TYR:O	1:C:348:THR:HG22	2.15	0.47
1:D:51:ASN:N	1:D:51:ASN:HD22	2.13	0.47
1:D:89:THR:HG22	1:D:281:GLN:NE2	2.30	0.47
1:D:172:LEU:CD2	1:F:172:LEU:N	2.74	0.47
1:D:226:THR:HA	1:E:236:GLN:HE22	1.78	0.47
1:E:295:LEU:HD23	1:F:432:ILE:HG21	1.96	0.47
1:E:385:THR:HG22	1:E:386:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:LEU:HD12	1:F:233:LEU:HA	1.66	0.47
1:F:235:ILE:HG23	1:F:236:GLN:N	2.30	0.47
1:F:376:GLU:HG3	1:F:380:THR:HG21	1.97	0.47
1:A:403:ASP:O	1:A:405:PRO:CD	2.63	0.47
1:B:101:ARG:HH22	1:C:247:ASP:CG	2.18	0.47
1:C:400:ARG:HD3	1:F:275:LEU:CD2	2.39	0.47
1:C:400:ARG:CZ	1:F:275:LEU:HD13	2.45	0.47
1:D:427:LEU:HD13	1:D:429:LEU:CD1	2.44	0.47
1:E:43:VAL:HG21	1:E:391:ILE:HG21	1.97	0.47
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.78	0.47
1:F:386:LEU:N	1:F:389:SER:O	2.47	0.47
1:A:330:ILE:HG22	1:A:330:ILE:O	2.14	0.47
1:B:349:ARG:NH2	1:C:305:THR:O	2.48	0.47
1:C:402:ALA:HA	1:F:282:LEU:HD22	1.96	0.47
1:C:403:ASP:CB	1:C:404:PRO:CD	2.90	0.47
1:D:252:LYS:NZ	1:D:252:LYS:HB3	2.30	0.47
1:E:53:TYR:CE2	1:E:268:LEU:HD21	2.49	0.47
1:F:220:VAL:HG12	1:F:221:PHE:CD1	2.50	0.47
1:F:397:THR:HG22	1:F:430:ASP:OD2	2.15	0.47
1:F:400:ARG:HB3	1:F:428:SER:OG	2.14	0.47
1:B:238:LEU:HD11	1:B:249:LEU:HD21	1.96	0.47
1:B:390:VAL:CG1	1:B:436:LEU:HD21	2.45	0.47
1:C:281:GLN:HA	1:C:281:GLN:OE1	2.15	0.47
1:D:99:ILE:HD11	1:D:273:PRO:HB2	1.97	0.47
1:E:315:ALA:HB1	1:E:372:TYR:HD2	1.80	0.47
1:F:403:ASP:CB	1:F:404:PRO:CD	2.88	0.47
1:A:326:VAL:HG23	1:B:379:LEU:CD1	2.45	0.46
1:B:352:THR:OG1	1:C:380:THR:HG22	2.14	0.46
1:B:428:SER:OG	1:B:433:THR:HG22	2.15	0.46
1:D:43:VAL:HG12	1:D:304:GLU:HB3	1.97	0.46
1:D:330:ILE:HG22	1:D:355:MET:HE1	1.97	0.46
1:E:179:VAL:O	1:E:183:GLN:HB3	2.14	0.46
1:E:429:LEU:O	1:E:430:ASP:O	2.32	0.46
1:F:337:TYR:O	1:F:348:THR:HG22	2.16	0.46
1:A:58:THR:O	1:B:439:GLU:HA	2.15	0.46
1:B:213:TYR:O	1:B:217:LEU:HB2	2.14	0.46
1:F:84:TYR:CD2	1:F:210:LEU:HG	2.50	0.46
1:C:406:GLY:HA2	1:F:62:ILE:HG21	1.96	0.46
1:D:72:ASP:O	1:D:74:GLU:N	2.48	0.46
1:D:172:LEU:N	1:E:172:LEU:HD21	2.31	0.46
1:E:281:GLN:HA	1:E:281:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD13	1:A:269:ILE:HG21	1.97	0.46
1:C:63:ILE:HD11	1:C:221:PHE:CD2	2.51	0.46
1:C:400:ARG:HG3	1:C:400:ARG:O	2.14	0.46
1:D:185:PHE:CD2	1:D:186:VAL:N	2.84	0.46
1:D:257:ASN:HD22	1:F:101:ARG:CB	2.28	0.46
1:F:74:GLU:HG2	1:F:75:ALA:N	2.30	0.46
1:A:76:CYS:O	1:A:203:THR:HG22	2.15	0.46
1:A:215:THR:CG2	1:B:215:THR:HG21	2.42	0.46
1:A:447:ASN:OD1	1:C:68:ASN:HB2	2.15	0.46
1:C:233:LEU:HG	1:C:237:ALA:HB3	1.97	0.46
1:C:403:ASP:O	1:C:405:PRO:N	2.48	0.46
1:D:87:THR:HG21	1:E:212:LEU:HB3	1.98	0.46
1:D:314:PHE:N	1:D:314:PHE:CD1	2.84	0.46
1:A:52:ILE:HD11	1:A:350:ILE:HG13	1.97	0.46
1:A:224:GLN:CD	1:A:224:GLN:H	2.18	0.46
1:A:315:ALA:HB1	1:A:372:TYR:CD2	2.51	0.46
1:A:450:ILE:HD11	1:C:73:LYS:CD	2.46	0.46
1:C:233:LEU:HD22	1:C:287:VAL:HG13	1.98	0.46
2:G:1:NAG:O6	2:G:2:NAG:C7	2.64	0.46
1:A:79:ALA:HB3	1:A:80:PRO:CD	2.45	0.46
1:A:383:TYR:CB	1:A:392:ALA:HB2	2.45	0.46
1:D:309:SER:O	1:D:312:LYS:N	2.39	0.46
1:E:318:LEU:HD21	1:E:373:SER:HB3	1.96	0.46
1:F:202:ILE:HG23	1:F:203:THR:N	2.31	0.46
1:B:197:LEU:HD23	1:C:197:LEU:HD21	1.95	0.46
1:C:383:TYR:CD1	1:C:429:LEU:HD23	2.51	0.46
1:C:386:LEU:HD23	1:C:391:ILE:HD11	1.98	0.46
1:D:79:ALA:HB3	1:D:80:PRO:CD	2.45	0.46
1:E:99:ILE:HD11	1:E:273:PRO:HB2	1.98	0.46
1:E:403:ASP:O	1:E:405:PRO:HD3	2.15	0.46
1:A:420:ASP:C	1:A:420:ASP:OD1	2.54	0.46
1:B:76:CYS:HB3	1:B:203:THR:HG23	1.97	0.46
1:C:312:LYS:C	1:C:314:PHE:N	2.69	0.46
1:F:360:TYR:CD1	1:F:360:TYR:C	2.90	0.46
1:A:257:ASN:HD22	1:C:101:ARG:CB	2.25	0.46
1:C:275:LEU:HD12	1:C:276:TYR:N	2.31	0.46
1:C:419:ILE:HG21	1:C:427:LEU:CG	2.42	0.46
1:D:93:THR:HB	1:D:94:PRO:HD3	1.98	0.46
1:D:172:LEU:CA	1:E:172:LEU:HD21	2.46	0.46
1:E:355:MET:HE1	1:E:363:LEU:HD12	1.98	0.46
1:E:426:ILE:HG22	1:E:426:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:PHE:CD2	1:F:374:LYS:HD3	2.51	0.46
1:A:298:MET:HG3	1:A:326:VAL:HG22	1.97	0.45
1:B:77:ALA:O	1:B:80:PRO:HD2	2.15	0.45
1:D:255:VAL:HG12	1:D:259:GLN:OE1	2.16	0.45
1:D:340:GLU:HB2	1:D:345:LEU:HD12	1.97	0.45
1:D:445:GLN:HB3	1:F:64:LYS:HD3	1.98	0.45
1:E:385:THR:CG2	1:E:386:LEU:N	2.79	0.45
1:A:223:PRO:HB2	1:A:224:GLN:NE2	2.30	0.45
1:A:240:ASN:HD22	1:B:444:TYR:HD1	1.64	0.45
1:B:316:SER:H	1:B:372:TYR:HB3	1.80	0.45
1:B:390:VAL:HG12	1:B:436:LEU:HD21	1.98	0.45
1:D:238:LEU:HD13	1:D:269:ILE:HG21	1.97	0.45
1:E:64:LYS:HZ1	1:F:445:GLN:NE2	2.13	0.45
1:E:311:THR:OG1	1:E:312:LYS:N	2.49	0.45
1:F:192:LYS:HD3	1:F:193:THR:N	2.31	0.45
1:F:220:VAL:HG22	1:F:236:GLN:HG3	1.97	0.45
1:F:349:ARG:CD	1:F:351:VAL:CG2	2.93	0.45
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.79	0.45
1:A:424:CYS:SG	1:A:425:ASN:N	2.89	0.45
1:C:259:GLN:O	1:C:263:LEU:HB2	2.16	0.45
1:D:445:GLN:HB3	1:F:64:LYS:HB2	1.97	0.45
1:E:255:VAL:HG12	1:E:259:GLN:OE1	2.16	0.45
1:A:325:GLN:HB2	1:A:329:VAL:O	2.17	0.45
1:B:47:ASP:C	1:B:48:LYS:HG3	2.36	0.45
1:C:332:GLU:O	1:C:352:THR:HB	2.16	0.45
1:E:44:VAL:O	1:E:44:VAL:HG12	2.15	0.45
1:E:260:LEU:O	1:E:260:LEU:HD12	2.16	0.45
1:E:435:ARG:HD3	1:E:437:SER:O	2.17	0.45
1:F:337:TYR:HB3	1:F:348:THR:HG23	1.98	0.45
1:A:200:ILE:HD13	1:B:200:ILE:CG2	2.45	0.45
1:E:44:VAL:HG22	1:E:303:LEU:CD2	2.47	0.45
1:F:54:THR:O	1:F:56:SER:N	2.44	0.45
1:F:454:GLN:N	1:F:454:GLN:CD	2.70	0.45
1:A:227:SER:HA	1:A:228:PRO:HD3	1.75	0.45
1:A:255:VAL:CG1	1:A:292:VAL:HG11	2.17	0.45
1:A:331:GLU:HB3	1:A:353:PHE:O	2.16	0.45
1:C:355:MET:CE	1:C:359:ILE:HG22	2.46	0.45
1:C:360:TYR:CD1	1:C:360:TYR:C	2.88	0.45
1:D:298:MET:HG3	1:D:326:VAL:CG2	2.46	0.45
1:E:74:GLU:O	1:E:77:ALA:N	2.50	0.45
1:F:266:SER:OG	1:F:268:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD22	1:A:428:SER:H	1.80	0.45
1:C:44:VAL:HG22	1:C:303:LEU:HD21	1.97	0.45
1:C:255:VAL:HG12	1:C:259:GLN:OE1	2.16	0.45
1:D:257:ASN:O	1:D:259:GLN:N	2.49	0.45
1:F:372:TYR:HD1	1:F:372:TYR:H	1.64	0.45
1:F:377:GLY:H	1:F:380:THR:CG2	2.30	0.45
1:A:349:ARG:NH2	1:B:305:THR:O	2.50	0.45
1:B:102:ILE:CD1	1:B:228:PRO:HB2	2.46	0.45
1:B:189:GLN:HB3	1:C:190:PHE:CZ	2.52	0.45
1:B:361:SER:HB3	1:B:369:ALA:CB	2.47	0.45
1:C:243:GLY:C	1:C:245:ASN:H	2.20	0.45
1:D:309:SER:HA	1:D:312:LYS:C	2.37	0.45
1:D:326:VAL:HG23	1:E:379:LEU:HD13	1.98	0.45
1:E:202:ILE:HD11	1:F:450:ILE:CD1	2.46	0.45
1:F:257:ASN:O	1:F:259:GLN:N	2.50	0.45
1:A:333:LEU:HD23	1:A:333:LEU:C	2.37	0.45
1:D:330:ILE:HG22	1:D:355:MET:CE	2.46	0.45
1:D:333:LEU:C	1:D:333:LEU:CD2	2.85	0.45
1:E:381:THR:HA	1:E:382:PRO:HD3	1.66	0.45
1:F:337:TYR:CD1	1:F:337:TYR:N	2.85	0.45
1:A:192:LYS:HD3	1:A:193:THR:H	1.80	0.45
1:A:75:ALA:HA	1:A:78:LYS:HZ2	1.82	0.44
1:A:275:LEU:HD12	1:A:276:TYR:H	1.82	0.44
1:B:73:LYS:CD	1:B:73:LYS:H	2.30	0.44
1:B:341:THR:HG23	1:B:342:ASP:N	2.32	0.44
1:B:386:LEU:HD12	1:B:386:LEU:C	2.38	0.44
1:C:51:ASN:CB	1:C:294:ASN:HA	2.40	0.44
1:C:311:THR:OG1	1:C:312:LYS:N	2.50	0.44
1:C:337:TYR:HB3	1:C:348:THR:HG23	1.99	0.44
1:C:383:TYR:CD1	1:C:383:TYR:C	2.90	0.44
1:E:189:GLN:OE1	1:E:189:GLN:HA	2.16	0.44
1:E:239:TYR:CZ	1:E:244:GLY:HA2	2.52	0.44
1:E:349:ARG:NH2	1:F:305:THR:O	2.50	0.44
1:A:101:ARG:HH11	1:B:257:ASN:ND2	2.11	0.44
1:A:257:ASN:O	1:A:259:GLN:N	2.49	0.44
1:B:88:LEU:HB3	1:B:281:GLN:NE2	2.32	0.44
1:D:242:ALA:O	1:D:243:GLY:C	2.56	0.44
1:F:75:ALA:HA	1:F:78:LYS:NZ	2.32	0.44
1:F:403:ASP:OD2	1:F:404:PRO:HD3	2.16	0.44
1:B:93:THR:HG21	3:H:3:BMA:H62	2.00	0.44
1:B:349:ARG:HG3	1:C:384:MET:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ILE:HG22	1:C:350:ILE:O	2.17	0.44
1:B:275:LEU:HD12	1:B:276:TYR:H	1.76	0.44
1:B:396:MET:O	1:B:397:THR:HG23	2.17	0.44
1:D:450:ILE:HD11	1:F:73:LYS:CD	2.47	0.44
1:F:51:ASN:OD1	1:F:259:GLN:NE2	2.50	0.44
1:F:361:SER:O	1:F:366:ASN:HB3	2.17	0.44
1:A:79:ALA:HB3	1:A:80:PRO:HD3	2.00	0.44
1:A:172:LEU:HD21	1:C:171:GLY:C	2.38	0.44
1:A:263:LEU:O	1:A:266:SER:HB3	2.17	0.44
1:A:427:LEU:CD1	1:A:429:LEU:HD21	2.37	0.44
1:D:83:ALA:HA	1:D:86:ARG:NH2	2.32	0.44
1:D:309:SER:HA	1:D:313:GLY:HA2	1.98	0.44
1:D:380:THR:HA	1:F:350:ILE:O	2.18	0.44
1:D:422:GLN:H	1:D:422:GLN:HG2	1.55	0.44
1:E:312:LYS:HB2	1:E:314:PHE:CD1	2.52	0.44
1:F:65:LEU:HD12	1:F:281:GLN:C	2.38	0.44
1:B:88:LEU:HB3	1:B:281:GLN:HE22	1.83	0.44
1:D:76:CYS:O	1:D:203:THR:HG22	2.17	0.44
1:F:334:ASP:OD2	1:F:337:TYR:HE1	2.00	0.44
1:D:92:LEU:N	1:D:92:LEU:HD23	2.33	0.44
1:D:184:GLN:CD	1:D:185:PHE:N	2.71	0.44
1:F:295:LEU:HD23	1:F:295:LEU:HA	1.86	0.44
1:A:403:ASP:CB	1:A:425:ASN:HB3	2.47	0.44
1:B:350:ILE:N	1:C:381:THR:CG2	2.81	0.44
1:C:410:GLN:H	1:C:410:GLN:HG2	1.55	0.44
1:D:197:LEU:HD21	1:E:197:LEU:HD21	1.98	0.44
1:D:212:LEU:HB3	1:F:87:THR:HG21	1.99	0.44
1:D:294:ASN:OD1	1:D:295:LEU:O	2.35	0.44
1:D:367:THR:O	1:D:370:CYS:HB2	2.17	0.44
1:A:257:ASN:HD21	1:C:101:ARG:NH1	2.16	0.44
1:B:48:LYS:HE2	1:B:342:ASP:O	2.18	0.44
1:B:98:SER:O	1:B:102:ILE:HG13	2.18	0.44
1:B:409:SER:C	1:B:410:GLN:HG2	2.38	0.44
1:B:454:GLN:N	1:B:454:GLN:CD	2.71	0.44
1:D:74:GLU:O	1:D:75:ALA:C	2.55	0.44
1:D:79:ALA:HB3	1:D:80:PRO:HD3	2.00	0.44
1:D:189:GLN:OE1	1:D:189:GLN:HA	2.17	0.44
1:E:49:ALA:HB2	1:E:299:ARG:HH12	1.83	0.44
1:A:74:GLU:O	1:A:75:ALA:C	2.55	0.43
1:B:403:ASP:O	1:B:404:PRO:C	2.53	0.43
1:B:419:ILE:HG21	1:B:427:LEU:CG	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ASN:HD21	1:F:101:ARG:NH1	2.17	0.43
1:E:403:ASP:OD2	1:E:404:PRO:HD3	2.18	0.43
1:A:366:ASN:OD1	1:A:369:ALA:N	2.44	0.43
1:B:184:GLN:CD	1:B:185:PHE:N	2.72	0.43
1:B:223:PRO:O	1:B:226:THR:HG22	2.18	0.43
1:B:377:GLY:H	1:B:380:THR:HG21	1.83	0.43
1:D:315:ALA:HB1	1:D:372:TYR:HD2	1.82	0.43
1:D:447:ASN:OD1	1:F:68:ASN:HB2	2.18	0.43
1:E:411:ASN:O	1:E:412:TYR:O	2.36	0.43
1:F:59:GLY:O	1:F:287:VAL:N	2.51	0.43
1:A:340:GLU:CG	1:A:340:GLU:O	2.65	0.43
1:C:349:ARG:CD	1:C:351:VAL:CG2	2.95	0.43
1:D:182:MET:HG3	1:E:182:MET:SD	2.57	0.43
1:F:262:SER:HA	1:F:341:THR:HG21	2.00	0.43
1:A:200:ILE:HD13	1:B:200:ILE:HG22	2.01	0.43
1:B:92:LEU:N	1:B:92:LEU:HD23	2.33	0.43
1:B:323:VAL:O	1:B:323:VAL:HG23	2.18	0.43
1:D:62:ILE:HG23	1:D:62:ILE:O	2.19	0.43
1:B:172:LEU:O	1:B:176:ALA:HB2	2.18	0.43
1:C:76:CYS:CB	1:C:202:ILE:CG2	2.97	0.43
1:C:182:MET:HE3	1:C:183:GLN:H	1.83	0.43
1:C:408:ILE:CD1	1:C:419:ILE:HG23	2.48	0.43
1:C:432:ILE:HD12	1:C:434:LEU:HD11	2.00	0.43
1:D:95:LEU:HD13	1:D:95:LEU:C	2.39	0.43
1:D:349:ARG:NH2	1:E:305:THR:O	2.51	0.43
1:D:440:PHE:HB3	1:F:241:LEU:HD11	2.00	0.43
1:E:414:GLU:O	1:E:415:ALA:HB3	2.18	0.43
1:F:325:GLN:HE21	1:F:325:GLN:HB2	1.64	0.43
1:A:239:TYR:CE2	1:A:244:GLY:HA2	2.53	0.43
1:A:408:ILE:HD11	1:A:424:CYS:HB2	1.99	0.43
1:B:76:CYS:O	1:B:203:THR:CG2	2.66	0.43
1:B:411:ASN:HB3	1:B:412:TYR:CD2	2.53	0.43
1:D:190:PHE:CZ	1:F:189:GLN:HB3	2.53	0.43
1:A:84:TYR:CE1	1:A:88:LEU:CD1	3.02	0.43
1:A:97:ASP:O	1:A:100:ARG:HB3	2.19	0.43
1:A:101:ARG:CD	1:B:257:ASN:ND2	2.78	0.43
1:A:176:ALA:HA	1:C:175:LEU:HD11	2.00	0.43
1:A:201:LYS:HG3	1:C:200:ILE:HD11	2.01	0.43
1:A:366:ASN:OD1	1:A:367:THR:N	2.51	0.43
1:A:421:ARG:CG	1:A:436:LEU:O	2.66	0.43
1:B:72:ASP:C	1:B:74:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:HG23	1:B:236:GLN:N	2.34	0.43
1:B:435:ARG:HD3	1:B:437:SER:O	2.18	0.43
1:D:72:ASP:C	1:D:74:GLU:N	2.70	0.43
1:D:241:LEU:HD22	1:D:287:VAL:HG21	2.01	0.43
1:D:381:THR:CG2	1:F:350:ILE:N	2.77	0.43
1:E:185:PHE:CD2	1:E:186:VAL:N	2.87	0.43
1:E:240:ASN:HD22	1:F:444:TYR:HD2	1.62	0.43
1:E:275:LEU:HD12	1:E:276:TYR:H	1.80	0.43
1:A:99:ILE:HD11	1:A:273:PRO:HB2	2.00	0.43
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.71	0.43
1:C:377:GLY:H	1:C:380:THR:CG2	2.32	0.43
1:D:181:LYS:O	1:D:182:MET:C	2.57	0.43
1:D:182:MET:SD	1:F:182:MET:HG3	2.59	0.43
1:D:450:ILE:HD11	1:F:73:LYS:HD2	2.01	0.43
1:E:184:GLN:CD	1:E:185:PHE:N	2.72	0.43
