Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 02:00 AM EDT

PDB ID	:	3K72
Title	:	Structure of integrin alphaX beta2
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Deposited on	:	2009-10-11
Resolution	:	3.70 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

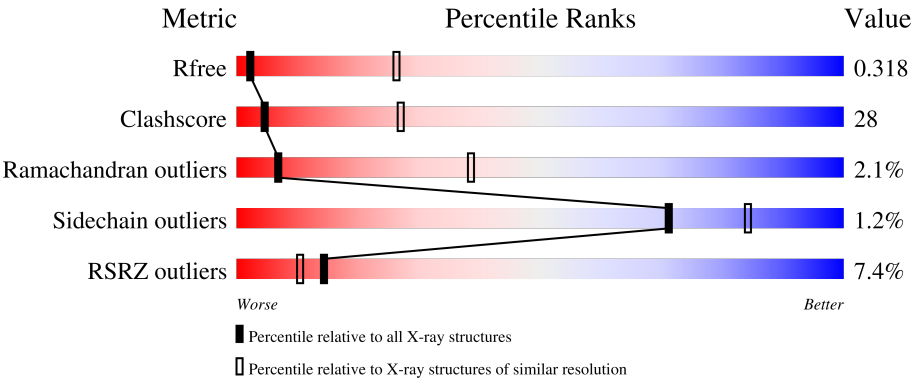
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	1095	3% 43% 35% 19%
1	C	1095	3% 44% 34% 19%
2	B	687	10% 62% 34%
2	D	687	13% 62% 34%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	I	2	
4	F	5	
4	J	5	
5	G	3	
5	H	3	
5	K	3	

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
3	NAG	I	2	-	-	-	X
4	NAG	F	1	X	-	-	-
4	MAN	F	3	X	-	-	-
4	MAN	F	4	-	-	-	X
4	NAG	J	1	X	-	-	-
4	MAN	J	3	X	-	-	-
5	MAN	G	3	X	-	-	-
5	MAN	H	3	X	-	-	X
5	NAG	K	1	-	-	X	-
5	MAN	K	3	X	-	-	-
6	NAG	B	3479	-	X	-	-
6	NAG	D	3094	-	-	-	X
8	MAN	C	3378	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 24382 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	884	Total	C	N	O	S	0	0	0
			6814	4305	1178	1297	34			
1	C	882	Total	C	N	O	S	0	0	0
			6802	4299	1176	1293	34			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702
C	1095	GLN	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	D	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			

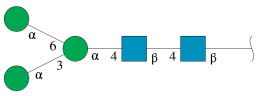
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	expression tag	UNP P05107
B	679	GLY	-	expression tag	UNP P05107
B	680	CYS	-	expression tag	UNP P05107
B	681	GLY	-	expression tag	UNP P05107
B	682	GLU	-	expression tag	UNP P05107
B	684	LEU	-	expression tag	UNP P05107
B	685	TYR	-	expression tag	UNP P05107
B	686	PHE	-	expression tag	UNP P05107
B	687	GLN	-	expression tag	UNP P05107
D	678	ASP	-	expression tag	UNP P05107
D	679	GLY	-	expression tag	UNP P05107
D	680	CYS	-	expression tag	UNP P05107
D	681	GLY	-	expression tag	UNP P05107
D	682	GLU	-	expression tag	UNP P05107
D	684	LEU	-	expression tag	UNP P05107
D	685	TYR	-	expression tag	UNP P05107
D	686	PHE	-	expression tag	UNP P05107
D	687	GLN	-	expression tag	UNP P05107

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

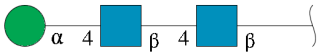
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



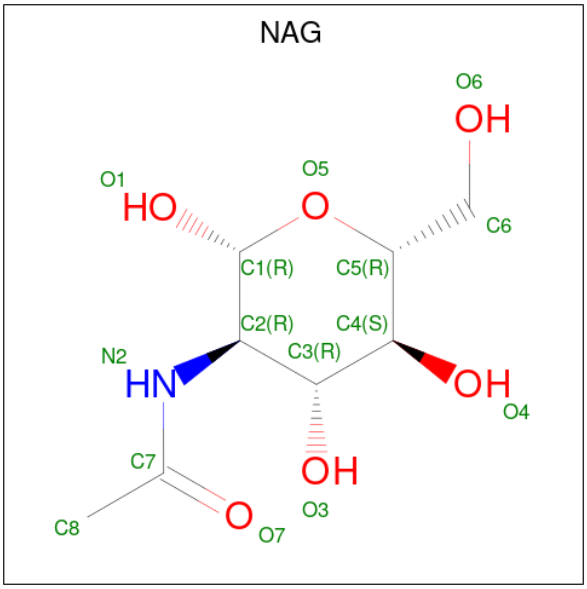
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	5	Total C N O 61 34 2 25	0	0	0
4	J	5	Total C N O 61 34 2 25	0	0	0

- Molecule 5 is an oligosaccharide called alpha-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
5	G	3	Total C N O 39 22 2 15	0	0	0
5	H	3	Total C N O 39 22 2 15	0	0	0
5	K	3	Total C N O 39 22 2 15	0	0	0

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

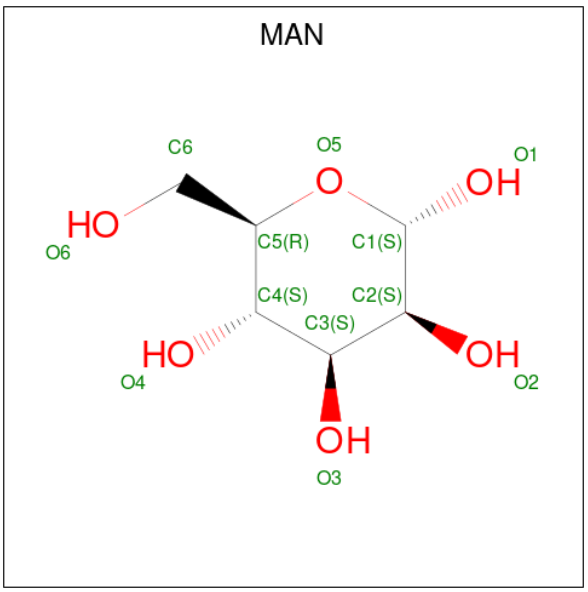


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Ca 3 3	0	0
7	B	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



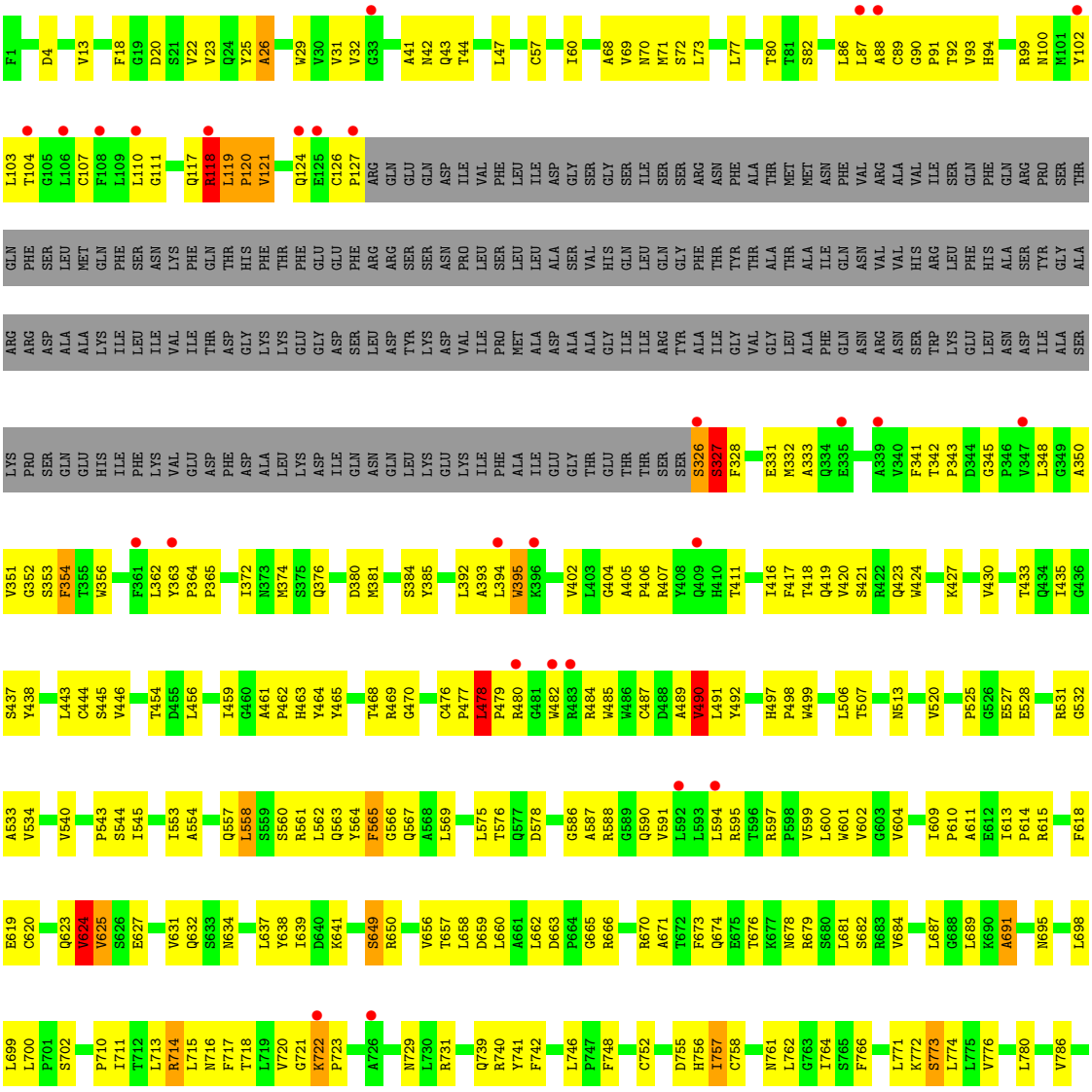
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		

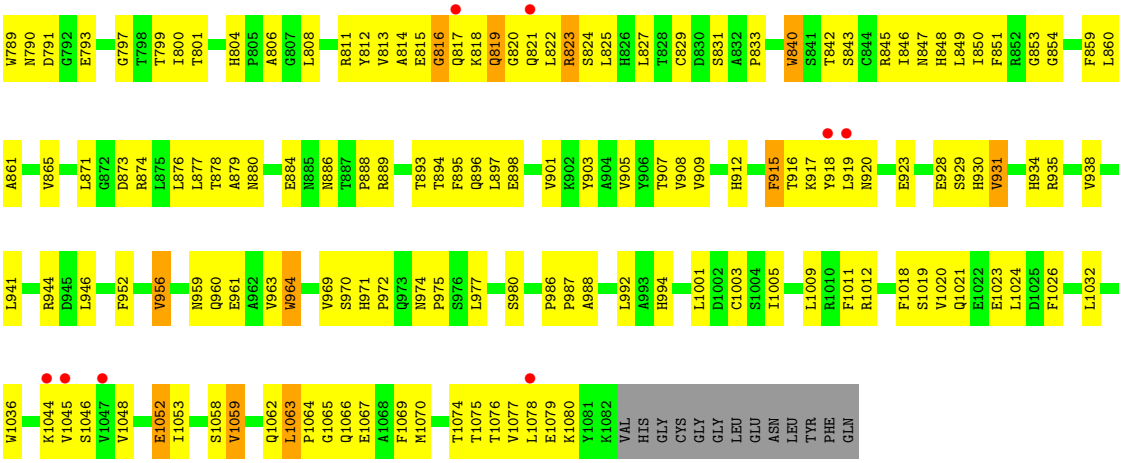
3 Residue-property plots (i)