1:E:197:LEU:HD23	1:F:197:LEU:HD21	2.01	0.43
1:F:255:VAL:CG1	1:F:292:VAL:HG11	2.46	0.43
1:A:84:TYR:HE1	1:A:88:LEU:HD12	1.83	0.43
1:A:408:ILE:O	1:A:408:ILE:HG22	2.18	0.43
1:A:450:ILE:HD11	1:C:73:LYS:HD2	2.00	0.43
1:B:249:LEU:O	1:B:250:LEU:C	2.57	0.43
1:E:104:GLU:OE1	1:E:104:GLU:CA	2.67	0.43
1:E:255:VAL:HG13	1:E:292:VAL:HG11	2.01	0.43
1:E:325:GLN:HE21	1:E:325:GLN:HB2	1.71	0.43
1:F:87:THR:HA	1:F:90:THR:HB	1.99	0.43
1:F:400:ARG:CB	1:F:400:ARG:HH11	2.32	0.43
1:A:172:LEU:HD21	1:C:172:LEU:H	1.83	0.43
1:A:298:MET:HG3	1:A:326:VAL:CG2	2.49	0.43
1:A:414:GLU:O	1:A:415:ALA:HB3	2.19	0.43
1:B:255:VAL:HG12	1:B:259:GLN:CD	2.40	0.43
1:D:72:ASP:C	1:D:74:GLU:H	2.23	0.43
1:E:68:ASN:HB2	1:F:447:ASN:OD1	2.19	0.43
1:E:73:LYS:CG	1:F:450:ILE:CD1	2.92	0.43
1:E:263:LEU:O	1:E:266:SER:HB3	2.19	0.43
1:F:36:PRO:CD	1:F:37:LEU:H	2.31	0.43
3:H:2:NAG:C3	3:H:3:BMA:H2	2.45	0.43
1:A:87:THR:HG21	1:B:212:LEU:HB3	2.01	0.42
1:A:350:ILE:HB	1:B:381:THR:CG2	2.39	0.42
1:A:361:SER:O	1:A:366:ASN:HB3	2.19	0.42
1:A:390:VAL:CG1	1:A:427:LEU:HD12	2.43	0.42
1:B:181:LYS:O	1:B:182:MET:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ARG:C	1:B:436:LEU:HD12	2.39	0.42
1:C:233:LEU:HA	1:C:233:LEU:HD12	1.65	0.42
1:D:84:TYR:HD1	1:D:85:ASN:N	2.17	0.42
1:D:325:GLN:HG3	1:D:325:GLN:O	2.19	0.42
1:F:76:CYS:HB3	1:F:203:THR:HG23	2.00	0.42
1:F:89:THR:CG2	2:N:1:NAG:H62	2.23	0.42
1:A:64:LYS:HD3	1:B:445:GLN:HB3	2.00	0.42
1:A:314:PHE:O	1:A:374:LYS:HB3	2.19	0.42
1:C:76:CYS:HB3	1:C:203:THR:HG23	1.99	0.42
1:C:183:GLN:O	1:C:186:VAL:HG22	2.19	0.42
1:D:312:LYS:O	1:D:314:PHE:N	2.52	0.42
1:D:356:SER:HB3	1:D:359:ILE:CG1	2.47	0.42
1:E:350:ILE:O	1:F:380:THR:HA	2.19	0.42
1:E:393:ASN:OD1	1:E:395:LYS:HB3	2.19	0.42
1:E:397:THR:HB	1:E:430:ASP:OD2	2.19	0.42
1:A:330:ILE:HG22	1:A:355:MET:CE	2.49	0.42
1:A:334:ASP:OD1	1:A:334:ASP:C	2.57	0.42
1:B:51:ASN:N	1:B:51:ASN:HD22	2.17	0.42
1:B:243:GLY:C	1:B:245:ASN:H	2.23	0.42
1:C:391:ILE:HA	1:C:417:SER:O	2.19	0.42
1:D:313:GLY:CA	1:D:396:MET:HE1	2.48	0.42
1:E:235:ILE:CG2	1:E:236:GLN:N	2.82	0.42
1:E:287:VAL:HG12	1:E:288:THR:N	2.33	0.42
1:F:435:ARG:HH11	1:F:435:ARG:CG	2.26	0.42
1:A:45:THR:HG23	1:A:304:GLU:HB2	2.01	0.42
1:A:89:THR:HG22	1:A:281:GLN:NE2	2.35	0.42
1:A:400:ARG:HG3	1:A:400:ARG:HH11	1.84	0.42
1:A:432:ILE:HD13	1:A:434:LEU:HD13	1.99	0.42
1:B:253:LEU:HD21	1:B:289:LEU:HB3	2.02	0.42
1:C:262:SER:HA	1:C:341:THR:HG21	2.00	0.42
1:D:88:LEU:HD23	1:D:88:LEU:HA	1.80	0.42
1:D:386:LEU:CD1	1:D:387:LYS:HG3	2.49	0.42
1:E:37:LEU:HD23	1:E:37:LEU:N	2.33	0.42
1:E:200:ILE:HD13	1:F:200:ILE:HG22	2.00	0.42
1:E:239:TYR:CE2	1:E:244:GLY:HA2	2.54	0.42
1:E:318:LEU:HD13	1:E:318:LEU:HA	1.85	0.42
1:E:448:ILE:HG22	1:E:449:SER:N	2.34	0.42
1:F:88:LEU:HB3	1:F:281:GLN:NE2	2.35	0.42
1:F:281:GLN:OE1	1:F:281:GLN:HA	2.19	0.42
1:F:328:SER:O	1:F:360:TYR:OH	2.33	0.42
1:A:381:THR:OG1	1:A:383:TYR:CE2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:SER:HA	1:D:228:PRO:HD3	1.71	0.42
1:E:79:ALA:HB3	1:E:80:PRO:CD	2.50	0.42
1:E:175:LEU:HD11	1:F:176:ALA:HA	2.01	0.42
1:E:410:GLN:HB2	1:E:414:GLU:CD	2.39	0.42
1:F:235:ILE:CG2	1:F:236:GLN:N	2.82	0.42
1:A:172:LEU:CD2	1:C:172:LEU:H	2.33	0.42
1:A:421:ARG:HG2	1:A:421:ARG:HH11	1.84	0.42
1:B:43:VAL:HG12	1:B:304:GLU:HB3	2.01	0.42
1:C:334:ASP:OD2	1:C:337:TYR:HE1	2.02	0.42
1:D:73:LYS:HD3	1:E:450:ILE:HD11	2.01	0.42
1:D:226:THR:HA	1:E:236:GLN:HE21	1.79	0.42
1:D:334:ASP:C	1:D:334:ASP:OD1	2.57	0.42
1:E:429:LEU:HD22	1:E:429:LEU:N	2.31	0.42
1:A:337:TYR:HB3	1:A:348:THR:HG23	2.02	0.42
1:C:407:ILE:O	1:C:408:ILE:C	2.58	0.42
1:D:279:GLN:OE1	2:L:2:NAG:H4	2.20	0.42
1:D:324:THR:HB	1:D:333:LEU:HD12	2.02	0.42
1:E:58:THR:OG1	1:E:59:GLY:N	2.53	0.42
1:F:42:ILE:HA	1:F:305:THR:HG22	2.01	0.42
1:A:259:GLN:O	1:A:263:LEU:HB2	2.19	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.88	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.77	0.42
1:B:325:GLN:HB2	1:B:329:VAL:O	2.19	0.42
1:B:424:CYS:SG	1:B:425:ASN:N	2.93	0.42
1:C:210:LEU:HD12	1:C:210:LEU:HA	1.87	0.42
1:E:396:MET:O	1:E:397:THR:HG23	2.19	0.42
1:F:182:MET:SD	1:F:183:GLN:N	2.93	0.42
1:A:184:GLN:CD	1:A:185:PHE:N	2.73	0.42
1:A:197:LEU:HD21	1:C:197:LEU:HD23	2.02	0.42
1:A:243:GLY:C	1:A:245:ASN:H	2.22	0.42
1:A:381:THR:HA	1:A:382:PRO:HD2	1.89	0.42
1:C:447:ASN:N	4:C:4471:NAG:H82	2.35	0.42
1:D:36:PRO:HD2	1:D:37:LEU:HD23	2.02	0.42
1:D:39:ALA:HA	1:D:415:ALA:HB3	2.02	0.42
1:D:172:LEU:O	1:D:176:ALA:HB2	2.20	0.42
1:E:77:ALA:O	1:E:80:PRO:HD2	2.19	0.42
1:E:350:ILE:N	1:F:381:THR:CG2	2.82	0.42
1:F:402:ALA:HB3	1:F:426:ILE:CG2	2.50	0.42
1:A:95:LEU:HD21	1:A:273:PRO:HG3	2.01	0.42
1:A:352:THR:OG1	1:B:380:THR:HG22	2.20	0.42
1:A:379:LEU:HD13	1:C:326:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HB3	1:C:190:PHE:CE2	2.55	0.42
1:B:255:VAL:HG12	1:B:259:GLN:OE1	2.19	0.42
1:C:224:GLN:HG2	1:C:285:ILE:CD1	2.50	0.42
1:C:311:THR:HG23	1:C:315:ALA:HB2	2.02	0.42
1:C:325:GLN:HE21	1:C:325:GLN:HB2	1.69	0.42
1:D:213:TYR:CZ	1:D:217:LEU:HD13	2.54	0.42
1:D:411:ASN:OD1	1:D:411:ASN:C	2.58	0.42
1:F:44:VAL:HG22	1:F:303:LEU:HD21	2.02	0.42
1:F:400:ARG:NH1	1:F:400:ARG:CB	2.83	0.42
1:A:236:GLN:HE21	1:C:226:THR:HA	1.85	0.41
1:A:242:ALA:O	1:A:243:GLY:C	2.58	0.41
1:A:340:GLU:HB2	1:A:345:LEU:HD12	2.02	0.41
1:A:403:ASP:O	1:A:405:PRO:N	2.53	0.41
1:A:440:PHE:HB3	1:C:241:LEU:HD11	2.02	0.41
1:B:54:THR:HA	1:C:385:THR:HG21	2.02	0.41
1:B:182:MET:HG3	1:C:182:MET:SD	2.60	0.41
1:D:101:ARG:NH1	1:E:257:ASN:HD21	2.18	0.41
1:D:210:LEU:HD12	1:D:210:LEU:HA	1.82	0.41
1:D:355:MET:CE	1:D:363:LEU:HD12	2.50	0.41
1:B:72:ASP:O	1:B:74:GLU:N	2.52	0.41
1:B:355:MET:HE1	1:B:363:LEU:HD12	2.02	0.41
1:D:403:ASP:O	1:D:404:PRO:C	2.57	0.41
1:E:183:GLN:O	1:E:186:VAL:HG22	2.20	0.41
1:E:352:THR:OG1	1:F:380:THR:HG22	2.20	0.41
1:F:47:ASP:OD1	1:F:47:ASP:C	2.58	0.41
1:F:191:ASN:O	1:F:195:GLN:HG3	2.20	0.41
1:A:438:GLY:O	1:A:439:GLU:HG3	2.20	0.41
1:B:54:THR:CG2	1:C:388:GLY:HA2	2.42	0.41
1:B:249:LEU:HD12	1:C:440:PHE:CE2	2.55	0.41
1:B:355:MET:HE3	1:B:359:ILE:HG22	2.01	0.41
1:B:366:ASN:OD1	1:B:368:SER:N	2.53	0.41
1:B:386:LEU:CD1	1:B:387:LYS:HG3	2.48	0.41
1:B:403:ASP:OD2	1:B:425:ASN:CB	2.68	0.41
1:C:184:GLN:O	1:C:187:ASN:HB2	2.20	0.41
1:D:361:SER:HB3	1:D:369:ALA:CB	2.50	0.41
1:D:432:ILE:HG23	1:F:295:LEU:HD23	2.01	0.41
1:A:202:ILE:HD11	1:B:450:ILE:CD1	2.49	0.41
1:B:248:TYR:O	1:B:251:THR:HB	2.20	0.41
1:C:45:THR:HG23	1:C:304:GLU:HB2	2.02	0.41
1:C:191:ASN:O	1:C:195:GLN:HG3	2.21	0.41
1:C:356:SER:HB3	1:C:359:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HA	1:E:305:THR:HG22	2.03	0.41
1:E:325:GLN:HB2	1:E:329:VAL:O	2.19	0.41
1:F:213:TYR:CZ	1:F:217:LEU:HD13	2.56	0.41
1:A:34:GLY:O	1:A:37:LEU:HD21	2.20	0.41
1:A:50:VAL:HG11	1:A:350:ILE:HD11	2.02	0.41
1:A:185:PHE:CD2	1:A:186:VAL:N	2.89	0.41
1:B:199:CYS:O	1:B:202:ILE:HG22	2.20	0.41
1:B:410:GLN:O	1:B:411:ASN:CG	2.59	0.41
1:D:381:THR:HG22	1:F:350:ILE:H	1.83	0.41
1:D:398:THR:HG22	1:D:400:ARG:HG2	2.01	0.41
1:F:84:TYR:O	1:F:86:ARG:N	2.53	0.41
1:A:51:ASN:HB3	1:A:294:ASN:HA	2.02	0.41
1:A:182:MET:SD	1:C:182:MET:CG	3.08	0.41
1:A:197:LEU:HD21	1:C:197:LEU:HD21	2.03	0.41
1:B:101:ARG:HD3	1:C:257:ASN:ND2	2.35	0.41
1:B:252:LYS:NZ	1:B:252:LYS:HB3	2.35	0.41
1:C:341:THR:HB	1:C:344:ASP:O	2.21	0.41
1:E:394:CYS:SG	1:E:417:SER:OG	2.72	0.41
1:F:443:THR:HG22	1:F:444:TYR:N	2.35	0.41
1:B:79:ALA:HB3	1:B:80:PRO:CD	2.51	0.41
1:C:318:LEU:CD2	1:C:371:MET:O	2.68	0.41
1:C:412:TYR:CZ	1:D:421:ARG:NH2	2.89	0.41
1:C:421:ARG:HB2	1:C:421:ARG:HH11	1.86	0.41
1:D:372:TYR:N	1:D:372:TYR:HD1	2.09	0.41
1:E:52:ILE:HA	1:E:347:CYS:O	2.21	0.41
1:E:73:LYS:N	1:E:73:LYS:CD	2.83	0.41
1:E:172:LEU:CA	1:F:172:LEU:HD21	2.51	0.41
1:E:248:TYR:OH	1:E:252:LYS:HE3	2.21	0.41
1:F:393:ASN:O	1:F:395:LYS:N	2.52	0.41
1:B:213:TYR:CE1	1:C:446:LYS:HB2	2.56	0.41
1:E:61:ILE:HD11	1:E:241:LEU:HB2	2.03	0.41
1:F:356:SER:HB3	1:F:359:ILE:HG12	2.03	0.41
1:A:176:ALA:HA	1:C:175:LEU:CD1	2.51	0.41
1:A:195:GLN:H	1:A:195:GLN:HG3	1.66	0.41
1:A:235:ILE:HG22	1:A:236:GLN:NE2	2.35	0.41
1:A:325:GLN:HB2	1:A:325:GLN:HE21	1.59	0.41
1:A:403:ASP:HB3	1:A:425:ASN:HB3	2.03	0.41
1:B:89:THR:HG21	2:I:1:NAG:H62	2.03	0.41
1:B:417:SER:HB2	1:B:419:ILE:CD1	2.50	0.41
1:B:418:LEU:HD23	1:B:418:LEU:O	2.21	0.41
1:D:64:LYS:HD3	1:E:445:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:THR:HG21	1:F:91:LEU:HD21	2.02	0.41
1:D:235:ILE:HG22	1:D:236:GLN:NE2	2.35	0.41
1:E:54:THR:CG2	1:F:388:GLY:CA	2.93	0.41
1:E:102:ILE:CD1	1:E:228:PRO:HB2	2.50	0.41
1:E:400:ARG:CB	1:E:400:ARG:NH1	2.84	0.41
1:F:66:LEU:HD23	1:F:66:LEU:HA	1.88	0.41
1:F:294:ASN:OD1	1:F:295:LEU:O	2.38	0.41
1:F:377:GLY:H	1:F:380:THR:HG21	1.85	0.41
1:F:393:ASN:C	1:F:395:LYS:H	2.24	0.41
2:G:2:NAG:O7	2:G:2:NAG:C3	2.69	0.41
1:B:54:THR:HG23	1:C:385:THR:HG23	2.03	0.41
1:C:87:THR:HA	1:C:90:THR:HB	2.02	0.41
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.21	0.41
1:C:312:LYS:CG	1:C:314:PHE:HB2	2.32	0.41
1:C:408:ILE:O	1:C:408:ILE:HG22	2.21	0.41
1:C:447:ASN:CB	4:C:4471:NAG:N2	2.83	0.41
1:D:314:PHE:O	1:D:374:LYS:HB3	2.21	0.41
1:D:350:ILE:O	1:E:380:THR:HA	2.21	0.41
1:E:175:LEU:CD1	1:F:176:ALA:HA	2.51	0.41
1:E:201:LYS:HD3	1:F:453:SER:CB	2.51	0.41
1:E:243:GLY:C	1:E:245:ASN:H	2.24	0.41
1:F:44:VAL:HG22	1:F:303:LEU:CD2	2.51	0.41
1:F:419:ILE:CD1	1:F:427:LEU:HD11	2.48	0.41
1:A:52:ILE:HA	1:A:347:CYS:O	2.21	0.40
1:B:43:VAL:HG11	1:B:384:MET:SD	2.61	0.40
1:B:410:GLN:O	1:B:411:ASN:ND2	2.54	0.40
1:C:370:CYS:HB3	1:C:372:TYR:CE1	2.55	0.40
1:C:408:ILE:HD13	1:C:419:ILE:HG12	2.03	0.40
1:D:274:ILE:HG12	1:D:284:GLY:O	2.21	0.40
1:E:79:ALA:HB3	1:E:80:PRO:HD3	2.04	0.40
1:E:182:MET:CG	1:F:182:MET:SD	3.08	0.40
1:E:224:GLN:CB	1:E:285:ILE:HD11	2.51	0.40
1:F:76:CYS:HB3	1:F:203:THR:HG22	2.00	0.40
1:F:419:ILE:HG21	1:F:427:LEU:HG	2.02	0.40
1:A:200:ILE:CG2	1:C:200:ILE:HD13	2.51	0.40
1:B:45:THR:HA	1:B:386:LEU:HD21	2.02	0.40
1:B:93:THR:HB	1:B:94:PRO:HD3	2.03	0.40
1:B:182:MET:HE3	1:B:182:MET:HB3	1.98	0.40
1:B:202:ILE:HD11	1:C:450:ILE:HD13	2.03	0.40
1:B:224:GLN:HG2	1:B:285:ILE:CD1	2.51	0.40
1:C:36:PRO:CD	1:C:37:LEU:H	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:ARG:CB	1:D:435:ARG:HH11	2.35	0.40
1:E:223:PRO:HB2	1:E:224:GLN:NE2	2.36	0.40
1:E:330:ILE:O	1:E:330:ILE:HG22	2.21	0.40
1:A:181:LYS:O	1:A:182:MET:C	2.59	0.40
1:A:325:GLN:O	1:A:325:GLN:HG3	2.22	0.40
1:C:35:ARG:HH22	1:C:418:LEU:HD13	1.84	0.40
1:C:238:LEU:O	1:C:239:TYR:C	2.60	0.40
1:D:340:GLU:O	1:D:340:GLU:CG	2.69	0.40
1:E:213:TYR:CE1	1:F:446:LYS:HB2	2.57	0.40
1:A:356:SER:HB3	1:A:359:ILE:CG1	2.50	0.40
1:B:400:ARG:HB2	1:B:400:ARG:NH1	2.36	0.40
1:D:63:ILE:HD11	1:D:221:PHE:CG	2.57	0.40
1:D:95:LEU:O	1:D:95:LEU:HD22	2.22	0.40
1:D:190:PHE:O	1:D:194:ALA:N	2.54	0.40
1:D:427:LEU:HD13	1:D:429:LEU:HD13	2.02	0.40
1:E:63:ILE:HB	1:E:283:LEU:HB3	2.02	0.40
1:A:252:LYS:HB3	1:A:252:LYS:HZ3	1.85	0.40
1:A:380:THR:HA	1:C:350:ILE:O	2.21	0.40
1:B:325:GLN:HB2	1:B:325:GLN:HE21	1.69	0.40
1:B:401:CYS:O	1:B:405:PRO:HA	2.22	0.40
1:B:427:LEU:HD13	1:B:429:LEU:HD11	2.04	0.40
1:C:235:ILE:HD12	1:C:235:ILE:HA	1.89	0.40
1:E:35:ARG:N	1:E:36:PRO:CD	2.84	0.40
1:E:48:LYS:HE2	1:E:342:ASP:O	2.22	0.40
1:E:51:ASN:N	1:E:51:ASN:HD22	2.19	0.40
1:E:447:ASN:O	4:E:4471:NAG:C8	2.69	0.40
1:F:255:VAL:HG12	1:F:259:GLN:OE1	2.21	0.40
1:F:414:GLU:O	1:F:415:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/481 (73%)	304 (86%)	40 (11%)	9 (2%)	5	27
1	B	353/481 (73%)	299 (85%)	40 (11%)	14 (4%)	3	18
1	C	353/481 (73%)	290 (82%)	56 (16%)	7 (2%)	7	32
1	D	353/481 (73%)	299 (85%)	48 (14%)	6 (2%)	9	35
1	E	353/481 (73%)	302 (86%)	40 (11%)	11 (3%)	4	23
1	F	353/481 (73%)	289 (82%)	56 (16%)	8 (2%)	6	29
All	All	2118/2886 (73%)	1783 (84%)	280 (13%)	55 (3%)	5	27