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: Integrin alpha-X

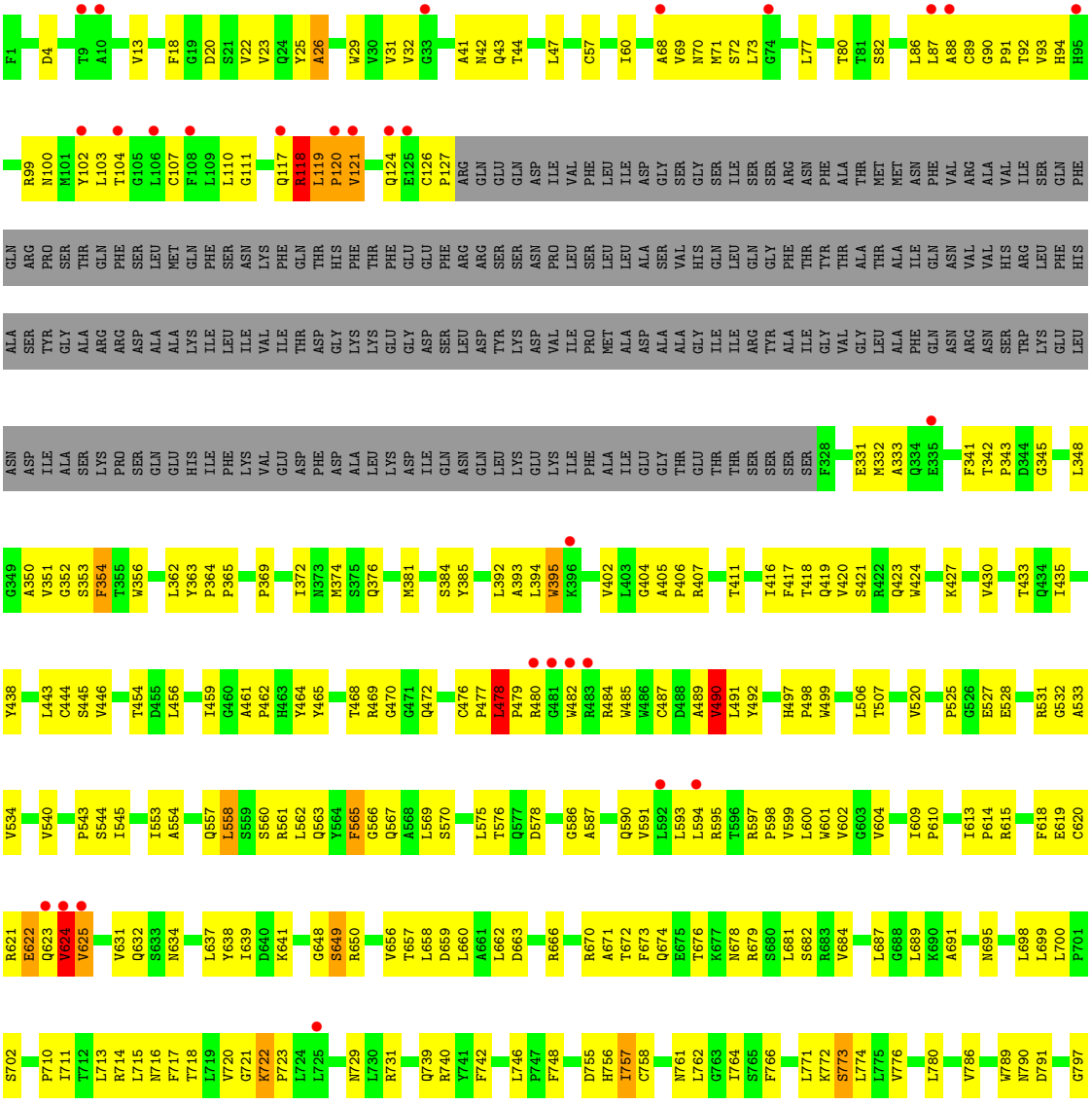
Chain A:

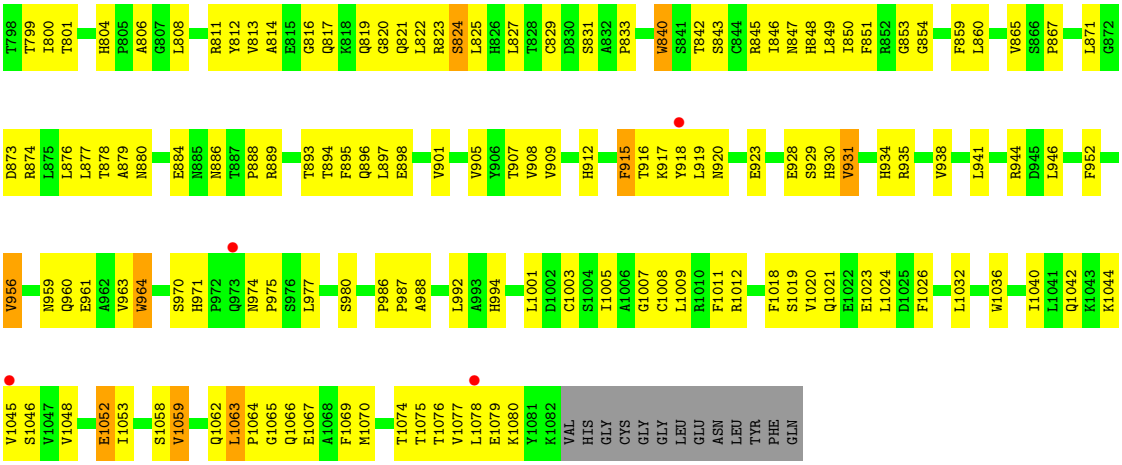




• Molecule 1: Integrin alpha-X

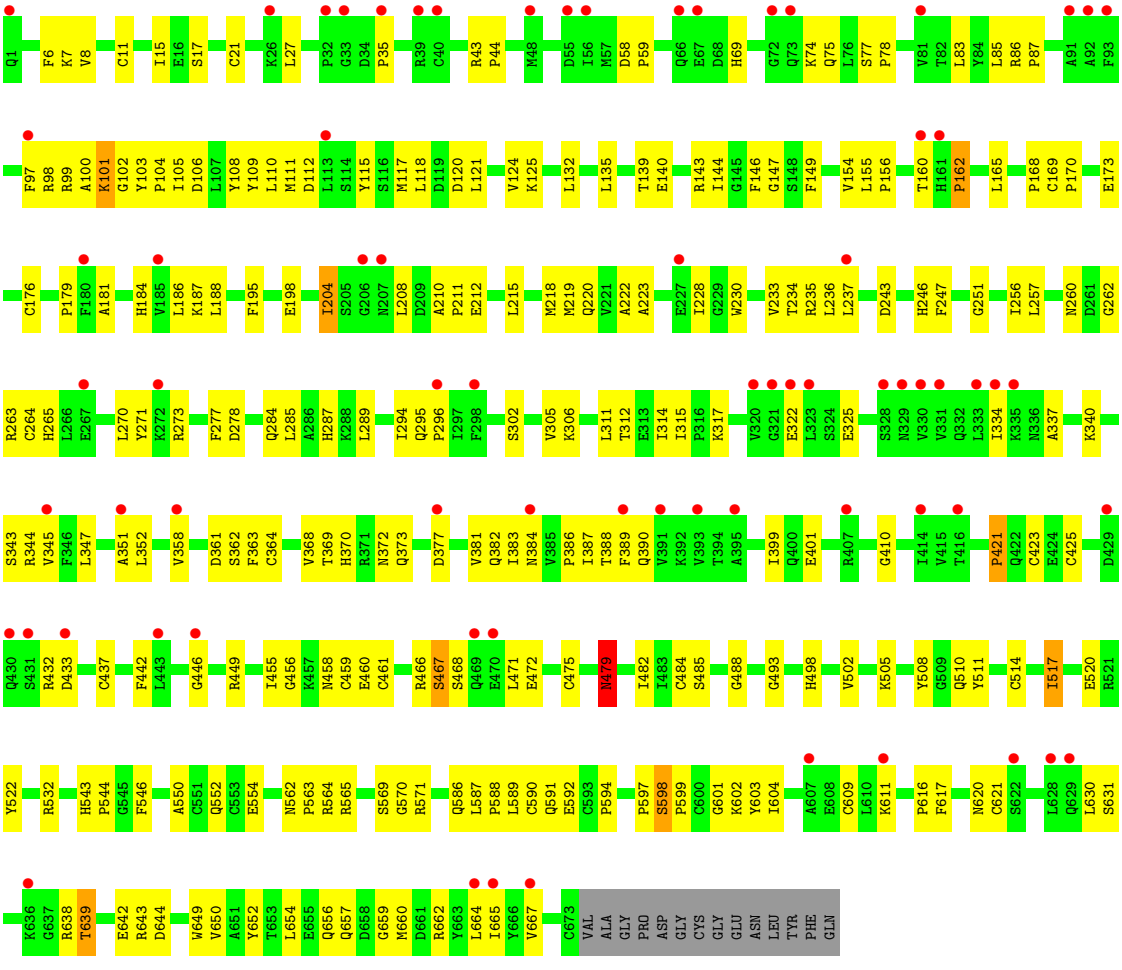
Chain C:





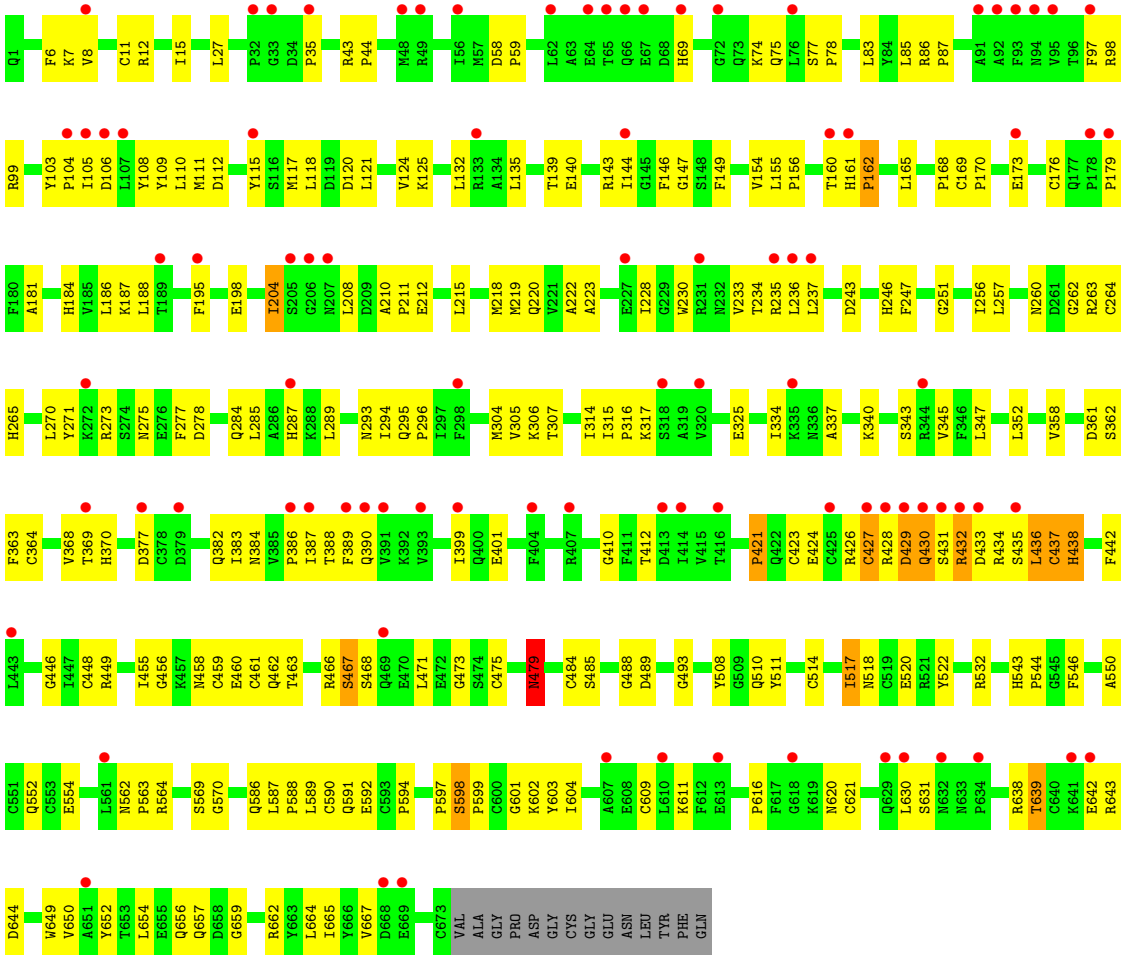
• Molecule 2: Integrin beta-2

Chain B:



• Molecule 2: Integrin beta-2

Chain D:



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

Chain E:

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

Chain I:

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

Chain F:

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

Chain J:

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

Chain G:

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

Chain H:

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

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	160.96Å 165.55Å 536.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.70 48.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.48-3.70) 99.4 (48.64-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.315 , 0.335 0.293 , 0.318	Depositor DCC
R_{free} test set	1136 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å^2)	92.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 151.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	24382	wwPDB-VP
Average B, all atoms (Å^2)	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	7/6969 (0.1%)	0.53	3/9480 (0.0%)
1	C	0.38	1/6957 (0.0%)	0.53	2/9464 (0.0%)
2	B	0.29	1/5273 (0.0%)	0.43	0/7119
2	D	0.31	1/5273 (0.0%)	0.43	0/7119
All	All	0.36	10/24472 (0.0%)	0.49	5/33182 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	C	0	15
2	B	0	2
2	D	0	3
All	All	0	33

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	479	ASN	CB-CG	7.36	1.68	1.51
2	B	479	ASN	CB-CG	6.92	1.67	1.51
1	A	326	SER	CB-OG	6.75	1.51	1.42
1	A	327	SER	CA-CB	6.62	1.62	1.52
1	A	326	SER	CA-CB	6.42	1.62	1.52
1	C	478	LEU	CG-CD1	-5.98	1.29	1.51
1	A	478	LEU	CG-CD1	-5.73	1.30	1.51
1	A	326	SER	C-O	5.67	1.34	1.23
1	A	326	SER	CA-C	5.49	1.67	1.52
1	A	327	SER	CB-OG	5.17	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	478	LEU	CA-CB-CG	8.42	134.66	115.30
1	A	478	LEU	CA-CB-CG	7.71	133.03	115.30
1	A	478	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	118	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	C	478	LEU	CB-CG-CD1	-5.06	102.39	111.00

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1063	LEU	Peptide
1	A	118	ARG	Peptide
1	A	326	SER	Peptide
1	A	327	SER	Peptide
1	A	490	VAL	Peptide
1	A	558	LEU	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
1	A	889	ARG	Peptide
2	B	100	ALA	Peptide
2	B	425	CYS	Peptide
1	C	1063	LEU	Peptide
1	C	118	ARG	Peptide
1	C	490	VAL	Peptide
1	C	558	LEU	Peptide
1	C	622	GLU	Peptide
1	C	624	VAL	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	817	GLN	Peptide
1	C	819	GLN	Peptide
1	C	82	SER	Peptide
1	C	820	GLY	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
1	C	889	ARG	Peptide
2	D	427	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	D	430	GLN	Peptide
2	D	431	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6814	0	6671	441	0
1	C	6802	0	6661	442	0
2	B	5177	0	4964	236	0
2	D	5177	0	4964	267	0
3	E	28	0	25	0	0
3	I	28	0	25	0	0
4	F	61	0	52	5	0
4	J	61	0	52	7	0
5	G	39	0	34	4	0
5	H	39	0	34	3	0
5	K	39	0	34	13	0
6	A	14	0	12	0	0
6	B	28	0	26	1	0
6	C	28	0	25	0	0
6	D	28	0	26	1	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
8	C	11	0	10	1	0
All	All	24382	0	23615	1353	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 28.