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ASP
1	B	403	ASP
1	B	412	TYR
1	C	403	ASP
1	D	310	THR
1	D	394	CYS
1	D	403	ASP
1	E	403	ASP
1	E	412	TYR
1	E	430	ASP
1	F	394	CYS
1	F	403	ASP
1	F	412	TYR
1	A	258	ASN
1	A	310	THR
1	B	73	LYS
1	B	310	THR
1	B	316	SER
1	C	310	THR
1	C	317	ALA
1	C	412	TYR
1	D	258	ASN
1	E	310	THR
1	E	316	SER
1	E	317	ALA
1	E	419	ILE
1	F	258	ASN
1	A	394	CYS
1	A	403	ASP
1	B	415	ALA

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Mol	Chain	Res	Type
1	B	430	ASP
1	C	430	ASP
1	F	313	GLY
1	F	317	ALA
1	A	330	ILE
1	A	419	ILE
1	B	313	GLY
1	C	72	ASP
1	D	312	LYS
1	D	330	ILE
1	A	72	ASP
1	A	312	LYS
1	B	317	ALA
1	B	419	ILE
1	F	85	ASN
1	C	419	ILE
1	E	313	GLY
1	F	312	LYS
1	A	244	GLY
1	B	405	PRO
1	B	426	ILE
1	E	244	GLY
1	E	404	PRO
1	E	330	ILE
1	B	244	GLY

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	307/406 (76%)	254 (83%)	53 (17%)	2 8
1	B	307/406 (76%)	256 (83%)	51 (17%)	2 10
1	C	307/406 (76%)	250 (81%)	57 (19%)	1 7
1	D	307/406 (76%)	249 (81%)	58 (19%)	1 6
1	E	307/406 (76%)	260 (85%)	47 (15%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	307/406 (76%)	251 (82%)	56 (18%)	1 7
All	All	1842/2436 (76%)	1520 (82%)	322 (18%)	2 8

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	43	VAL
1	A	47	ASP
1	A	51	ASN
1	A	57	GLN
1	A	58	THR
1	A	74	GLU
1	A	78	LYS
1	A	90	THR
1	A	95	LEU
1	A	172	LEU
1	A	183	GLN
1	A	184	GLN
1	A	188	ASP
1	A	190	PHE
1	A	192	LYS
1	A	195	GLN
1	A	196	GLU
1	A	197	LEU
1	A	199	CYS
1	A	215	THR
1	A	226	THR
1	A	231	THR
1	A	232	GLN
1	A	236	GLN
1	A	240	ASN
1	A	251	THR
1	A	266	SER
1	A	318	LEU
1	A	322	VAL
1	A	325	GLN
1	A	329	VAL
1	A	340	GLU
1	A	348	THR
1	A	349	ARG
1	A	350	ILE

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Mol	Chain	Res	Type
1	A	375	THR
1	A	376	GLU
1	A	380	THR
1	A	389	SER
1	A	390	VAL
1	A	407	ILE
1	A	422	GLN
1	A	427	LEU
1	A	430	ASP
1	A	434	LEU
1	A	436	LEU
1	A	437	SER
1	A	441	ASP
1	A	449	SER
1	A	451	GLN
1	A	452	ASP
1	A	454	GLN
1	B	37	LEU
1	B	43	VAL
1	B	51	ASN
1	B	58	THR
1	B	71	LYS
1	B	73	LYS
1	B	82	GLU
1	B	90	THR
1	B	172	LEU
1	B	183	GLN
1	B	184	GLN
1	B	188	ASP
1	B	192	LYS
1	B	195	GLN
1	B	196	GLU
1	B	197	LEU
1	B	199	CYS
1	B	215	THR
1	B	226	THR
1	B	231	THR
1	B	232	GLN
1	B	236	GLN
1	B	251	THR
1	B	266	SER
1	B	292	VAL

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Mol	Chain	Res	Type
1	B	318	LEU
1	B	325	GLN
1	B	329	VAL
1	B	341	THR
1	B	348	THR
1	B	349	ARG
1	B	355	MET
1	B	370	CYS
1	B	372	TYR
1	B	376	GLU
1	B	380	THR
1	B	381	THR
1	B	386	LEU
1	B	390	VAL
1	B	395	LYS
1	B	396	MET
1	B	400	ARG
1	B	416	VAL
1	B	417	SER
1	B	433	THR
1	B	434	LEU
1	B	435	ARG
1	B	441	ASP
1	B	445	GLN
1	B	451	GLN
1	B	452	ASP
1	C	37	LEU
1	C	43	VAL
1	C	47	ASP
1	C	51	ASN
1	C	58	THR
1	C	74	GLU
1	C	82	GLU
1	C	172	LEU
1	C	183	GLN
1	C	184	GLN
1	C	188	ASP
1	C	190	PHE
1	C	192	LYS
1	C	195	GLN
1	C	196	GLU
1	C	197	LEU

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Mol	Chain	Res	Type
1	C	198	ASP
1	C	199	CYS
1	C	215	THR
1	C	226	THR
1	C	231	THR
1	C	232	GLN
1	C	236	GLN
1	C	251	THR
1	C	266	SER
1	C	292	VAL
1	C	311	THR
1	C	318	LEU
1	C	322	VAL
1	C	325	GLN
1	C	329	VAL
1	C	336	SER
1	C	348	THR
1	C	349	ARG
1	C	355	MET
1	C	360	TYR
1	C	370	CYS
1	C	372	TYR
1	C	376	GLU
1	C	380	THR
1	C	390	VAL
1	C	396	MET
1	C	397	THR
1	C	400	ARG
1	C	408	ILE
1	C	420	ASP
1	C	422	GLN
1	C	427	LEU
1	C	429	LEU
1	C	434	LEU
1	C	435	ARG
1	C	439	GLU
1	C	441	ASP
1	C	445	GLN
1	C	449	SER
1	C	452	ASP
1	C	453	SER
1	D	37	LEU

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Mol	Chain	Res	Type
1	D	43	VAL
1	D	47	ASP
1	D	51	ASN
1	D	57	GLN
1	D	58	THR
1	D	74	GLU
1	D	78	LYS
1	D	90	THR
1	D	172	LEU
1	D	183	GLN
1	D	184	GLN
1	D	188	ASP
1	D	190	PHE
1	D	192	LYS
1	D	195	GLN
1	D	196	GLU
1	D	197	LEU
1	D	199	CYS
1	D	206	VAL
1	D	215	THR
1	D	226	THR
1	D	231	THR
1	D	232	GLN
1	D	236	GLN
1	D	240	ASN
1	D	251	THR
1	D	266	SER
1	D	275	LEU
1	D	298	MET
1	D	314	PHE
1	D	318	LEU
1	D	322	VAL
1	D	325	GLN
1	D	329	VAL
1	D	340	GLU
1	D	348	THR
1	D	349	ARG
1	D	350	ILE
1	D	355	MET
1	D	370	CYS
1	D	372	TYR
1	D	375	THR

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Mol	Chain	Res	Type
1	D	376	GLU
1	D	380	THR
1	D	389	SER
1	D	396	MET
1	D	418	LEU
1	D	425	ASN
1	D	427	LEU
1	D	429	LEU
1	D	434	LEU
1	D	436	LEU
1	D	437	SER
1	D	441	ASP
1	D	449	SER
1	D	451	GLN
1	D	452	ASP
1	E	37	LEU
1	E	43	VAL
1	E	51	ASN
1	E	58	THR
1	E	71	LYS
1	E	73	LYS
1	E	82	GLU
1	E	90	THR
1	E	172	LEU
1	E	183	GLN
1	E	184	GLN
1	E	188	ASP
1	E	192	LYS
1	E	195	GLN
1	E	196	GLU
1	E	197	LEU
1	E	199	CYS
1	E	215	THR
1	E	226	THR
1	E	231	THR
1	E	232	GLN
1	E	236	GLN
1	E	251	THR
1	E	266	SER
1	E	292	VAL
1	E	318	LEU
1	E	325	GLN

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Mol	Chain	Res	Type
1	E	329	VAL
1	E	341	THR
1	E	348	THR
1	E	349	ARG
1	E	355	MET
1	E	370	CYS
1	E	372	TYR
1	E	376	GLU
1	E	380	THR
1	E	381	THR
1	E	390	VAL
1	E	395	LYS
1	E	427	LEU
1	E	429	LEU
1	E	430	ASP
1	E	435	ARG
1	E	441	ASP
1	E	445	GLN
1	E	451	GLN
1	E	452	ASP
1	F	37	LEU
1	F	43	VAL
1	F	47	ASP
1	F	51	ASN
1	F	58	THR
1	F	74	GLU
1	F	82	GLU
1	F	172	LEU
1	F	183	GLN
1	F	184	GLN
1	F	188	ASP
1	F	190	PHE
1	F	192	LYS
1	F	195	GLN
1	F	196	GLU
1	F	197	LEU
1	F	198	ASP
1	F	199	CYS
1	F	215	THR
1	F	226	THR
1	F	231	THR
1	F	232	GLN

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Mol	Chain	Res	Type
1	F	236	GLN
1	F	251	THR
1	F	266	SER
1	F	275	LEU
1	F	290	PRO
1	F	292	VAL
1	F	318	LEU
1	F	322	VAL
1	F	325	GLN
1	F	329	VAL
1	F	348	THR
1	F	349	ARG
1	F	355	MET
1	F	360	TYR
1	F	370	CYS
1	F	372	TYR
1	F	376	GLU
1	F	380	THR
1	F	390	VAL
1	F	397	THR
1	F	416	VAL
1	F	418	LEU
1	F	420	ASP
1	F	424	CYS
1	F	427	LEU
1	F	429	LEU
1	F	434	LEU
1	F	435	ARG
1	F	437	SER
1	F	439	GLU
1	F	441	ASP
1	F	445	GLN
1	F	449	SER
1	F	452	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	103	GLN
1	A	184	GLN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	224	GLN
1	A	236	GLN
1	A	257	ASN
1	A	286	GLN
1	A	325	GLN
1	A	422	GLN
1	B	57	GLN
1	B	103	GLN
1	B	184	GLN
1	B	187	ASN
1	B	205	GLN
1	B	211	ASN
1	B	224	GLN
1	B	236	GLN
1	B	257	ASN
1	B	286	GLN
1	B	325	GLN
1	B	410	GLN
1	B	451	GLN
1	C	57	GLN
1	C	103	GLN
1	C	184	GLN
1	C	205	GLN
1	C	236	GLN
1	C	257	ASN
1	C	325	GLN
1	C	422	GLN
1	C	445	GLN
1	D	57	GLN
1	D	103	GLN
1	D	184	GLN
1	D	205	GLN
1	D	224	GLN
1	D	232	GLN
1	D	236	GLN
1	D	257	ASN
1	D	286	GLN
1	D	325	GLN
1	D	425	ASN
1	E	57	GLN
1	E	103	GLN