All (1353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ILE:HG23	2:B:86:ARG:CZ	1.67	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:430:GLN:HB3	2:D:434:ARG:NH2	1.61	1.14
2:D:430:GLN:HG3	2:D:442:PHE:CB	1.78	1.14
2:D:430:GLN:CB	2:D:434:ARG:HH21	1.62	1.10
2:D:430:GLN:HG3	2:D:442:PHE:HB2	1.13	1.09
5:K:1:NAG:H83	5:K:1:NAG:H3	1.33	1.08
2:D:430:GLN:HB3	2:D:434:ARG:HH21	0.95	1.07
2:D:15:ILE:HG23	2:D:86:ARG:CZ	1.85	1.07
2:B:15:ILE:HG23	2:B:86:ARG:NH2	1.69	1.06
1:C:94:HIS:NE2	2:D:155:LEU:HD21	1.70	1.06
5:K:1:NAG:H3	5:K:1:NAG:C8	1.87	1.04
1:A:94:HIS:NE2	2:B:155:LEU:HD21	1.72	1.03
1:C:822:LEU:HG	1:C:823:ARG:H	1.22	1.02
1:A:119:LEU:N	1:A:120:PRO:HA	1.79	0.97
1:C:119:LEU:N	1:C:120:PRO:HA	1.80	0.96
2:D:430:GLN:CG	2:D:442:PHE:CB	2.43	0.95
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.46	0.94
1:A:119:LEU:HD21	1:A:124:GLN:HE21	1.32	0.94
1:C:103:LEU:HD11	2:D:155:LEU:HD13	1.47	0.94
1:C:659:ASP:OD2	5:K:1:NAG:C8	2.18	0.92
1:C:119:LEU:HD21	1:C:124:GLN:HE21	1.33	0.92
2:D:437:CYS:HA	2:D:458:ASN:O	1.71	0.90
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.02	0.90
2:D:430:GLN:CB	2:D:434:ARG:NH2	2.28	0.90
2:D:430:GLN:CG	2:D:442:PHE:HB2	2.00	0.90
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.54	0.89
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.55	0.89
1:C:1063:LEU:HD12	1:C:1064:PRO:N	1.87	0.89
1:A:1063:LEU:HD12	1:A:1064:PRO:N	1.87	0.89
1:A:484:ARG:NH1	2:B:586:GLN:HG3	1.89	0.88
1:C:659:ASP:OD2	5:K:1:NAG:C7	2.21	0.88
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.02	0.88
1:A:623:GLN:O	1:A:624:VAL:HG22	1.72	0.88
1:C:118:ARG:HG2	1:C:120:PRO:HB3	1.57	0.87
1:C:624:VAL:HG12	1:C:625:VAL:H	1.40	0.87
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.09	0.87
1:C:624:VAL:HG12	1:C:625:VAL:N	1.90	0.86
2:D:15:ILE:HG23	2:D:86:ARG:NH2	1.89	0.86
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.12	0.84
1:A:817:GLN:N	1:A:818:LYS:HA	1.92	0.83
5:K:2:NAG:O3	5:K:3:MAN:H2	1.78	0.83
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HG2	1:A:120:PRO:HB3	1.61	0.81
2:B:15:ILE:CG2	2:B:86:ARG:CZ	2.54	0.81
2:D:430:GLN:CG	2:D:442:PHE:HB3	2.10	0.81
2:D:430:GLN:HG2	2:D:442:PHE:HB3	1.61	0.81
1:A:756:HIS:O	1:A:757:ILE:HG22	1.80	0.81
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.17	0.80
2:D:317:LYS:HE3	2:D:410:GLY:CA	2.11	0.80
2:D:317:LYS:HE3	2:D:410:GLY:HA3	1.63	0.79
1:A:731:ARG:HG3	1:A:731:ARG:O	1.83	0.79
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.17	0.79
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.12	0.79
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.63	0.78
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.64	0.78
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.13	0.78
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.66	0.78
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.64	0.77
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.66	0.77
1:A:328:PHE:O	1:A:354:PHE:HA	1.84	0.77
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.19	0.77
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.66	0.77
1:A:822:LEU:HG	1:A:823:ARG:H	1.49	0.77
1:C:731:ARG:O	1:C:731:ARG:HG3	1.86	0.76
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.66	0.76
8:C:3378:MAN:C1	4:J:5:MAN:H4	2.15	0.76
1:C:822:LEU:CG	1:C:823:ARG:H	1.99	0.75
1:C:721:GLY:C	1:C:723:PRO:HD3	2.07	0.75
1:A:103:LEU:CD1	2:B:155:LEU:HD13	2.16	0.75
1:C:756:HIS:O	1:C:757:ILE:HG22	1.85	0.74
1:C:621:ARG:HH12	1:C:623:GLN:HG2	1.51	0.74
5:K:1:NAG:H83	5:K:1:NAG:C3	2.15	0.74
1:A:721:GLY:C	1:A:723:PRO:HD3	2.08	0.74
2:D:471:LEU:O	2:D:493:GLY:HA2	1.88	0.74
1:C:103:LEU:CD1	2:D:155:LEU:HD13	2.17	0.73
2:B:27:LEU:HD21	2:B:446:GLY:HA2	1.70	0.73
2:B:546:PHE:CD2	2:B:554:GLU:O	2.41	0.72
1:C:117:GLN:HB2	1:C:121:VAL:HG21	1.71	0.72
1:A:119:LEU:H	1:A:120:PRO:HA	1.53	0.72
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.10	0.72
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.09	0.72
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.72	0.72
1:A:484:ARG:NH1	2:B:586:GLN:CG	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.72	0.71
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.09	0.71
2:D:436:LEU:O	2:D:437:CYS:CB	2.39	0.71
1:A:103:LEU:HD13	2:B:156:PRO:HG3	1.73	0.70
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.71	0.70
5:H:1:NAG:H61	5:H:2:NAG:O5	1.91	0.70
1:A:117:GLN:HB2	1:A:121:VAL:HG21	1.70	0.70
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.72	0.70
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.74	0.69
1:C:394:LEU:HD23	1:C:395:TRP:N	2.08	0.69
2:D:427:CYS:HB3	2:D:428:ARG:HB2	1.74	0.69
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.23	0.69
1:C:119:LEU:H	1:C:120:PRO:HA	1.55	0.69
1:C:721:GLY:C	1:C:723:PRO:CD	2.62	0.68
1:A:394:LEU:HD23	1:A:395:TRP:N	2.08	0.68
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.28	0.68
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.75	0.68
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.75	0.68
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.29	0.68
1:A:721:GLY:C	1:A:723:PRO:CD	2.62	0.68
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.75	0.68
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.28	0.68
1:A:623:GLN:O	1:A:624:VAL:CG2	2.42	0.67
2:D:437:CYS:SG	2:D:458:ASN:HA	2.33	0.67
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.30	0.67
2:B:597:PRO:O	2:B:598:SER:HB2	1.93	0.67
1:C:103:LEU:HD13	2:D:156:PRO:HG3	1.76	0.67
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.25	0.67
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.30	0.67
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.76	0.67
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.30	0.67
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.76	0.66
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.31	0.66
2:B:312:THR:CG2	2:B:344:ARG:HH22	2.09	0.66
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.78	0.66
1:C:599:VAL:HG23	1:C:599:VAL:O	1.96	0.66
1:C:825:LEU:HD12	1:C:859:PHE:HB3	1.78	0.66
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.30	0.66
1:A:1064:PRO:HG2	1:A:1067:GLU:HG3	1.76	0.66
2:D:436:LEU:O	2:D:437:CYS:SG	2.53	0.66
1:A:813:VAL:HB	1:A:823:ARG:HH21	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.24	0.65
1:C:119:LEU:HD21	1:C:124:GLN:NE2	2.08	0.65
1:A:822:LEU:CG	1:A:823:ARG:H	2.10	0.65
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.27	0.65
1:C:624:VAL:CG1	1:C:625:VAL:HG13	2.26	0.65
1:C:722:LYS:N	1:C:723:PRO:CD	2.60	0.65
1:A:484:ARG:HH12	2:B:586:GLN:HG3	1.60	0.65
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.78	0.65
2:D:437:CYS:O	2:D:459:CYS:HB2	1.97	0.65
1:A:119:LEU:HD21	1:A:124:GLN:NE2	2.08	0.65
1:C:103:LEU:CD1	2:D:156:PRO:HG3	2.27	0.65
1:C:1064:PRO:HG2	1:C:1067:GLU:HG3	1.77	0.65
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.79	0.64
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.79	0.64
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.27	0.64
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.64
1:C:812:TYR:HE2	1:C:814:ALA:HB2	1.61	0.64
2:D:546:PHE:CD2	2:D:554:GLU:O	2.50	0.64
1:A:722:LYS:N	1:A:723:PRO:CD	2.60	0.64
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.27	0.64
2:B:479:ASN:OD1	6:B:3479:NAG:O5	2.12	0.64
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.79	0.64
2:D:12:ARG:NH1	2:D:424:GLU:OE2	2.30	0.64
5:H:2:NAG:H62	5:H:3:MAN:O5	1.98	0.64
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.28	0.64
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.28	0.64
2:D:597:PRO:O	2:D:598:SER:CB	2.46	0.64
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.27	0.64
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.78	0.63
2:B:15:ILE:CG2	2:B:86:ARG:NH2	2.55	0.63
2:D:154:VAL:HA	2:D:160:THR:HG22	1.80	0.63
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.29	0.63
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.63
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.33	0.63
1:A:4:ASP:CG	1:A:597:ARG:NH2	2.51	0.63
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.33	0.63
2:D:532:ARG:HD3	2:D:554:GLU:CD	2.19	0.63
2:B:154:VAL:HA	2:B:160:THR:HG22	1.81	0.63
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.79	0.63
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.33	0.63
2:D:437:CYS:CA	2:D:458:ASN:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.80	0.62
1:C:44:THR:HG22	1:C:71:MET:HG2	1.81	0.62
1:C:621:ARG:NH1	1:C:623:GLN:HG2	2.14	0.62
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.28	0.62
1:C:47:LEU:HD11	1:C:88:ALA:CB	2.29	0.62
2:B:27:LEU:CD2	2:B:446:GLY:HA2	2.29	0.62
2:D:436:LEU:O	2:D:437:CYS:HB2	1.98	0.62
2:B:571:ARG:HH21	2:B:660:MET:CG	2.13	0.62
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.34	0.62
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.81	0.62
2:B:597:PRO:O	2:B:598:SER:CB	2.47	0.61
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.35	0.61
4:F:2:NAG:O3	4:F:3:MAN:H2	2.01	0.61
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.30	0.61
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.82	0.61
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.82	0.61
1:A:599:VAL:HG23	1:A:599:VAL:O	1.99	0.61
2:B:571:ARG:HH21	2:B:660:MET:HG3	1.65	0.61
1:C:43:GLN:HA	1:C:70:ASN:H	1.66	0.61
1:A:362:LEU:HD23	1:A:363:TYR:N	2.16	0.61
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.36	0.61
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	1.83	0.61
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.82	0.61
1:C:118:ARG:HA	1:C:120:PRO:HB3	1.82	0.61
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.01	0.61
1:C:919:LEU:O	2:D:643:ARG:NH1	2.34	0.61
5:G:1:NAG:H61	5:G:2:NAG:O5	2.01	0.61
1:A:928:GLU:HG3	1:A:929:SER:N	2.16	0.61
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.36	0.60
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.36	0.60
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.82	0.60
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.83	0.60
1:C:822:LEU:HG	1:C:823:ARG:N	2.06	0.60
1:A:43:GLN:HA	1:A:70:ASN:H	1.65	0.60
1:C:928:GLU:HG3	1:C:929:SER:N	2.17	0.60
1:A:44:THR:HG22	1:A:71:MET:HG2	1.83	0.60
1:A:941:LEU:HD12	1:A:941:LEU:N	2.16	0.60
1:C:941:LEU:N	1:C:941:LEU:HD12	2.16	0.60
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.02	0.60
2:B:466:ARG:O	2:B:467:SER:OG	2.19	0.60
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HG	1:C:119:LEU:O	2.02	0.59
1:C:833:PRO:HA	1:C:840:TRP:CB	2.32	0.59
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.83	0.59
1:C:824:SER:H	1:C:825:LEU:HG	1.67	0.59
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.83	0.59
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.38	0.59
1:C:362:LEU:HD23	1:C:363:TYR:N	2.17	0.59
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.43	0.59
2:D:597:PRO:O	2:D:598:SER:HB2	2.03	0.59
1:A:833:PRO:HA	1:A:840:TRP:CB	2.32	0.59
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.32	0.59
1:A:820:GLY:N	1:A:822:LEU:HB3	2.18	0.59
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.37	0.59
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.33	0.59