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Mol	Chain	Res	Type
1	E	184	GLN
1	E	205	GLN
1	E	211	ASN
1	E	224	GLN
1	E	236	GLN
1	E	257	ASN
1	E	286	GLN
1	E	325	GLN
1	E	451	GLN
1	F	57	GLN
1	F	103	GLN
1	F	184	GLN
1	F	204	GLN
1	F	205	GLN
1	F	236	GLN
1	F	257	ASN
1	F	281	GLN
1	F	297	ASN
1	F	325	GLN
1	F	422	GLN
1	F	445	GLN

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)

17 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	$\#\|Z\|>2$
2	NAG	G	1	1,2	14,14,15	0.56	0	17,19,21	0.77	1 (5%)
2	NAG	G	2	2	14,14,15	0.48	0	17,19,21	0.66	0
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	0.66	0
3	NAG	H	2	3	14,14,15	1.06	1 (7%)	17,19,21	1.28	2 (11%)
3	BMA	H	3	3	11,11,12	0.59	0	15,15,17	0.61	0
2	NAG	I	1	1,2	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
2	NAG	I	2	2	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.83	0	17,19,21	1.22	3 (17%)
2	NAG	J	2	2	14,14,15	0.80	0	17,19,21	0.71	0
2	NAG	K	1	1,2	14,14,15	0.54	0	17,19,21	0.67	0
2	NAG	K	2	2	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.58	0	17,19,21	0.68	1 (5%)
2	NAG	L	2	2	14,14,15	0.66	0	17,19,21	0.68	0
2	NAG	M	1	1,2	14,14,15	0.66	0	17,19,21	0.63	0
2	NAG	M	2	2	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
2	NAG	N	1	1,2	14,14,15	0.56	0	17,19,21	0.71	0
2	NAG	N	2	2	14,14,15	0.52	0	17,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C1-C2	2.98	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	NAG	C1-O5-C5	2.72	115.88	112.19
3	H	2	NAG	O5-C1-C2	2.72	115.58	111.29
2	K	2	NAG	C2-N2-C7	-2.50	119.35	122.90
2	I	1	NAG	C2-N2-C7	-2.35	119.55	122.90
2	J	1	NAG	C4-C3-C2	-2.33	107.60	111.02
3	H	2	NAG	C1-O5-C5	2.29	115.30	112.19
2	M	2	NAG	C2-N2-C7	-2.20	119.78	122.90
2	J	1	NAG	C2-N2-C7	-2.19	119.78	122.90
2	I	2	NAG	C2-N2-C7	-2.10	119.91	122.90
2	G	1	NAG	C2-N2-C7	-2.10	119.91	122.90
2	L	1	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	M	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6

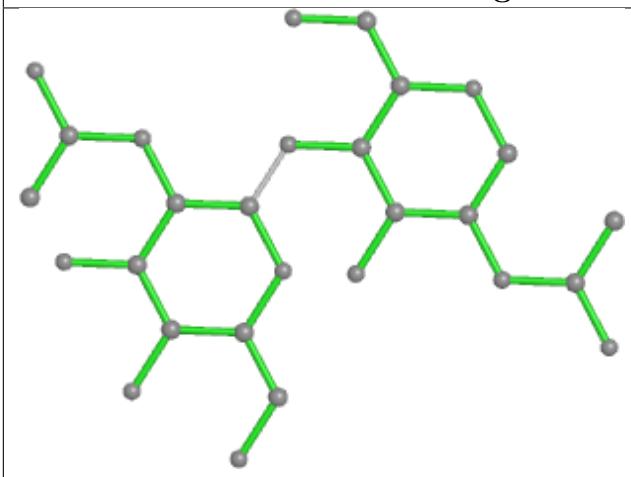
There are no ring outliers.

13 monomers are involved in 21 short contacts:

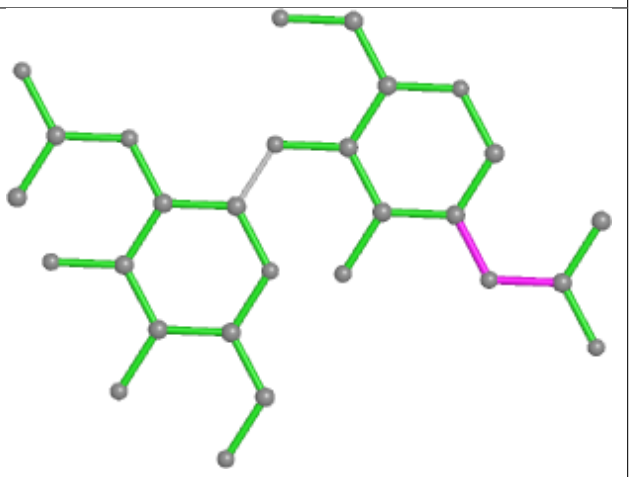
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	2	NAG	1	0
3	H	1	NAG	2	0
3	H	3	BMA	3	0
2	J	1	NAG	3	0
2	N	1	NAG	2	0
3	H	2	NAG	2	0
2	M	2	NAG	1	0
2	I	2	NAG	1	0
2	G	2	NAG	5	0
2	J	2	NAG	3	0
2	I	1	NAG	1	0
2	G	1	NAG	2	0
2	K	2	NAG	1	0

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

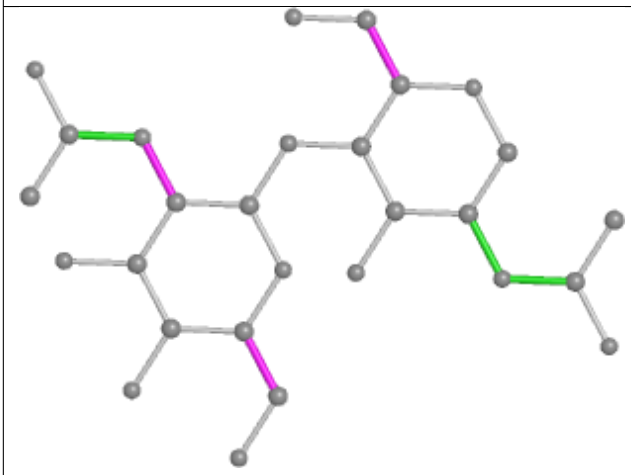
Oligosaccharide Chain G



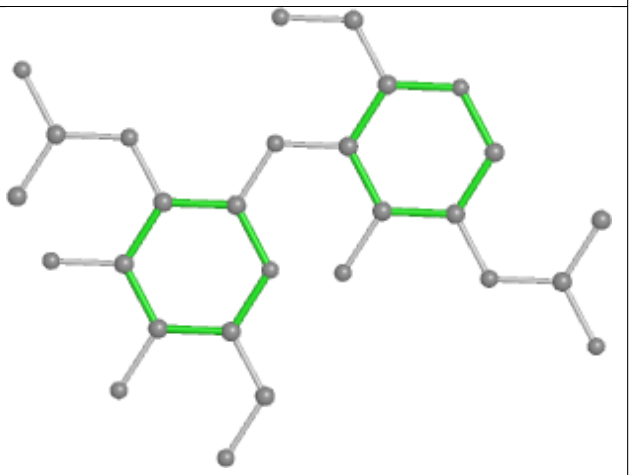
Bond lengths



Bond angles

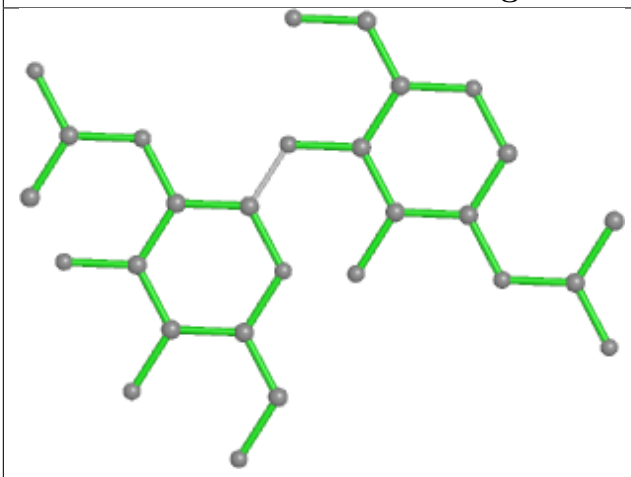


Torsions

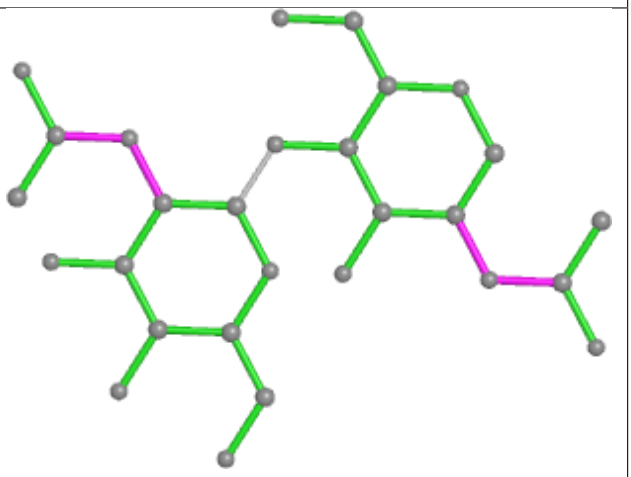


Rings

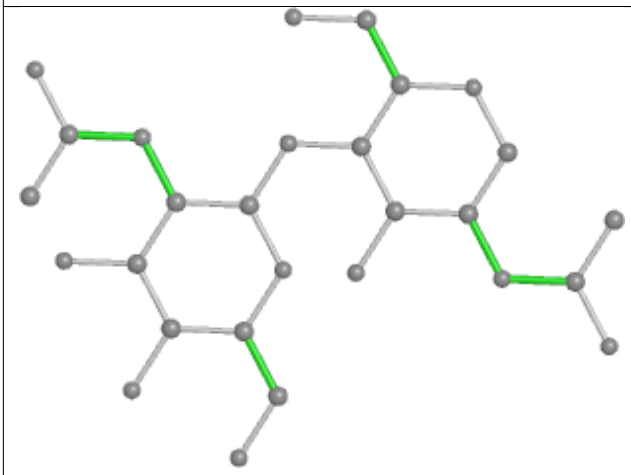
Oligosaccharide Chain I



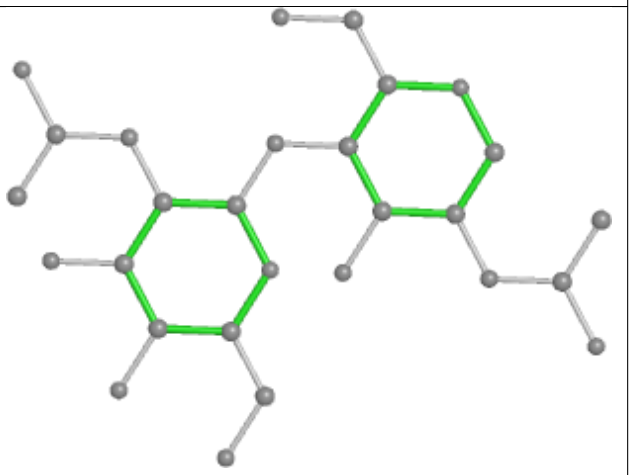
Bond lengths



Bond angles

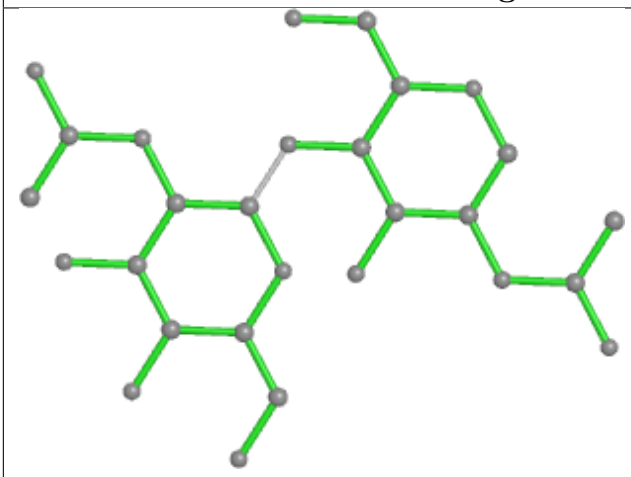


Torsions

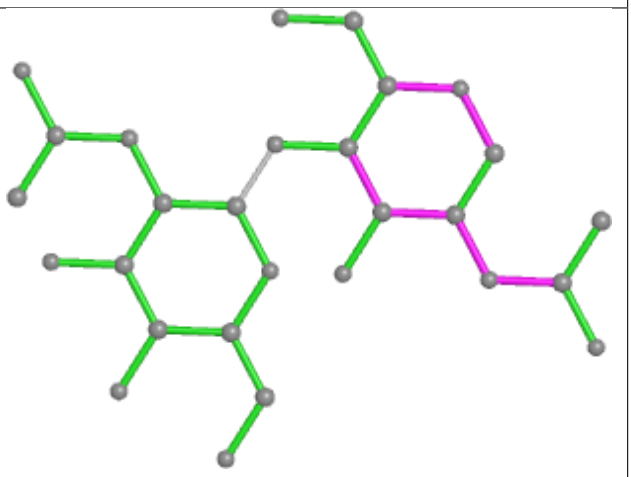


Rings

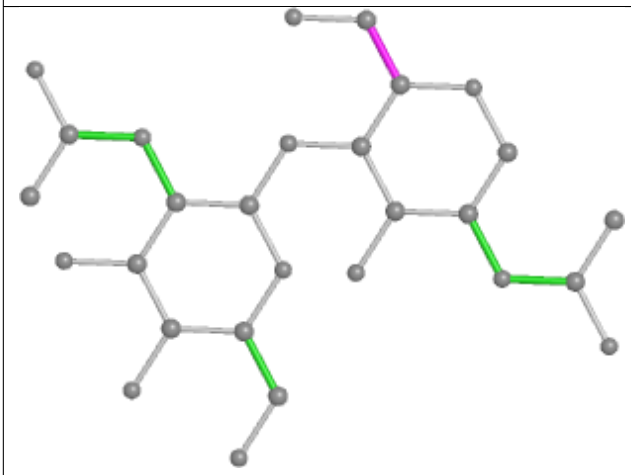
Oligosaccharide Chain J



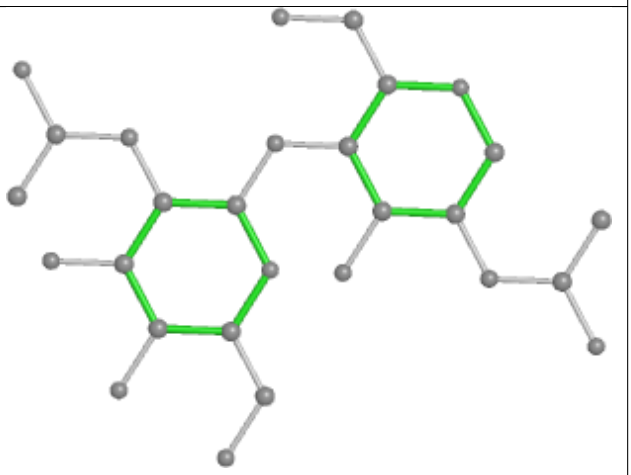
Bond lengths



Bond angles

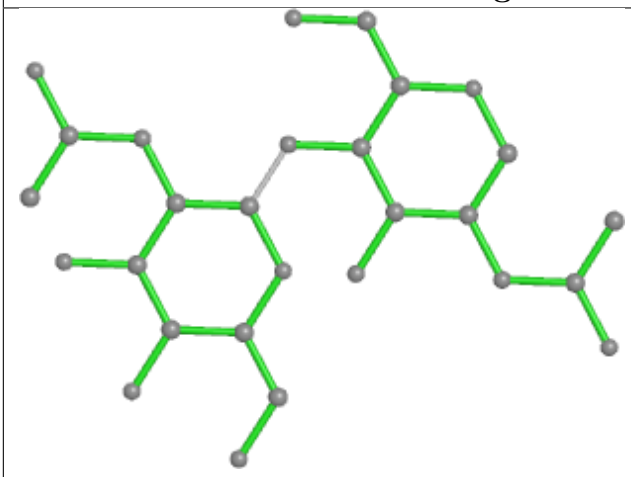


Torsions

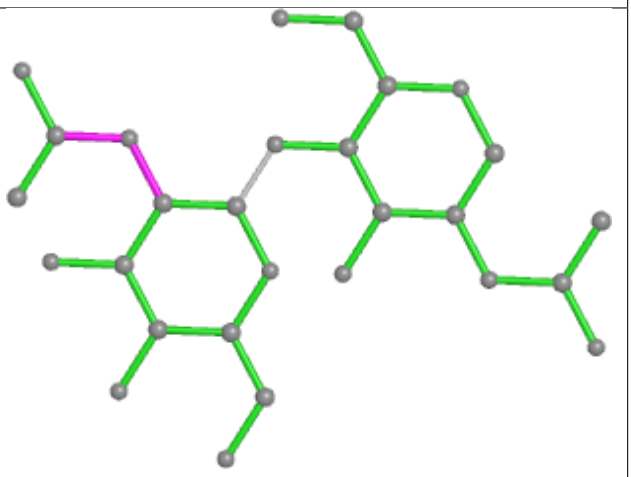


Rings

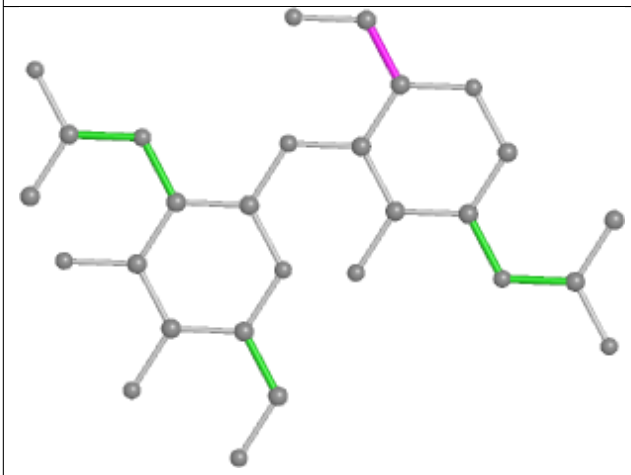
Oligosaccharide Chain K



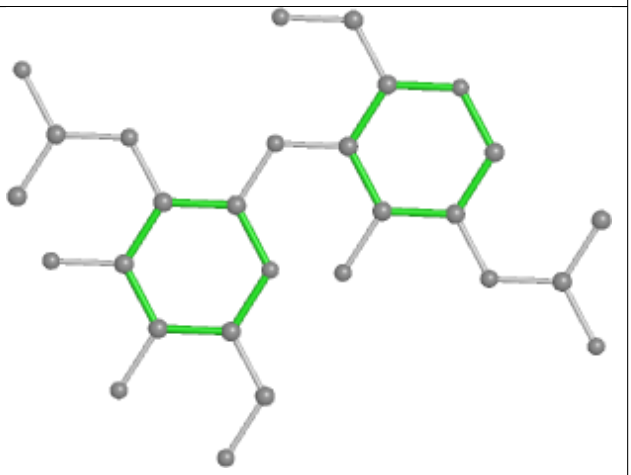
Bond lengths



Bond angles

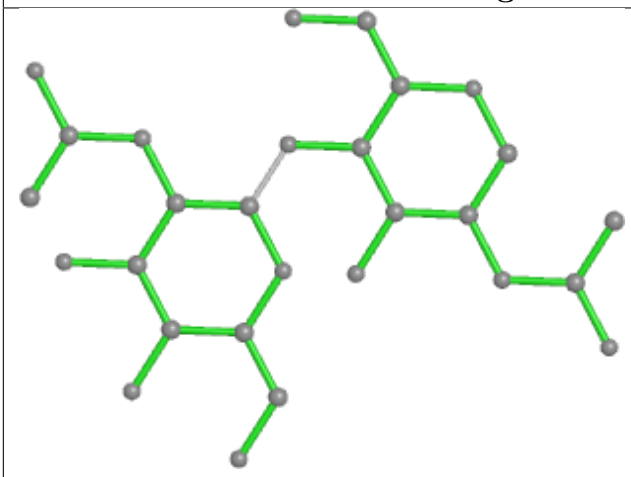


Torsions

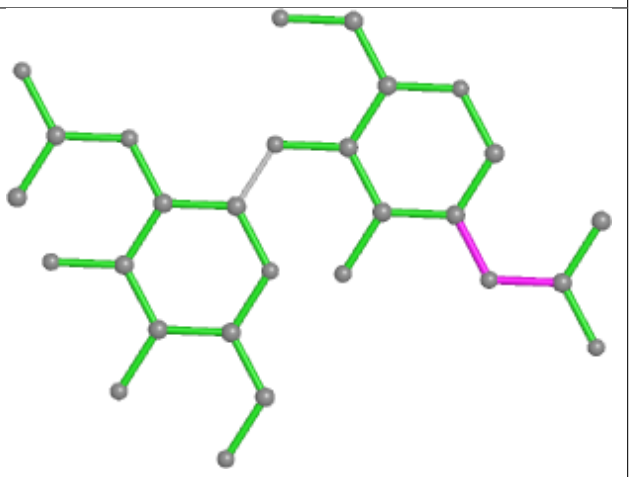


Rings

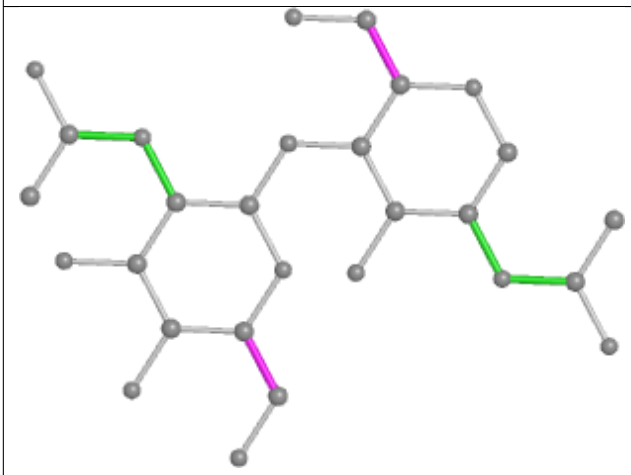
Oligosaccharide Chain L



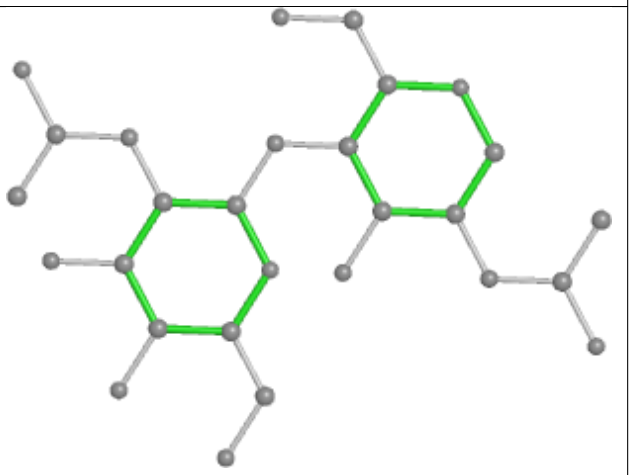
Bond lengths



Bond angles

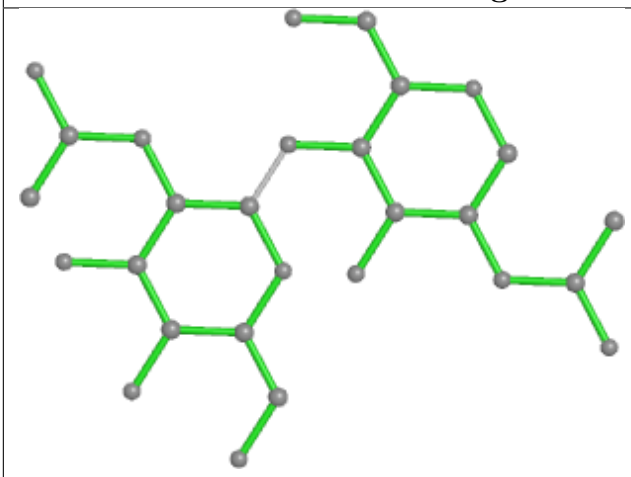


Torsions

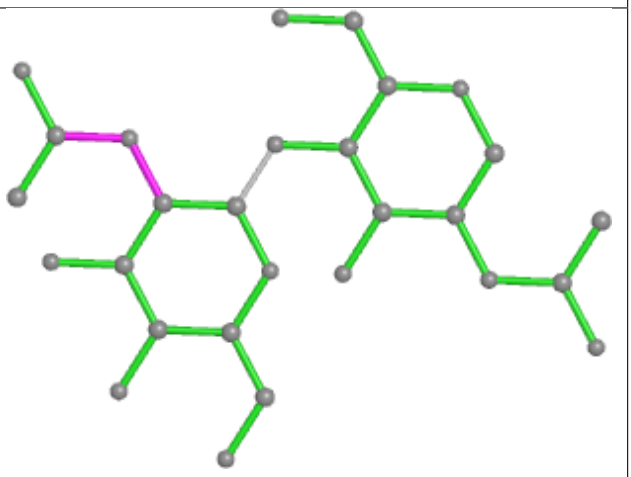


Rings

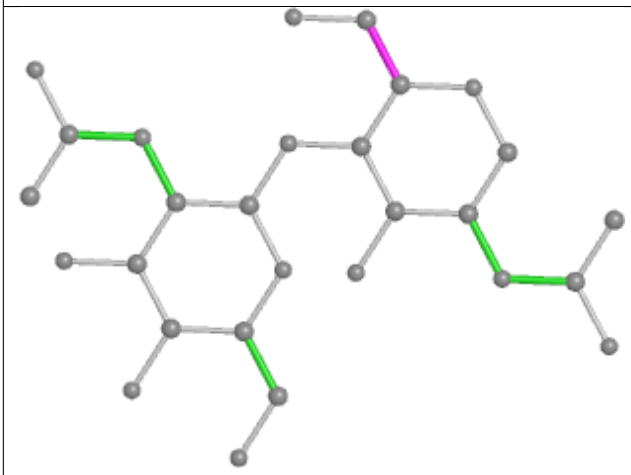
Oligosaccharide Chain M



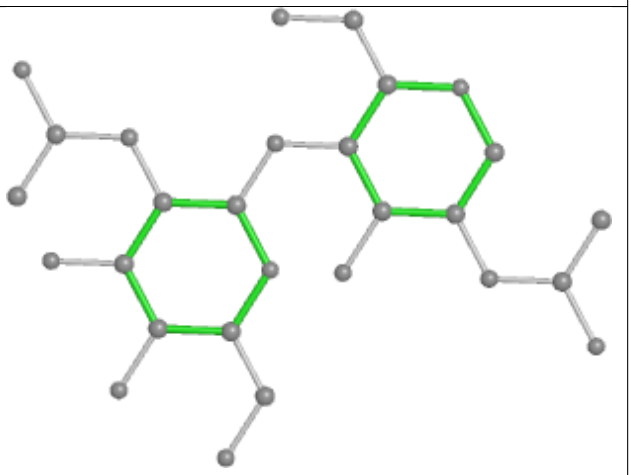
Bond lengths



Bond angles

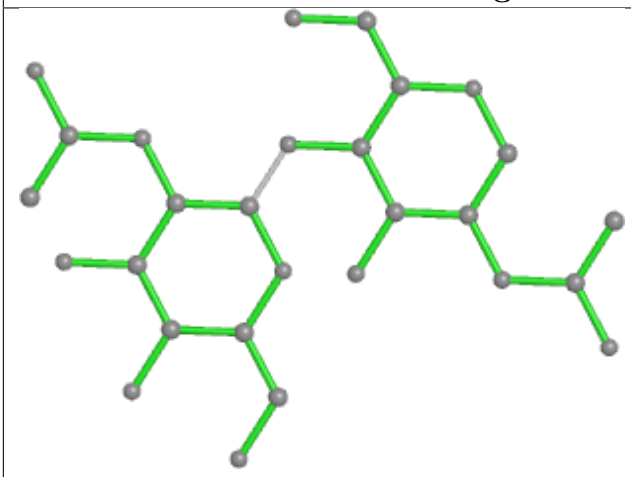


Torsions

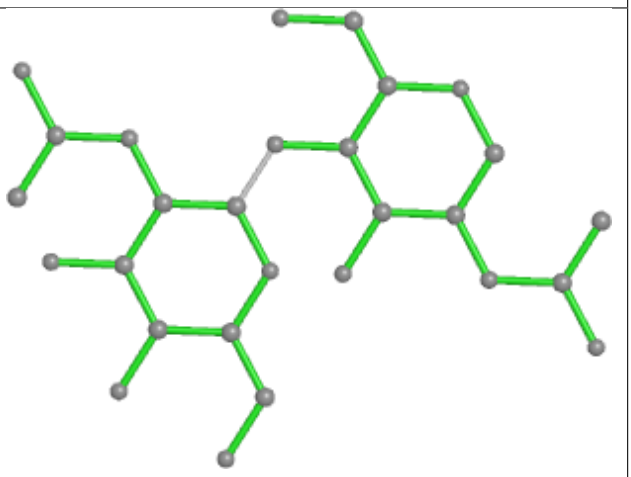


Rings

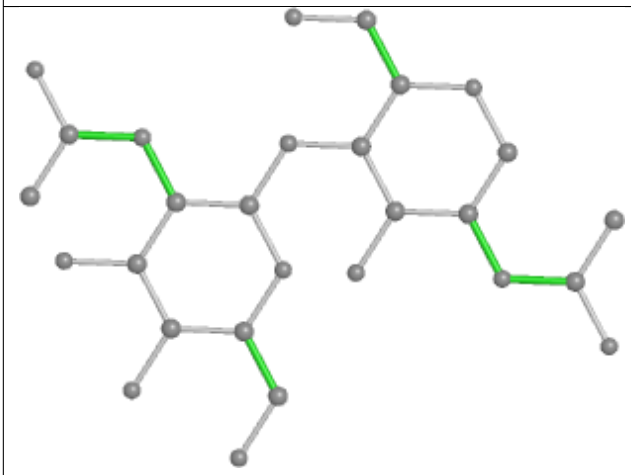
Oligosaccharide Chain N



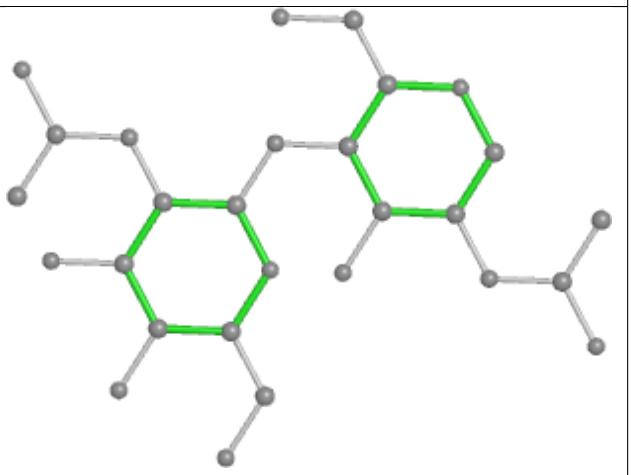
Bond lengths



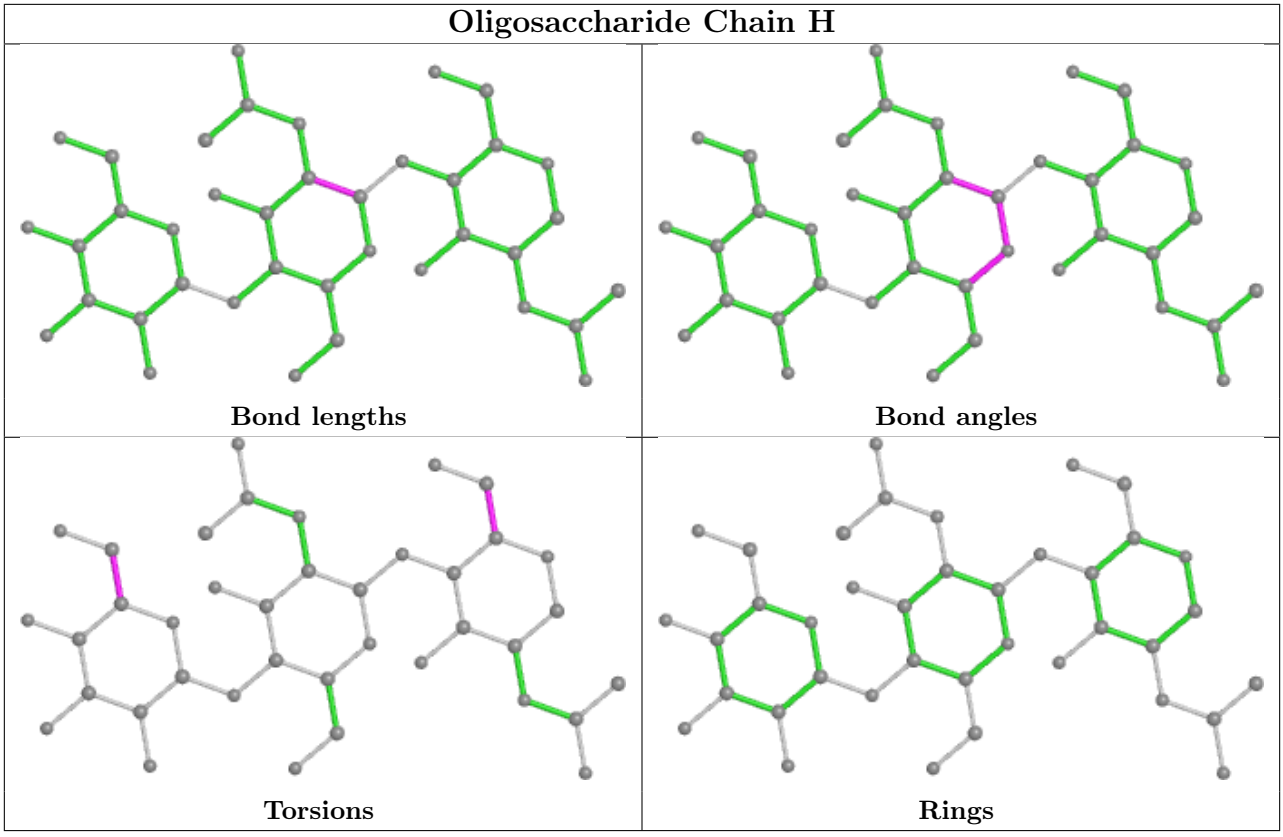
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1911	1	14,14,15	0.76	0	17,19,21	0.57	0
4	NAG	C	4471	1	14,14,15	0.53	0	17,19,21	0.65	1 (5%)
4	NAG	D	1911	1	14,14,15	0.55	0	17,19,21	0.66	0
4	NAG	E	4471	1	14,14,15	0.76	1 (7%)	17,19,21	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1911	1	-	2/6/23/26	0/1/1/1
4	NAG	C	4471	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1911	1	-	2/6/23/26	0/1/1/1
4	NAG	E	4471	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4471	NAG	C1-C2	2.02	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	4471	NAG	C2-N2-C7	-2.03	120.02	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	4471	NAG	O5-C5-C6-O6
4	F	1911	NAG	O5-C5-C6-O6
4	D	1911	NAG	O5-C5-C6-O6
4	E	4471	NAG	C4-C5-C6-O6
4	C	4471	NAG	O5-C5-C6-O6
4	C	4471	NAG	C4-C5-C6-O6
4	F	1911	NAG	C4-C5-C6-O6
4	D	1911	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4471	NAG	7	0