2:D:430:GLN:HB2	2:D:434:ARG:NH2	2.17	0.59
1:A:715:LEU:O	1:A:715:LEU:HD12	2.03	0.59
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.38	0.59
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.33	0.59
1:A:659:ASP:OD2	5:G:1:NAG:N2	2.35	0.59
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.83	0.59
1:C:374:MET:HG3	1:C:381:MET:SD	2.43	0.59
2:B:35:PRO:HG2	2:B:510:GLN:CD	2.23	0.58
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.03	0.58
1:A:20:ASP:OD1	1:A:567:GLN:OE1	2.21	0.58
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.85	0.58
4:J:2:NAG:O3	4:J:3:MAN:H2	2.03	0.58
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.85	0.58
1:A:118:ARG:HA	1:A:120:PRO:HB3	1.84	0.58
1:A:121:VAL:HG12	1:A:121:VAL:O	2.04	0.58
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.39	0.58
1:A:374:MET:HG3	1:A:381:MET:SD	2.43	0.58
1:C:715:LEU:HD12	1:C:715:LEU:O	2.04	0.58
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.34	0.58
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.39	0.58
1:A:119:LEU:HG	1:A:119:LEU:O	2.03	0.57
1:A:602:VAL:HG23	1:A:638:TYR:O	2.04	0.57
2:B:461:CYS:SG	2:B:466:ARG:HD3	2.43	0.57
2:B:592:GLU:O	2:B:594:PRO:HD3	2.04	0.57
1:C:20:ASP:OD1	1:C:567:GLN:OE1	2.22	0.57
1:C:602:VAL:HG23	1:C:638:TYR:O	2.04	0.57
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.40	0.57
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.39	0.57
2:D:15:ILE:CG2	2:D:86:ARG:CZ	2.74	0.57
1:C:119:LEU:N	1:C:120:PRO:CA	2.61	0.57
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.39	0.57
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.05	0.57
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.38	0.57
1:C:490:VAL:HG12	1:C:491:LEU:N	2.19	0.57
1:A:822:LEU:HG	1:A:823:ARG:N	2.19	0.57
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.40	0.57
1:A:490:VAL:HG12	1:A:491:LEU:N	2.18	0.57
1:A:831:SER:CB	1:A:842:THR:HG22	2.35	0.57
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.34	0.57
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.04	0.57
1:C:659:ASP:OD2	5:K:1:NAG:H81	2.02	0.57
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.40	0.57
2:B:461:CYS:SG	2:B:466:ARG:CD	2.93	0.57
1:C:659:ASP:OD2	5:K:1:NAG:O7	2.23	0.57
2:D:35:PRO:HG2	2:D:510:GLN:CD	2.25	0.57
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.40	0.56
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.39	0.56
2:D:165:LEU:HD12	2:D:179:PRO:HG2	1.87	0.56
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.86	0.56
1:A:919:LEU:CD1	2:B:643:ARG:NH1	2.68	0.56
2:B:570:GLY:HA2	2:B:659:GLY:HA2	1.87	0.56
1:C:624:VAL:HG12	1:C:625:VAL:HG13	1.86	0.56
1:A:772:LYS:HG3	1:A:772:LYS:O	2.04	0.56
2:B:165:LEU:HD12	2:B:179:PRO:HG2	1.87	0.56
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.86	0.56
1:C:121:VAL:HG12	1:C:121:VAL:O	2.04	0.56
1:C:772:LYS:HG3	1:C:772:LYS:O	2.05	0.56
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.36	0.56
2:B:162:PRO:O	2:B:165:LEU:HB3	2.05	0.56
2:B:471:LEU:O	2:B:493:GLY:HA2	2.06	0.56
2:D:74:LYS:HD2	2:D:103:TYR:OH	2.06	0.56
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.21	0.56
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.06	0.56
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.87	0.56
2:D:135:LEU:HD11	2:D:139:THR:HB	1.88	0.56
2:D:317:LYS:CE	2:D:410:GLY:HA3	2.33	0.56
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:ARG:CD	2:B:554:GLU:HG3	2.36	0.56
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.41	0.56
2:D:162:PRO:O	2:D:165:LEU:HB3	2.05	0.56
1:C:619:GLU:O	1:C:620:CYS:SG	2.64	0.56
2:D:654:LEU:HD13	2:D:665:ILE:HG13	1.88	0.56
1:A:780:LEU:O	1:A:865:VAL:HG12	2.06	0.55
2:B:468:SER:HB2	2:B:471:LEU:HG	1.87	0.55
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.21	0.55
1:C:780:LEU:O	1:C:865:VAL:HG12	2.06	0.55
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.42	0.55
2:D:468:SER:HB2	2:D:471:LEU:HG	1.87	0.55
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.21	0.55
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.89	0.55
1:C:89:CYS:O	1:C:91:PRO:HD3	2.07	0.55
1:C:621:ARG:HG2	1:C:622:GLU:H	1.72	0.55
1:C:395:TRP:CH2	1:C:480:ARG:HD3	2.41	0.55
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.21	0.55
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.41	0.55
2:B:87:PRO:CD	2:B:423:CYS:SG	2.94	0.55
1:C:332:MET:SD	2:D:208:LEU:HD13	2.46	0.55
1:C:812:TYR:CE2	1:C:814:ALA:CB	2.84	0.55
1:C:831:SER:CB	1:C:842:THR:HG22	2.35	0.55
1:A:89:CYS:O	1:A:91:PRO:HD3	2.06	0.55
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.06	0.55
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.88	0.55
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.42	0.55
1:C:575:LEU:HD12	1:C:576:THR:N	2.21	0.55
5:K:2:NAG:C3	5:K:3:MAN:H2	2.36	0.55
1:A:575:LEU:HD12	1:A:576:THR:N	2.22	0.55
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.89	0.55
1:C:118:ARG:HA	1:C:120:PRO:CB	2.37	0.55
1:C:722:LYS:N	1:C:723:PRO:HD2	2.22	0.55
2:B:58:ASP:N	2:B:59:PRO:HD3	2.21	0.55
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.89	0.55
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.22	0.55
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.37	0.55
2:D:437:CYS:O	2:D:438:HIS:HB2	2.06	0.55
1:A:491:LEU:HD12	1:A:491:LEU:C	2.27	0.54
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.42	0.54
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.90	0.54
1:A:722:LYS:N	1:A:723:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.42	0.54
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.42	0.54
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.89	0.54
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.37	0.54
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.37	0.54
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.42	0.54
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.89	0.54
1:C:1063:LEU:HD12	1:C:1064:PRO:HA	1.84	0.54
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.90	0.54
1:A:649:SER:O	1:A:650:ARG:HB3	2.07	0.54
1:C:4:ASP:CG	1:C:597:ARG:NH2	2.61	0.54
1:C:491:LEU:C	1:C:491:LEU:HD12	2.28	0.54
2:B:135:LEU:HD11	2:B:139:THR:HB	1.90	0.54
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.43	0.54
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.89	0.54
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.28	0.54
2:D:461:CYS:HB3	2:D:466:ARG:HD3	1.88	0.54
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.38	0.54
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.43	0.54
2:B:587:LEU:HD12	2:B:587:LEU:N	2.23	0.54
2:D:112:ASP:O	2:D:117:MET:HG3	2.08	0.54
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.90	0.54
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.43	0.54
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.88	0.54
2:B:27:LEU:HD21	2:B:446:GLY:CA	2.37	0.54
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.90	0.54
2:D:654:LEU:CD1	2:D:665:ILE:HG13	2.38	0.54
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.27	0.54
1:A:80:THR:HB	1:A:341:PHE:CG	2.43	0.53
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.42	0.53
2:B:659:GLY:O	2:B:662:ARG:HG2	2.09	0.53
1:C:364:PRO:CB	1:C:365:PRO:CD	2.86	0.53
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.89	0.53
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.89	0.53
2:D:429:ASP:OD1	2:D:429:ASP:N	2.36	0.53
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.90	0.53
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.43	0.53
2:B:520:GLU:HB3	2:B:550:ALA:HB2	1.89	0.53
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.43	0.53
2:D:98:ARG:O	2:D:98:ARG:HG2	2.09	0.53
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.38	0.53
2:D:520:GLU:HB3	2:D:550:ALA:HB2	1.89	0.53
1:A:364:PRO:CB	1:A:365:PRO:CD	2.86	0.53
1:A:659:ASP:OD2	5:G:1:NAG:C7	2.56	0.53
1:A:812:TYR:CE2	1:A:814:ALA:CB	2.89	0.53
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.89	0.53
2:B:343:SER:HA	2:B:381:VAL:O	2.08	0.53
2:D:461:CYS:CB	2:D:466:ARG:HD3	2.38	0.53
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.91	0.53
2:B:654:LEU:HD13	2:B:665:ILE:HG13	1.89	0.53
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.90	0.53
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.38	0.53
1:A:657:THR:HG23	1:A:720:VAL:HB	1.90	0.53
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.91	0.53
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.89	0.53
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.90	0.53
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.91	0.53
2:D:74:LYS:HZ2	2:D:103:TYR:HE2	1.57	0.53
2:D:462:GLN:HG2	2:D:463:THR:N	2.24	0.53
2:D:659:GLY:O	2:D:662:ARG:HG2	2.09	0.53
1:A:595:ARG:HB2	1:A:597:ARG:HH12	1.74	0.53
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.38	0.53
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.44	0.53
1:C:80:THR:HB	1:C:341:PHE:CG	2.44	0.53
1:C:621:ARG:HG2	1:C:622:GLU:N	2.24	0.53
1:C:649:SER:O	1:C:650:ARG:HB3	2.09	0.53
1:C:1053:ILE:CG2	1:C:1070:MET:HB2	2.39	0.53
2:D:87:PRO:CD	2:D:423:CYS:SG	2.97	0.53
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.91	0.53
1:A:876:LEU:C	1:A:876:LEU:HD12	2.30	0.53
2:B:98:ARG:O	2:B:98:ARG:HG2	2.09	0.53
1:C:657:THR:HG23	1:C:720:VAL:HB	1.91	0.53
1:C:772:LYS:O	1:C:773:SER:HB3	2.09	0.53
2:D:155:LEU:H	2:D:160:THR:CG2	2.22	0.53
1:C:595:ARG:HB2	1:C:597:ARG:HH12	1.74	0.52
2:D:466:ARG:O	2:D:467:SER:OG	2.26	0.52
2:D:587:LEU:HD12	2:D:587:LEU:N	2.24	0.52
1:A:755:ASP:O	1:A:756:HIS:HB3	2.09	0.52
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.91	0.52
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.92	0.52
1:A:118:ARG:HA	1:A:120:PRO:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.90	0.52
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.38	0.52
1:C:681:LEU:C	1:C:681:LEU:HD12	2.30	0.52
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.92	0.52
2:D:423:CYS:O	2:D:424:GLU:HG2	2.10	0.52
1:A:4:ASP:HB2	1:A:597:ARG:CZ	2.40	0.52
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.91	0.52
2:B:155:LEU:H	2:B:160:THR:CG2	2.23	0.52
2:B:599:PRO:HB2	2:B:603:TYR:HE2	1.74	0.52
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.91	0.52
2:B:638:ARG:HB2	2:B:654:LEU:O	2.09	0.52
2:B:654:LEU:CD1	2:B:665:ILE:HG13	2.39	0.52
2:D:340:LYS:HA	2:D:343:SER:HB2	1.90	0.52
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.44	0.52
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.92	0.52
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.92	0.52
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.92	0.52
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.39	0.52
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.92	0.52
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.45	0.52
1:A:772:LYS:O	1:A:773:SER:HB3	2.09	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
1:C:623:GLN:O	1:C:624:VAL:HB	2.10	0.52
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.39	0.52
1:A:681:LEU:C	1:A:681:LEU:HD12	2.31	0.52
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.90	0.52
2:B:460:GLU:HG2	2:B:461:CYS:N	2.24	0.52
1:C:624:VAL:CG1	1:C:625:VAL:N	2.61	0.52
2:D:461:CYS:SG	2:D:466:ARG:NE	2.83	0.52
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.44	0.52
1:A:332:MET:SD	2:B:208:LEU:HD13	2.50	0.52
1:A:831:SER:HA	1:A:842:THR:HG22	1.92	0.52
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.45	0.52
1:A:812:TYR:HE2	1:A:814:ALA:HB2	1.68	0.52
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.45	0.52
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.45	0.52
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.93	0.52
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.45	0.51
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.91	0.51
2:D:638:ARG:HB2	2:D:654:LEU:O	2.10	0.51
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:ARG:HD3	2:D:433:ASP:N	2.25	0.51
1:A:848:HIS:HB2	2:B:485:SER:HB3	1.92	0.51
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.75	0.51
1:A:461:ALA:N	1:A:462:PRO:HD3	2.26	0.51
1:A:484:ARG:HH12	2:B:586:GLN:CG	2.19	0.51
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.41	0.51
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.91	0.51
1:A:569:LEU:HD12	1:A:569:LEU:O	2.10	0.51
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.92	0.51
1:A:71:MET:CG	1:A:90:GLY:HA3	2.40	0.51
1:A:553:ILE:HG23	1:A:557:GLN:HG3	1.93	0.51
1:C:461:ALA:N	1:C:462:PRO:HD3	2.26	0.51
1:C:470:GLY:HA2	1:C:497:HIS:O	2.09	0.51
1:C:531:ARG:HA	1:C:563:GLN:O	2.11	0.51
1:C:656:VAL:HG13	1:C:718:THR:O	2.11	0.51
1:A:71:MET:SD	1:A:90:GLY:HA3	2.50	0.51
1:A:93:VAL:HB	1:A:104:THR:CG2	2.40	0.51
1:C:118:ARG:HA	1:C:120:PRO:HA	1.93	0.51
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.46	0.51
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.93	0.51
1:A:119:LEU:N	1:A:120:PRO:CA	2.60	0.51
1:A:797:GLY:HA3	1:A:884:GLU:HB2	1.93	0.51
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.93	0.51
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.41	0.51
1:C:569:LEU:O	1:C:569:LEU:HD12	2.10	0.51
1:C:620:CYS:HB3	1:C:702:SER:O	2.11	0.51
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.45	0.51
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.93	0.51
2:D:423:CYS:O	2:D:424:GLU:CG	2.58	0.51
1:A:625:VAL:HG23	1:A:627:GLU:N	2.26	0.51
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.92	0.51
1:C:831:SER:HA	1:C:842:THR:HG22	1.92	0.51
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.46	0.51
2:B:105:ILE:HG12	2:B:106:ASP:N	2.26	0.51
1:C:345:GLY:HA3	1:C:363:TYR:O	2.11	0.51
1:A:470:GLY:HA2	1:A:497:HIS:O	2.10	0.50
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.93	0.50
1:C:876:LEU:C	1:C:876:LEU:HD12	2.32	0.50
2:D:110:LEU:HD13	2:D:218:MET:SD	2.50	0.50
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.93	0.50
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.09	0.50
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.93	0.50
1:A:89:CYS:C	1:A:91:PRO:HD3	2.32	0.50
1:A:93:VAL:O	1:A:103:LEU:HA	2.11	0.50
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.46	0.50
1:C:93:VAL:O	1:C:103:LEU:HA	2.12	0.50
1:C:848:HIS:O	1:C:849:LEU:HB3	2.12	0.50
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.92	0.50
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.41	0.50
2:B:110:LEU:HD13	2:B:218:MET:SD	2.51	0.50
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.80	0.50
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.11	0.50
1:A:531:ARG:HA	1:A:563:GLN:O	2.11	0.50
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.76	0.50
1:A:848:HIS:O	1:A:849:LEU:HB3	2.12	0.50
2:B:99:ARG:O	2:B:383:ILE:O	2.30	0.50
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.92	0.50
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.94	0.50
2:B:659:GLY:O	2:B:662:ARG:CG	2.60	0.50
1:C:873:ASP:C	1:C:901:VAL:HG12	2.33	0.50
2:D:659:GLY:O	2:D:662:ARG:CG	2.60	0.50
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.42	0.50
1:A:820:GLY:H	1:A:822:LEU:HB3	1.76	0.50
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.94	0.50
2:D:154:VAL:HG23	2:D:160:THR:HG21	1.92	0.50
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.93	0.50
2:B:532:ARG:HD3	2:B:554:GLU:CG	2.42	0.50
1:A:465:TYR:CG	1:A:469:ARG:CG	2.95	0.49
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.93	0.49
2:B:154:VAL:HG23	2:B:160:THR:HG21	1.92	0.49
1:C:419:GLN:HA	1:C:424:TRP:HA	1.94	0.49
1:C:716:ASN:OD1	1:C:716:ASN:C	2.49	0.49
1:C:908:VAL:O	1:C:938:VAL:HG23	2.12	0.49
2:D:592:GLU:O	2:D:594:PRO:HD3	2.12	0.49
1:A:659:ASP:OD2	5:G:1:NAG:O7	2.30	0.49
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.93	0.49
2:D:383:ILE:HG22	2:D:384:ASN:N	2.27	0.49
2:D:532:ARG:CD	2:D:554:GLU:HG3	2.43	0.49
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.47	0.49
1:A:126:CYS:HB3	1:A:127:PRO:CD	2.42	0.49
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:MET:SD	1:C:90:GLY:HA3	2.52	0.49
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.42	0.49
2:D:58:ASP:N	2:D:59:PRO:HD3	2.26	0.49
2:D:105:ILE:HG12	2:D:106:ASP:N	2.27	0.49
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.93	0.49
1:A:345:GLY:HA3	1:A:363:TYR:O	2.12	0.49
2:B:437:CYS:HA	2:B:458:ASN:O	2.12	0.49
2:B:532:ARG:HD3	2:B:554:GLU:HG3	1.95	0.49
1:C:93:VAL:HB	1:C:104:THR:CG2	2.41	0.49
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.95	0.49
1:A:666:ARG:HB3	2:B:498:HIS:CD2	2.48	0.49
2:B:6:PHE:O	2:B:8:VAL:HG23	2.11	0.49
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.10	0.49
2:B:546:PHE:HE2	2:B:554:GLU:HG2	1.76	0.49
1:C:126:CYS:HB3	1:C:127:PRO:CD	2.43	0.49
1:C:553:ILE:HG23	1:C:557:GLN:HG3	1.93	0.49
1:C:964:TRP:HB2	1:C:1032:LEU:HA	1.94	0.49
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.13	0.49
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.47	0.49
1:A:578:ASP:O	1:A:578:ASP:OD1	2.31	0.49
2:B:112:ASP:O	2:B:117:MET:HG3	2.12	0.49
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.47	0.49
2:D:11:CYS:O	2:D:15:ILE:HG12	2.13	0.49
2:D:401:GLU:HA	2:D:421:PRO:HD3	1.94	0.49
1:A:873:ASP:C	1:A:901:VAL:HG12	2.32	0.49
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.12	0.49
2:B:656:GLN:HG2	2:B:657:GLN:N	2.28	0.49
1:C:681:LEU:HD12	1:C:682:SER:N	2.28	0.49
1:C:89:CYS:C	1:C:91:PRO:HD3	2.33	0.49
1:C:465:TYR:CG	1:C:469:ARG:CG	2.96	0.49
2:D:6:PHE:CG	2:D:7:LYS:N	2.81	0.49
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.48	0.49
1:A:362:LEU:HD23	1:A:362:LEU:C	2.33	0.49
1:A:491:LEU:HD12	1:A:492:TYR:N	2.28	0.49
1:A:850:ILE:HG22	1:A:851:PHE:N	2.27	0.49
1:A:1053:ILE:CG2	1:A:1070:MET:HB2	2.42	0.49
2:B:77:SER:HA	2:B:78:PRO:C	2.32	0.49
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.13	0.49
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.94	0.49
2:D:135:LEU:CD1	2:D:139:THR:HB	2.42	0.49
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:460:GLU:HG2	2:D:461:CYS:N	2.28	0.49
1:A:986:PRO:CB	1:A:987:PRO:CD	2.91	0.49
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.13	0.49
2:B:6:PHE:CG	2:B:7:LYS:N	2.81	0.49
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.48	0.49
2:B:455:ILE:HG22	2:B:456:GLY:N	2.28	0.49
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.48	0.49
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.43	0.49
1:C:624:VAL:HG13	1:C:625:VAL:HG13	1.93	0.49
1:A:395:TRP:CH2	1:A:480:ARG:HD3	2.47	0.48
1:A:681:LEU:HD12	1:A:682:SER:N	2.28	0.48
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.34	0.48
2:B:401:GLU:HA	2:B:421:PRO:HD3	1.94	0.48
1:C:118:ARG:HA	1:C:120:PRO:CA	2.43	0.48
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.95	0.48
2:D:6:PHE:O	2:D:8:VAL:HG23	2.12	0.48
2:D:479:ASN:HB3	6:D:3479:NAG:O7	2.13	0.48
2:D:546:PHE:CE2	2:D:554:GLU:HG2	2.48	0.48
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.43	0.48
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.94	0.48
2:B:11:CYS:O	2:B:15:ILE:HG12	2.12	0.48
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.81	0.48
1:C:77:LEU:HD23	1:C:88:ALA:HA	1.95	0.48
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.94	0.48
1:C:986:PRO:CB	1:C:987:PRO:CD	2.90	0.48
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.95	0.48
1:A:118:ARG:HA	1:A:120:PRO:HA	1.95	0.48
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.29	0.48
2:B:135:LEU:CD1	2:B:139:THR:HB	2.43	0.48
1:C:71:MET:CG	1:C:90:GLY:HA3	2.44	0.48
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.28	0.48
1:A:656:VAL:HG13	1:A:718:THR:O	2.12	0.48
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.94	0.48
2:B:383:ILE:HG22	2:B:384:ASN:N	2.28	0.48
2:D:77:SER:HA	2:D:78:PRO:C	2.34	0.48
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.48	0.48
1:A:928:GLU:HG3	1:A:929:SER:H	1.77	0.48
2:B:121:LEU:O	2:B:125:LYS:HB3	2.13	0.48
1:C:20:ASP:OD1	2:D:257:LEU:HD22	2.13	0.48
1:A:716:ASN:C	1:A:716:ASN:OD1	2.52	0.48
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:ILE:HG22	1:C:851:PHE:N	2.28	0.48
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.94	0.48
1:C:918:TYR:C	2:D:643:ARG:NH2	2.67	0.48
2:D:99:ARG:O	2:D:383:ILE:O	2.31	0.48
2:D:461:CYS:SG	2:D:466:ARG:HD3	2.53	0.48
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.48	0.48
1:A:776:VAL:HG21	1:A:903:TYR:CE1	2.49	0.48
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.94	0.48
1:A:992:LEU:C	1:A:992:LEU:HD23	2.34	0.48
2:B:432:ARG:O	2:B:433:ASP:HB2	2.14	0.48
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.54	0.48
1:C:491:LEU:HD12	1:C:492:TYR:N	2.29	0.48
1:C:928:GLU:HG3	1:C:929:SER:H	1.77	0.48
2:D:285:LEU:O	2:D:289:LEU:HB3	2.14	0.48
2:D:432:ARG:HG2	2:D:432:ARG:HH11	1.78	0.48
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.48
1:A:639:ILE:HG13	1:A:689:LEU:HA	1.96	0.48
2:B:591:GLN:HG2	2:B:592:GLU:N	2.29	0.48
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.28	0.48
1:C:1058:SER:O	1:C:1059:VAL:HB	2.14	0.48
2:D:43:ARG:N	2:D:44:PRO:CD	2.77	0.48
2:D:162:PRO:O	2:D:165:LEU:CB	2.62	0.48
2:D:437:CYS:HA	2:D:458:ASN:HB3	1.95	0.48
2:D:437:CYS:O	2:D:458:ASN:O	2.32	0.48
1:A:964:TRP:HB2	1:A:1032:LEU:HA	1.94	0.48
1:C:987:PRO:O	1:C:988:ALA:HB3	2.14	0.48
2:D:591:GLN:HG2	2:D:592:GLU:N	2.29	0.48
2:B:43:ARG:N	2:B:44:PRO:CD	2.77	0.48
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.48	0.48
1:C:755:ASP:O	1:C:756:HIS:HB3	2.13	0.48
5:K:1:NAG:H61	5:K:2:NAG:O5	2.13	0.48
1:A:812:TYR:HD2	1:A:814:ALA:HB2	1.77	0.47
1:A:822:LEU:CG	1:A:823:ARG:N	2.77	0.47
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.77	0.47
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.14	0.47
1:A:1058:SER:O	1:A:1059:VAL:HB	2.13	0.47
2:B:285:LEU:O	2:B:289:LEU:HB3	2.14	0.47
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.43	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HG	1.96	0.47
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.34	0.47
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:VAL:HG23	1:A:430:VAL:O	2.14	0.47
1:A:631:VAL:HG11	1:A:746:LEU:HD11	1.96	0.47
1:C:411:THR:HG22	1:C:435:ILE:HA	1.96	0.47
1:C:905:VAL:CG1	1:C:946:LEU:HD21	2.44	0.47
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.15	0.47
2:D:656:GLN:HG2	2:D:657:GLN:N	2.28	0.47
1:A:118:ARG:CG	1:A:120:PRO:HB3	2.40	0.47
1:A:476:CYS:CB	1:A:487:CYS:HA	2.43	0.47
1:A:698:LEU:N	1:A:698:LEU:HD12	2.29	0.47