4	E	4471	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	357/481 (74%)	-0.24	12 (3%)	45	43	7, 34, 87, 100	0
1	B	357/481 (74%)	-0.20	10 (2%)	53	51	3, 35, 88, 100	0
1	C	357/481 (74%)	-0.21	14 (3%)	39	37	7, 33, 90, 100	0
1	D	357/481 (74%)	-0.25	13 (3%)	42	40	6, 33, 88, 100	0
1	E	357/481 (74%)	-0.19	11 (3%)	49	48	7, 34, 86, 100	0
1	F	357/481 (74%)	-0.25	6 (1%)	70	68	5, 33, 87, 99	0
All	All	2142/2886 (74%)	-0.22	66 (3%)	49	48	3, 34, 88, 100	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	173	SER	11.0
1	B	173	SER	4.8
1	F	174	GLN	4.1
1	E	172	LEU	4.1
1	C	173	SER	4.0
1	C	172	LEU	4.0
1	E	412	TYR	3.8
1	B	310	THR	3.8
1	C	314	PHE	3.8
1	F	173	SER	3.7
1	C	413	GLY	3.6
1	D	172	LEU	3.4
1	A	454	GLN	3.3
1	C	183	GLN	3.3
1	C	171	GLY	3.2
1	D	412	TYR	3.2
1	A	173	SER	3.2
1	E	73	LYS	3.1
1	C	310	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	THR	3.0
1	F	171	GLY	3.0
1	A	181	LYS	3.0
1	D	191	ASN	3.0
1	D	180	GLY	3.0
1	E	193	THR	3.0
1	A	412	TYR	3.0
1	B	174	GLN	3.0
1	B	375	THR	3.0
1	F	411	ASN	2.9
1	C	412	TYR	2.9
1	F	375	THR	2.9
1	D	171	GLY	2.8
1	E	179	VAL	2.8
1	A	309	SER	2.7
1	C	176	ALA	2.7
1	B	180	GLY	2.7
1	B	78	LYS	2.6
1	C	175	LEU	2.6
1	E	452	ASP	2.5
1	B	172	LEU	2.4
1	D	374	LYS	2.4
1	E	451	GLN	2.4
1	A	172	LEU	2.4
1	E	375	THR	2.4
1	D	413	GLY	2.4
1	C	375	THR	2.4
1	D	72	ASP	2.4
1	E	192	LYS	2.3
1	D	195	GLN	2.3
1	A	297	ASN	2.3
1	D	314	PHE	2.3
1	B	72	ASP	2.3
1	E	194	ALA	2.2
1	C	371	MET	2.2
1	D	177	VAL	2.1
1	B	75	ALA	2.1
1	E	450	ILE	2.1
1	C	313	GLY	2.1
1	D	311	THR	2.1
1	A	171	GLY	2.0
1	B	411	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	314	PHE	2.0
1	A	184	GLN	2.0
1	A	177	VAL	2.0
1	A	411	ASN	2.0
1	C	411	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)

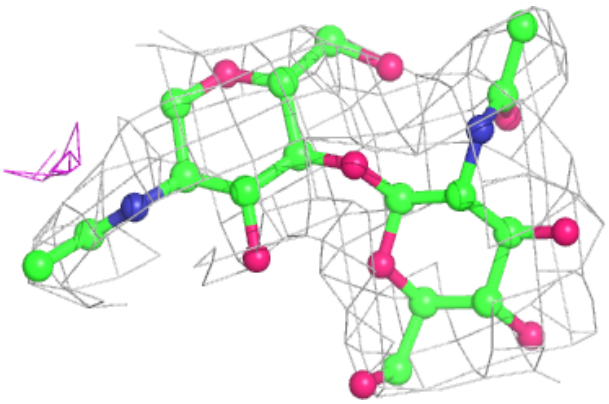
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

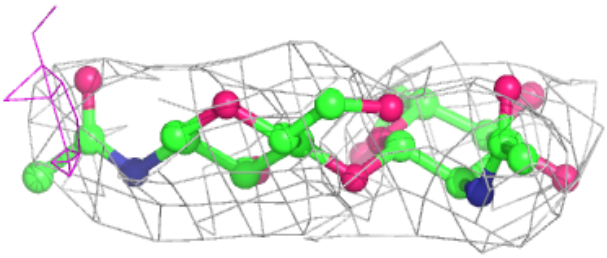
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	1	14/15	0.41	0.77	90,95,98,98	0
2	NAG	J	2	14/15	0.47	0.91	93,100,100,100	0
3	NAG	H	2	14/15	0.52	0.99	97,100,100,100	0
3	BMA	H	3	11/12	0.72	0.81	98,100,100,100	0
2	NAG	J	1	14/15	0.76	0.65	84,90,95,96	0
2	NAG	L	2	14/15	0.85	0.29	66,72,73,75	0
2	NAG	N	2	14/15	0.87	0.32	48,49,54,57	0
2	NAG	I	2	14/15	0.87	0.32	55,60,63,68	0
2	NAG	G	2	14/15	0.89	0.43	61,66,75,77	0
2	NAG	M	2	14/15	0.89	0.29	66,70,75,79	0
2	NAG	L	1	14/15	0.89	0.24	48,59,71,73	0
2	NAG	M	1	14/15	0.90	0.16	49,55,64,64	0
2	NAG	G	1	14/15	0.90	0.39	49,55,64,65	0
2	NAG	K	2	14/15	0.90	0.43	40,43,48,53	0
2	NAG	K	1	14/15	0.92	0.26	34,40,49,52	0
2	NAG	I	1	14/15	0.94	0.13	46,53,56,59	0
2	NAG	N	1	14/15	0.94	0.18	38,45,53,56	0