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.50	0.47
1:A:77:LEU:HD23	1:A:88:ALA:HA	1.96	0.47
1:A:419:GLN:HA	1:A:424:TRP:HA	1.95	0.47
1:A:445:SER:HB2	1:A:454:THR:HG21	1.97	0.47
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.95	0.47
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.44	0.47
1:C:1053:ILE:CG2	1:C:1070:MET:CB	2.92	0.47
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.50	0.47
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.49	0.47
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.44	0.47
1:C:600:LEU:O	1:C:600:LEU:HD12	2.15	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.95	0.47
2:D:223:ALA:HB1	2:D:263:ARG:HA	1.97	0.47
1:A:110:LEU:HD12	1:A:110:LEU:N	2.29	0.47
2:B:143:ARG:C	2:B:144:ILE:HD12	2.35	0.47
1:C:362:LEU:HD23	1:C:362:LEU:C	2.34	0.47
1:A:848:HIS:HB2	2:B:485:SER:O	2.14	0.47
1:A:880:ASN:OD1	1:A:894:THR:HG22	2.14	0.47
1:A:970:SER:O	1:A:1026:PHE:HB2	2.14	0.47
2:B:121:LEU:O	2:B:121:LEU:HD23	2.14	0.47
1:C:395:TRP:HH2	1:C:480:ARG:CG	2.28	0.47
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.44	0.47
1:C:575:LEU:HD12	1:C:576:THR:HG23	1.96	0.47
1:C:578:ASP:OD1	1:C:578:ASP:O	2.33	0.47
1:C:748:PHE:CD1	1:C:748:PHE:N	2.82	0.47
1:C:797:GLY:HA3	1:C:884:GLU:HB2	1.95	0.47
1:C:822:LEU:CG	1:C:823:ARG:N	2.72	0.47
1:C:886:ASN:O	1:C:888:PRO:HD3	2.15	0.47
2:D:121:LEU:HD23	2:D:121:LEU:O	2.14	0.47
4:J:1:NAG:H3	4:J:2:NAG:N2	2.30	0.47
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.49	0.47
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PRO:O	2:B:165:LEU:CB	2.62	0.47
2:B:562:ASN:OD1	2:B:564:ARG:HB2	2.15	0.47
1:C:476:CYS:CB	1:C:487:CYS:HA	2.44	0.47
2:D:455:ILE:HG22	2:D:456:GLY:N	2.29	0.47
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.30	0.47
1:A:840:TRP:CD1	1:A:840:TRP:N	2.81	0.47
1:C:430:VAL:HG13	1:C:485:TRP:CE3	2.50	0.47
1:C:601:TRP:CZ2	1:C:641:LYS:HG2	2.50	0.47
1:C:812:TYR:CE2	1:C:814:ALA:CA	2.98	0.47
1:C:813:VAL:HG23	1:C:823:ARG:NH1	2.30	0.47
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.78	0.47
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.95	0.47
2:D:121:LEU:O	2:D:125:LYS:HB3	2.14	0.47
1:A:964:TRP:HB3	1:A:1032:LEU:HG	1.96	0.47
1:A:987:PRO:O	1:A:988:ALA:HB3	2.15	0.47
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.96	0.47
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.55	0.47
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.50	0.47
1:C:663:ASP:HB3	1:C:666:ARG:HD3	1.97	0.47
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.97	0.47
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.50	0.46
1:A:811:ARG:HG3	1:A:811:ARG:O	2.14	0.46
1:A:831:SER:HB3	1:A:842:THR:HG22	1.97	0.46
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.15	0.46
1:A:1063:LEU:HD12	1:A:1064:PRO:CB	2.46	0.46
2:B:382:GLN:HG3	2:B:383:ILE:H	1.80	0.46
1:C:812:TYR:HE2	1:C:814:ALA:CB	2.23	0.46
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.15	0.46
1:A:118:ARG:HA	1:A:120:PRO:CA	2.45	0.46
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.45	0.46
1:C:376:GLN:HB2	4:J:1:NAG:O4	2.15	0.46
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.46	0.46
1:C:639:ILE:HG13	1:C:689:LEU:HA	1.96	0.46
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.55	0.46
1:A:20:ASP:OD1	2:B:257:LEU:HD22	2.16	0.46
1:A:601:TRP:CZ2	1:A:641:LYS:HG2	2.50	0.46
2:B:15:ILE:HG23	2:B:86:ARG:NH1	2.22	0.46
1:C:721:GLY:O	1:C:723:PRO:HD3	2.15	0.46
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.45	0.46
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.97	0.46
1:A:477:PRO:HG2	1:A:489:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.63	0.46
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.46	0.46
2:B:256:ILE:HG13	2:B:256:ILE:O	2.15	0.46
1:C:430:VAL:HG22	1:C:485:TRP:HZ3	1.80	0.46
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	1.98	0.46
1:A:25:TYR:CG	1:A:26:ALA:N	2.83	0.46
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.98	0.46
1:C:780:LEU:C	1:C:780:LEU:HD23	2.36	0.46
1:C:1053:ILE:HG22	1:C:1070:MET:HB2	1.96	0.46
2:D:154:VAL:HA	2:D:160:THR:CG2	2.45	0.46
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.45	0.46
2:D:437:CYS:HA	2:D:458:ASN:C	2.35	0.46
2:D:468:SER:HB2	2:D:471:LEU:CG	2.45	0.46
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.51	0.46
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.98	0.46
1:A:333:ALA:HA	1:A:352:GLY:H	1.80	0.46
1:A:456:LEU:HA	1:A:477:PRO:HA	1.97	0.46
1:A:490:VAL:HG12	1:A:491:LEU:CA	2.46	0.46
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.96	0.46
1:A:908:VAL:O	1:A:938:VAL:HG23	2.15	0.46
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.81	0.46
1:A:790:ASN:O	1:A:854:GLY:HA2	2.16	0.46
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.56	0.46
1:A:874:ARG:NH2	1:C:894:THR:O	2.49	0.46
2:B:155:LEU:HB2	2:B:156:PRO:CA	2.38	0.46
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.46	0.46
1:C:25:TYR:CG	1:C:26:ALA:N	2.84	0.46
1:C:490:VAL:HG12	1:C:491:LEU:CA	2.46	0.46
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.46
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.97	0.46
2:D:120:ASP:OD1	2:D:325:GLU:O	2.33	0.46
1:A:894:THR:O	1:C:874:ARG:NH2	2.49	0.46
2:B:468:SER:HB2	2:B:471:LEU:CG	2.46	0.46
1:C:333:ALA:HA	1:C:352:GLY:H	1.81	0.46
1:C:445:SER:HB2	1:C:454:THR:HG21	1.97	0.46
1:C:831:SER:HB3	1:C:842:THR:HG22	1.98	0.46
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.97	0.46
2:D:382:GLN:HG3	2:D:383:ILE:H	1.79	0.46
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.46	0.46
1:A:766:PHE:CE2	1:A:895:PHE:HD2	2.34	0.46
1:A:780:LEU:C	1:A:780:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ASN:O	1:A:888:PRO:HD3	2.15	0.46
2:B:270:LEU:HD23	2:B:271:TYR:O	2.16	0.46
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.97	0.46
1:C:631:VAL:HG11	1:C:746:LEU:HD11	1.98	0.46
1:C:676:THR:HG23	1:C:678:ASN:H	1.81	0.46
1:C:840:TRP:CD1	1:C:840:TRP:N	2.84	0.46
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.97	0.46
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.97	0.46
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.46	0.46
1:A:1065:GLY:O	1:A:1066:GLN:HG3	2.16	0.46
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.46	0.46
1:C:634:ASN:HB2	1:C:695:ASN:HB3	1.97	0.46
1:C:771:LEU:HD11	1:C:774:LEU:HB2	1.97	0.46
1:C:1063:LEU:HD12	1:C:1064:PRO:CB	2.46	0.46
2:D:461:CYS:SG	2:D:466:ARG:CD	3.04	0.46
4:F:1:NAG:H3	4:F:2:NAG:N2	2.31	0.46
1:A:73:LEU:HA	1:A:90:GLY:HA2	1.98	0.45
1:A:756:HIS:HA	1:C:1052:GLU:OE1	2.16	0.45
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	1.98	0.45
1:C:110:LEU:HD12	1:C:110:LEU:N	2.31	0.45
1:C:456:LEU:HA	1:C:477:PRO:HA	1.97	0.45
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.98	0.45
1:C:698:LEU:N	1:C:698:LEU:HD12	2.31	0.45
1:C:766:PHE:CD1	1:C:766:PHE:C	2.89	0.45
2:D:345:VAL:HG11	2:D:387:ILE:HD11	1.98	0.45
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.98	0.45
2:D:562:ASN:OD1	2:D:564:ARG:HB2	2.16	0.45
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.98	0.45
2:D:143:ARG:C	2:D:144:ILE:HD12	2.37	0.45
1:A:376:GLN:HB2	4:F:1:NAG:O4	2.16	0.45
1:A:395:TRP:HH2	1:A:480:ARG:CG	2.29	0.45
1:A:676:THR:HG23	1:A:678:ASN:H	1.81	0.45
2:B:169:CYS:HB2	2:B:173:GLU:HA	1.98	0.45
1:C:353:SER:C	1:C:354:PHE:CG	2.90	0.45
1:C:766:PHE:CE2	1:C:895:PHE:HD2	2.34	0.45
1:C:959:ASN:O	1:C:960:GLN:HB3	2.17	0.45
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.56	0.45
5:K:1:NAG:H3	5:K:1:NAG:H82	1.88	0.45
1:A:25:TYR:HD2	1:A:29:TRP:HB2	1.81	0.45
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.16	0.45
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:SER:HB2	2:B:370:HIS:HB2	1.98	0.45
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.51	0.45
1:C:790:ASN:O	1:C:854:GLY:HA2	2.16	0.45
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.65	0.45
2:D:643:ARG:NH2	2:D:649:TRP:HZ2	2.14	0.45
1:A:663:ASP:HB3	1:A:666:ARG:HD3	1.97	0.45
1:A:799:THR:HA	1:A:845:ARG:HA	1.99	0.45
1:A:897:LEU:C	1:A:897:LEU:HD12	2.37	0.45
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.97	0.45
1:C:823:ARG:NH1	1:C:860:LEU:O	2.49	0.45
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.46	0.45
1:A:721:GLY:O	1:A:723:PRO:HD3	2.16	0.45
1:A:764:ILE:HD12	1:A:800:ILE:HD13	1.98	0.45
1:A:800:ILE:HD12	1:A:880:ASN:O	2.17	0.45
1:A:819:GLN:HA	1:A:820:GLY:HA2	1.78	0.45
2:B:345:VAL:HG11	2:B:387:ILE:HD11	1.99	0.45
2:B:472:GLU:HA	2:B:475:CYS:CB	2.46	0.45
1:C:970:SER:O	1:C:1026:PHE:HB2	2.16	0.45
1:C:1048:VAL:HG22	1:C:1075:THR:HB	1.99	0.45
2:D:428:ARG:NH1	2:D:428:ARG:HG3	2.32	0.45
1:A:25:TYR:O	1:A:26:ALA:C	2.54	0.45
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.94	0.45
1:A:959:ASN:O	1:A:960:GLN:HB3	2.17	0.45
2:B:223:ALA:HB1	2:B:263:ARG:HA	1.97	0.45
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.98	0.45
1:C:71:MET:O	1:C:72:SER:C	2.54	0.45
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.46	0.45
1:A:797:GLY:N	1:A:884:GLU:HB2	2.32	0.45
1:A:1063:LEU:N	1:A:1064:PRO:CD	2.80	0.45
1:C:25:TYR:OH	1:C:111:GLY:HA2	2.16	0.45
1:C:31:VAL:HG21	1:C:86:LEU:CD1	2.47	0.45
1:C:430:VAL:O	1:C:430:VAL:HG23	2.17	0.45
1:C:800:ILE:HD12	1:C:880:ASN:O	2.16	0.45
1:C:880:ASN:OD1	1:C:894:THR:HG22	2.17	0.45
2:D:109:TYR:CE2	2:D:111:MET:HB2	2.52	0.45
2:D:256:ILE:HG13	2:D:256:ILE:O	2.17	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.32	0.45
1:A:987:PRO:HA	1:C:619:GLU:OE1	2.16	0.45
2:B:599:PRO:O	2:B:603:TYR:CD2	2.70	0.45
1:C:20:ASP:CG	2:D:257:LEU:HD22	2.38	0.45
1:C:73:LEU:HA	1:C:90:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:ILE:HD12	1:C:800:ILE:HD13	1.99	0.45
1:C:897:LEU:C	1:C:897:LEU:HD12	2.38	0.45
2:D:6:PHE:CD2	2:D:7:LYS:N	2.85	0.45
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.99	0.45
2:D:169:CYS:HB2	2:D:173:GLU:HA	1.98	0.45
4:J:3:MAN:O2	4:J:4:MAN:C1	2.65	0.45
1:A:352:GLY:HA2	1:A:356:TRP:HA	1.99	0.45
1:A:634:ASN:HB2	1:A:695:ASN:HB3	1.98	0.45
2:B:305:VAL:HG13	2:B:306:LYS:N	2.31	0.45
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.98	0.45
1:C:342:THR:OG1	1:C:343:PRO:HD2	2.17	0.45
1:C:908:VAL:HG12	1:C:909:VAL:N	2.32	0.45
1:A:631:VAL:HG11	1:A:746:LEU:CD1	2.47	0.44
1:A:748:PHE:N	1:A:748:PHE:CD1	2.84	0.44
1:A:827:LEU:HD12	1:A:827:LEU:O	2.16	0.44
2:B:6:PHE:CD2	2:B:7:LYS:N	2.85	0.44
2:B:83:LEU:HD12	2:B:83:LEU:O	2.16	0.44
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.99	0.44
2:B:437:CYS:HB3	2:B:459:CYS:SG	2.58	0.44
2:B:643:ARG:NH2	2:B:649:TRP:HZ2	2.15	0.44
1:C:624:VAL:HG12	1:C:625:VAL:HG22	1.99	0.44
2:D:285:LEU:C	2:D:287:HIS:N	2.71	0.44
1:A:374:MET:SD	1:A:417:PHE:CZ	3.10	0.44
1:A:762:LEU:HD23	1:A:790:ASN:HA	1.99	0.44
1:C:621:ARG:CG	1:C:622:GLU:H	2.30	0.44
1:C:790:ASN:O	1:C:853:GLY:O	2.35	0.44
1:C:980:SER:HB3	1:C:1012:ARG:HB3	2.00	0.44
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.16	0.44
2:D:222:ALA:HB2	2:D:294:ILE:CD1	2.47	0.44
1:A:348:LEU:N	1:A:348:LEU:HD12	2.32	0.44
1:A:764:ILE:CD1	1:A:800:ILE:CD1	2.95	0.44
1:A:1053:ILE:CG2	1:A:1070:MET:CB	2.95	0.44
2:B:334:ILE:HA	2:B:337:ALA:CB	2.48	0.44
2:B:569:SER:HB2	2:B:590:CYS:O	2.18	0.44
1:C:25:TYR:HD2	1:C:29:TRP:HB2	1.83	0.44
1:C:418:THR:HB	1:C:427:LYS:CG	2.47	0.44
1:C:419:GLN:CG	1:C:424:TRP:CD1	3.00	0.44