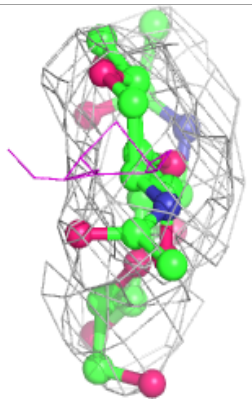
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

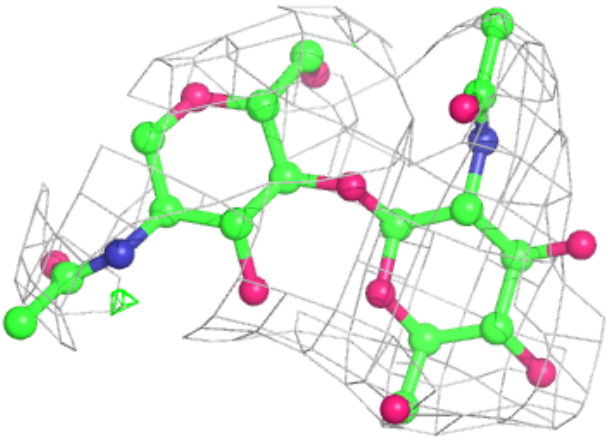


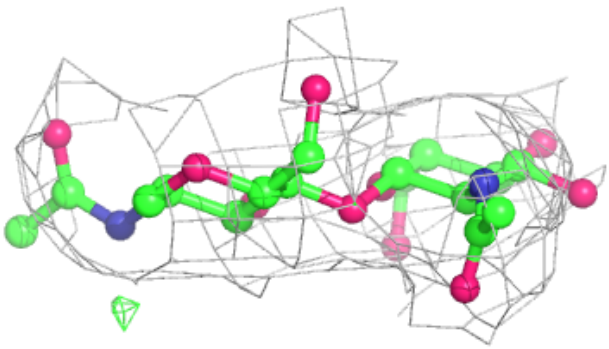


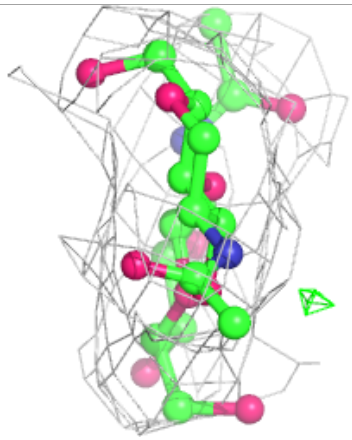


Electron density around Chain I:

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

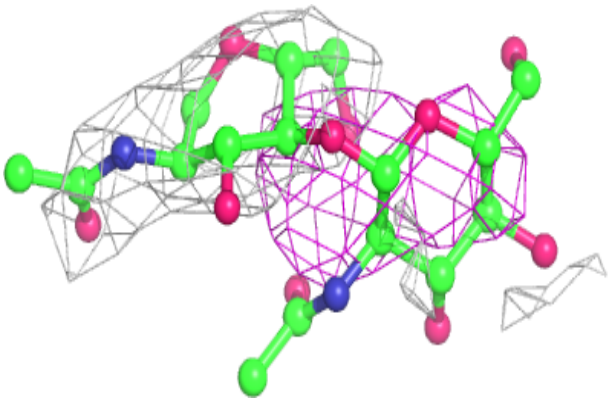


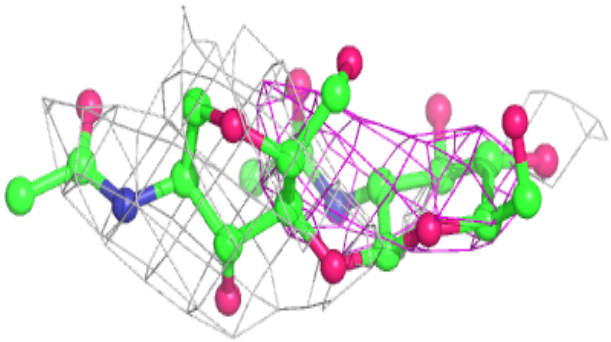


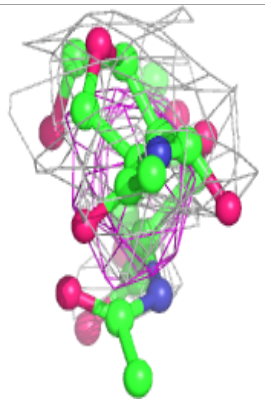


Electron density around Chain J:

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

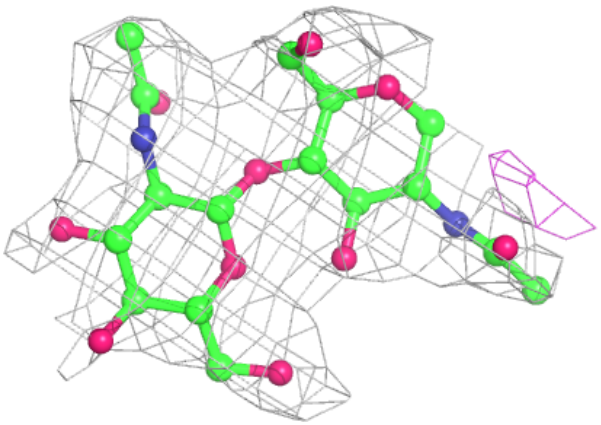


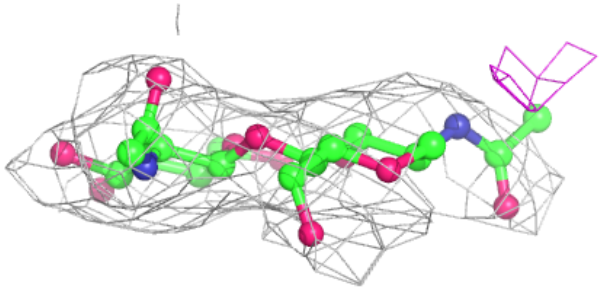


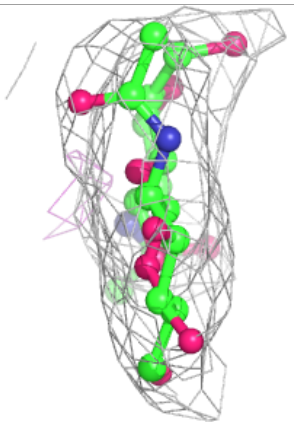


Electron density around Chain K:

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

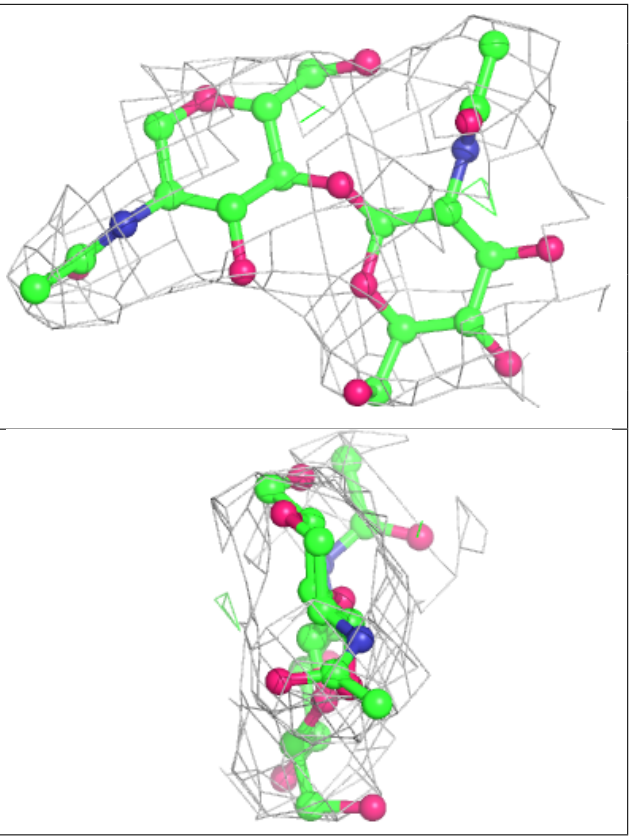






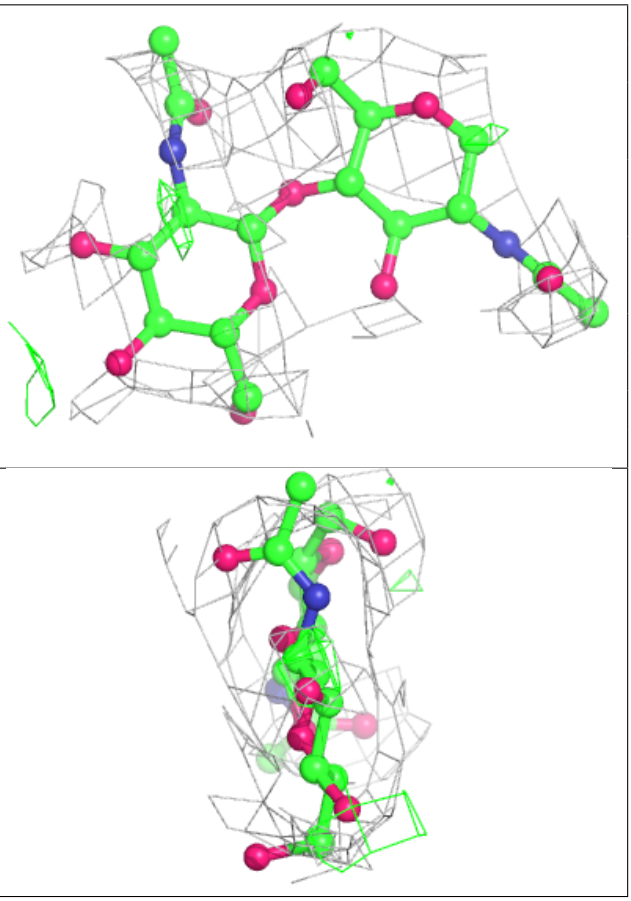
Electron density around Chain L:

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



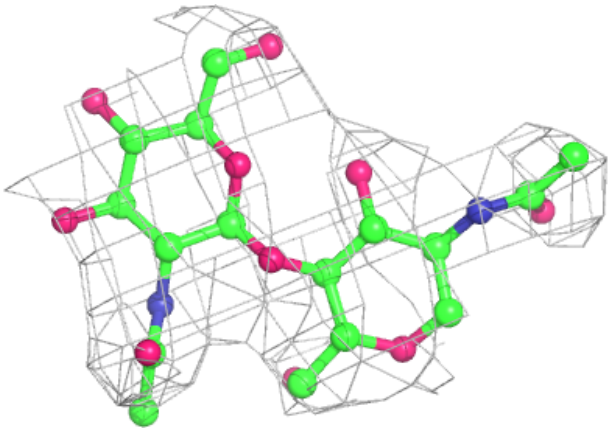
Electron density around Chain M:

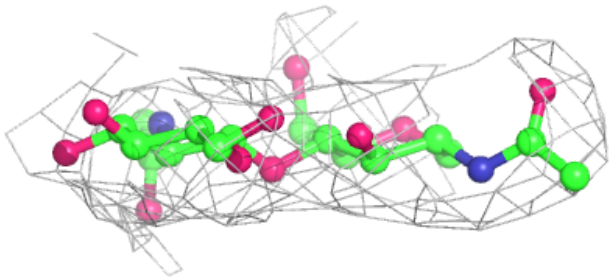
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

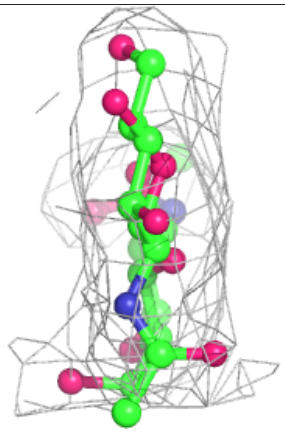


Electron density around Chain N:

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

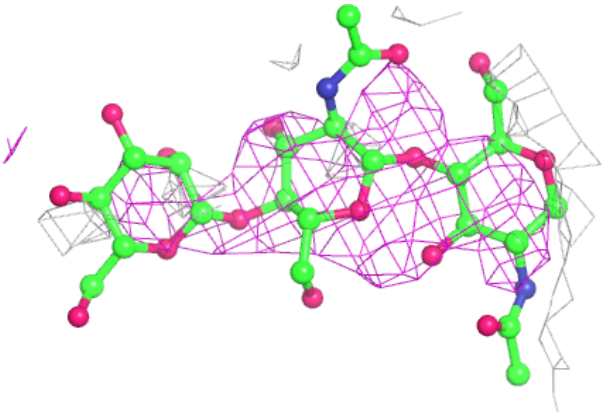


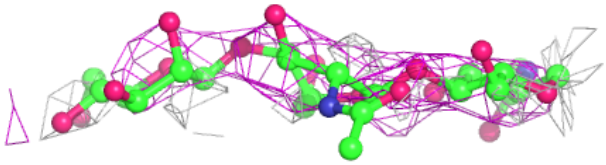




Electron density around Chain H:

$2mF_o$-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
4	NAG	D	1911	14/15	0.70	0.67	99,100,100,100	0
4	NAG	E	4471	14/15	0.74	0.55	84,90,100,100	0
4	NAG	C	4471	14/15	0.79	0.48	79,86,91,92	0
4	NAG	F	1911	14/15	0.81	0.46	91,95,100,100	0

6.5 Other polymers

There are no such residues in this entry.