2:D:75:GLN:O	2:D:97:PHE:CD1	2.71	0.44
2:D:149:PHE:HA	2:D:181:ALA:O	2.17	0.44
1:A:22:VAL:HG22	1:A:23:VAL:N	2.32	0.44
1:A:1048:VAL:HG22	1:A:1075:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:GLU:OE2	1:C:757:ILE:HB	2.17	0.44
2:B:154:VAL:HA	2:B:160:THR:CG2	2.46	0.44
1:C:477:PRO:HG2	1:C:489:ALA:HB2	1.99	0.44
1:C:1065:GLY:O	1:C:1066:GLN:HG3	2.17	0.44
2:D:273:ARG:O	2:D:277:PHE:HB3	2.18	0.44
2:D:361:ASP:HB2	2:D:390:GLN:HB3	1.98	0.44
2:D:639:THR:HG23	2:D:639:THR:O	2.18	0.44
5:H:1:NAG:O3	5:H:1:NAG:H82	2.17	0.44
1:A:513:ASN:HA	1:A:599:VAL:HG21	2.00	0.44
2:B:543:HIS:HB3	2:B:544:PRO:HD2	1.99	0.44
2:D:139:THR:HG22	2:D:140:GLU:N	2.33	0.44
2:D:543:HIS:HB3	2:D:544:PRO:HD2	1.99	0.44
1:A:25:TYR:OH	1:A:111:GLY:HA2	2.17	0.44
1:A:93:VAL:HB	1:A:104:THR:HG22	2.00	0.44
1:A:430:VAL:HG22	1:A:485:TRP:HZ3	1.83	0.44
1:A:771:LEU:HD11	1:A:774:LEU:HB2	1.99	0.44
2:B:75:GLN:O	2:B:97:PHE:CD1	2.71	0.44
2:B:222:ALA:HB2	2:B:294:ILE:CD1	2.48	0.44
2:B:479:ASN:OD1	2:B:479:ASN:N	2.43	0.44
1:C:25:TYR:O	1:C:26:ALA:C	2.55	0.44
1:C:107:CYS:SG	1:C:348:LEU:HD21	2.58	0.44
1:C:348:LEU:N	1:C:348:LEU:HD12	2.32	0.44
1:C:631:VAL:HG11	1:C:746:LEU:CD1	2.48	0.44
1:C:873:ASP:O	1:C:901:VAL:HG12	2.17	0.44
2:D:27:LEU:HG	2:D:446:GLY:HA2	2.00	0.44
1:A:812:TYR:HE2	1:A:814:ALA:CB	2.31	0.44
1:A:848:HIS:O	1:A:848:HIS:ND1	2.50	0.44
1:A:873:ASP:O	1:A:901:VAL:HG12	2.17	0.44
2:B:109:TYR:CE2	2:B:111:MET:HB2	2.52	0.44
2:B:665:ILE:N	2:B:665:ILE:HD12	2.33	0.44
1:C:73:LEU:HD12	1:C:73:LEU:C	2.38	0.44
2:D:479:ASN:OD1	2:D:479:ASN:N	2.41	0.44
2:D:569:SER:HB2	2:D:590:CYS:O	2.17	0.44
1:A:87:LEU:HD21	1:A:348:LEU:HD11	1.98	0.44
1:A:1001:LEU:O	1:A:1001:LEU:HD23	2.17	0.44
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	2.00	0.44
2:B:169:CYS:CB	2:B:173:GLU:HA	2.48	0.44
2:B:219:MET:HE2	2:B:262:GLY:HA2	2.00	0.44
2:B:285:LEU:C	2:B:287:HIS:N	2.71	0.44
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.53	0.44
1:C:87:LEU:HD21	1:C:348:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLY:HA2	1:C:356:TRP:HA	1.99	0.44
1:C:560:SER:O	1:C:561:ARG:HG2	2.18	0.44
1:C:876:LEU:HB3	1:C:898:GLU:HG3	2.00	0.44
2:D:83:LEU:HD12	2:D:83:LEU:O	2.18	0.44
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.53	0.44
1:A:31:VAL:HG21	1:A:86:LEU:CD1	2.48	0.44
1:A:741:TYR:CD2	2:B:502:VAL:HG22	2.52	0.44
2:B:149:PHE:HA	2:B:181:ALA:O	2.18	0.44
1:C:420:VAL:HG12	1:C:421:SER:N	2.32	0.44
1:C:507:THR:HG22	1:C:569:LEU:CD1	2.48	0.44
1:C:650:ARG:HD3	1:C:729:ASN:CB	2.48	0.44
1:C:764:ILE:CD1	1:C:800:ILE:CD1	2.96	0.44
1:C:813:VAL:CG2	1:C:823:ARG:NH1	2.81	0.44
4:F:2:NAG:C3	4:F:3:MAN:H2	2.47	0.44
1:A:73:LEU:HD12	1:A:73:LEU:C	2.39	0.43
1:A:419:GLN:CG	1:A:424:TRP:CD1	3.00	0.43
1:A:671:ALA:HB2	1:A:700:LEU:HD23	2.00	0.43
1:A:786:VAL:CG1	1:A:859:PHE:CZ	2.99	0.43
2:B:87:PRO:HD3	2:B:423:CYS:SG	2.59	0.43
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.48	0.43
1:C:1053:ILE:HG22	1:C:1070:MET:CB	2.48	0.43
2:D:237:LEU:HD13	2:D:294:ILE:HG23	2.00	0.43
2:D:270:LEU:HD23	2:D:271:TYR:O	2.17	0.43
2:D:432:ARG:HD3	2:D:433:ASP:H	1.83	0.43
2:D:437:CYS:SG	2:D:448:CYS:CB	3.05	0.43
2:D:437:CYS:O	2:D:438:HIS:CB	2.66	0.43
1:A:484:ARG:NH1	2:B:586:GLN:CB	2.81	0.43
1:A:658:LEU:O	1:A:659:ASP:OD1	2.36	0.43
1:A:815:GLU:HB3	1:A:819:GLN:NE2	2.33	0.43
2:B:340:LYS:HA	2:B:343:SER:HB2	1.98	0.43
1:C:22:VAL:HG22	1:C:23:VAL:N	2.33	0.43
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.48	0.43
2:D:132:LEU:HA	2:D:135:LEU:HB3	1.99	0.43
2:D:169:CYS:CB	2:D:173:GLU:HA	2.48	0.43
2:D:304:MET:HE3	2:D:307:THR:HG21	2.00	0.43
1:A:68:ALA:HA	1:A:93:VAL:HG13	1.99	0.43
1:A:107:CYS:SG	1:A:348:LEU:HD21	2.58	0.43
1:A:525:PRO:HA	1:A:532:GLY:HA2	1.99	0.43
1:A:893:THR:HG23	1:A:893:THR:O	2.18	0.43
2:B:132:LEU:HA	2:B:135:LEU:HB3	1.99	0.43
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:THR:HG21	1:C:1053:ILE:HD13	2.00	0.43
2:D:665:ILE:HD12	2:D:665:ILE:N	2.33	0.43
1:A:13:VAL:HG21	1:A:57:CYS:HB2	2.01	0.43
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.53	0.43
1:A:420:VAL:HG12	1:A:421:SER:N	2.32	0.43
1:A:649:SER:O	1:A:650:ARG:CB	2.67	0.43
1:A:801:THR:HG22	1:A:843:SER:CB	2.49	0.43
2:B:273:ARG:O	2:B:277:PHE:HB3	2.18	0.43
1:C:20:ASP:OD2	2:D:257:LEU:HD22	2.18	0.43
1:C:658:LEU:O	1:C:659:ASP:OD1	2.37	0.43
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.52	0.43
1:C:848:HIS:HB2	2:D:485:SER:HB3	2.01	0.43
1:C:1001:LEU:O	1:C:1001:LEU:HD23	2.18	0.43
1:C:1003:CYS:HB3	1:C:1008:CYS:HB2	1.88	0.43
2:D:87:PRO:HD3	2:D:423:CYS:SG	2.59	0.43
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.99	0.43
2:D:285:LEU:O	2:D:287:HIS:N	2.51	0.43
1:A:71:MET:O	1:A:72:SER:C	2.55	0.43
1:A:560:SER:O	1:A:561:ARG:HG2	2.18	0.43
1:A:600:LEU:HD12	1:A:600:LEU:O	2.17	0.43
1:A:619:GLU:O	1:A:620:CYS:SG	2.76	0.43
1:A:934:HIS:ND1	1:A:1074:THR:HB	2.33	0.43
2:B:120:ASP:OD1	2:B:325:GLU:O	2.36	0.43
1:C:4:ASP:HB2	1:C:597:ARG:CZ	2.49	0.43
1:C:992:LEU:C	1:C:992:LEU:HD23	2.39	0.43
2:D:532:ARG:O	2:D:543:HIS:HB2	2.19	0.43
2:D:601:GLY:O	2:D:602:LYS:HB2	2.19	0.43
2:D:631:SER:HB3	2:D:664:LEU:HD11	2.01	0.43
1:A:41:ALA:O	1:A:42:ASN:C	2.56	0.43
1:A:93:VAL:HB	1:A:104:THR:HG23	2.01	0.43
1:A:650:ARG:HD3	1:A:729:ASN:CB	2.48	0.43
1:A:711:ILE:HD11	1:A:746:LEU:HD13	2.00	0.43
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.07	0.43
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.48	0.43
1:C:41:ALA:O	1:C:42:ASN:C	2.57	0.43
1:C:757:ILE:O	1:C:758:CYS:HB2	2.19	0.43
1:C:762:LEU:HD23	1:C:790:ASN:HA	1.99	0.43
1:C:848:HIS:O	1:C:848:HIS:ND1	2.51	0.43
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.48	0.43
2:D:334:ILE:HA	2:D:337:ALA:CB	2.49	0.43
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG12	1:A:70:ASN:N	2.34	0.43
1:A:372:ILE:O	1:A:372:ILE:HG13	2.19	0.43
2:B:639:THR:O	2:B:639:THR:HG23	2.19	0.43
2:B:652:TYR:HB3	2:B:667:VAL:HA	1.99	0.43
1:C:13:VAL:HG21	1:C:57:CYS:HB2	2.01	0.43
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.83	0.43
2:D:643:ARG:CZ	2:D:649:TRP:CZ2	3.02	0.43
1:A:374:MET:SD	1:A:417:PHE:CE2	3.12	0.43
2:B:154:VAL:HG22	2:B:155:LEU:N	2.34	0.43
2:B:188:LEU:HD12	2:B:230:TRP:HA	2.00	0.43
1:C:671:ALA:HB2	1:C:700:LEU:HD23	2.01	0.43
1:C:944:ARG:N	1:C:1020:VAL:HG21	2.34	0.43
2:D:154:VAL:HG22	2:D:155:LEU:N	2.34	0.43
1:A:99:ARG:HG3	1:A:100:ASN:OD1	2.18	0.43
1:A:392:LEU:HG	1:A:393:ALA:N	2.33	0.43
1:A:507:THR:HG22	1:A:569:LEU:CD1	2.48	0.43
1:A:566:GLY:O	1:A:567:GLN:C	2.56	0.43
1:A:575:LEU:HD12	1:A:576:THR:HG23	1.99	0.43
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.53	0.43
2:B:508:TYR:CZ	2:B:514:CYS:HB3	2.54	0.43
1:C:69:VAL:HG12	1:C:70:ASN:N	2.34	0.43
1:C:392:LEU:HG	1:C:393:ALA:N	2.34	0.43
1:C:402:VAL:HG12	1:C:443:LEU:HD22	2.01	0.43
1:C:609:ILE:CD1	1:C:632:GLN:OE1	2.66	0.43
1:C:621:ARG:CG	1:C:622:GLU:N	2.82	0.43
1:C:757:ILE:HD12	1:C:757:ILE:HA	1.91	0.43
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.58	0.43
2:D:75:GLN:O	2:D:97:PHE:HA	2.19	0.43
2:D:363:PHE:HB2	2:D:388:THR:HB	2.00	0.43
1:A:353:SER:C	1:A:354:PHE:CG	2.91	0.43
1:A:418:THR:HB	1:A:427:LYS:CG	2.48	0.43
1:A:919:LEU:HG	2:B:643:ARG:CZ	2.49	0.43
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.54	0.43
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.49	0.43
2:B:120:ASP:O	2:B:124:VAL:HB	2.18	0.43
2:B:234:THR:HG22	2:B:235:ARG:N	2.34	0.43
1:C:404:GLY:O	1:C:406:PRO:HD3	2.19	0.43
1:C:525:PRO:HA	1:C:532:GLY:HA2	2.00	0.43
1:C:594:LEU:HD12	1:C:594:LEU:N	2.34	0.43
1:C:786:VAL:CG1	1:C:859:PHE:CZ	2.99	0.43
1:C:1023:GLU:O	1:C:1024:LEU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:652:TYR:HB3	2:D:667:VAL:HA	2.00	0.43
5:K:1:NAG:O3	5:K:2:NAG:H2	2.19	0.43
1:A:620:CYS:HB3	1:A:702:SER:O	2.19	0.42
1:A:660:LEU:CD2	1:A:715:LEU:HB3	2.49	0.42
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.54	0.42
1:A:1018:PHE:O	1:A:1019:SER:C	2.57	0.42
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.53	0.42
2:B:601:GLY:O	2:B:602:LYS:HB2	2.19	0.42
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.54	0.42
1:C:575:LEU:CD1	1:C:576:THR:HG23	2.49	0.42
1:C:609:ILE:HB	1:C:610:PRO:CD	2.46	0.42
1:C:797:GLY:H	1:C:884:GLU:HB2	1.84	0.42
1:C:797:GLY:N	1:C:884:GLU:HB2	2.33	0.42
1:C:1018:PHE:O	1:C:1019:SER:C	2.55	0.42
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.54	0.42
2:D:120:ASP:O	2:D:124:VAL:HB	2.19	0.42
2:D:219:MET:HE2	2:D:262:GLY:HA2	2.01	0.42
2:D:432:ARG:HG2	2:D:432:ARG:NH1	2.34	0.42
4:F:3:MAN:O2	4:F:4:MAN:C1	2.66	0.42
1:A:790:ASN:O	1:A:853:GLY:O	2.37	0.42
1:A:905:VAL:O	1:A:1062:GLN:HG3	2.18	0.42
2:B:139:THR:HG22	2:B:140:GLU:N	2.34	0.42
2:B:631:SER:HB3	2:B:664:LEU:HD11	2.00	0.42
1:C:659:ASP:OD2	5:K:1:NAG:H82	2.11	0.42
1:C:799:THR:HA	1:C:845:ARG:HA	2.00	0.42
1:C:812:TYR:HD2	1:C:814:ALA:HB2	1.81	0.42
2:D:473:GLY:C	2:D:475:CYS:H	2.22	0.42
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.01	0.42
1:A:444:CYS:HB2	1:A:506:LEU:HD12	2.02	0.42
1:A:477:PRO:C	1:A:479:PRO:HD3	2.40	0.42
1:A:908:VAL:HG12	1:A:909:VAL:N	2.33	0.42
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.54	0.42
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.96	0.42
1:C:527:GLU:HG3	1:C:533:ALA:CB	2.50	0.42
1:C:660:LEU:CD2	1:C:715:LEU:HB3	2.49	0.42
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.54	0.42
1:A:594:LEU:HD12	1:A:594:LEU:N	2.35	0.42
2:B:98:ARG:HD2	2:B:384:ASN:OD1	2.19	0.42
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.01	0.42
1:C:68:ALA:HA	1:C:93:VAL:HG13	2.01	0.42
1:C:93:VAL:HB	1:C:104:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ARG:HG2	2:D:247:PHE:CZ	2.54	0.42
1:C:459:ILE:HD12	1:C:487:CYS:SG	2.60	0.42
1:C:813:VAL:HG23	1:C:823:ARG:HH12	1.84	0.42
2:D:438:HIS:ND1	2:D:460:GLU:HA	2.34	0.42
1:A:351:VAL:HG23	1:A:352:GLY:N	2.35	0.42
1:A:402:VAL:HG12	1:A:443:LEU:HD22	2.02	0.42
1:A:446:VAL:HG12	1:A:456:LEU:HD11	2.01	0.42
1:A:491:LEU:HD21	1:A:545:ILE:HG12	2.02	0.42
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.53	0.42
1:A:797:GLY:H	1:A:884:GLU:HB2	1.85	0.42
1:A:876:LEU:HB3	1:A:898:GLU:HG3	2.01	0.42
1:A:1023:GLU:O	1:A:1024:LEU:C	2.58	0.42
1:A:1058:SER:O	1:A:1059:VAL:CB	2.67	0.42
2:B:176:CYS:HB2	2:B:204:ILE:O	2.19	0.42
2:B:285:LEU:O	2:B:287:HIS:N	2.52	0.42
2:B:643:ARG:CZ	2:B:649:TRP:CZ2	3.02	0.42
1:C:372:ILE:HG13	1:C:372:ILE:O	2.19	0.42
2:D:428:ARG:HG3	2:D:428:ARG:HH11	1.84	0.42
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.54	0.42
1:C:102:TYR:CG	1:C:331:GLU:HB3	2.55	0.42
1:C:351:VAL:HG23	1:C:352:GLY:N	2.34	0.42
1:C:374:MET:SD	1:C:417:PHE:CZ	3.12	0.42
1:C:446:VAL:HG12	1:C:456:LEU:HD11	2.00	0.42
1:C:801:THR:HG22	1:C:843:SER:CB	2.49	0.42
1:C:893:THR:O	1:C:893:THR:HG23	2.20	0.42
2:D:188:LEU:HD12	2:D:230:TRP:HA	2.01	0.42
1:A:609:ILE:CD1	1:A:632:GLN:OE1	2.67	0.42
2:B:219:MET:CE	2:B:262:GLY:HA2	2.50	0.42
2:B:237:LEU:HD13	2:B:294:ILE:HG23	2.01	0.42
1:C:93:VAL:HB	1:C:104:THR:HG23	2.02	0.42
1:C:597:ARG:HA	1:C:598:PRO:HD3	1.90	0.42
1:C:772:LYS:O	1:C:773:SER:CB	2.68	0.42
2:D:27:LEU:CD2	2:D:446:GLY:HA2	2.50	0.42
2:D:186:LEU:HD21	2:D:198:GLU:HB2	2.02	0.42
2:D:234:THR:HG22	2:D:235:ARG:N	2.34	0.42
2:D:315:ILE:HA	2:D:316:PRO:HD3	1.87	0.42
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.02	0.42
1:A:975:PRO:HG2	1:A:977:LEU:HD11	2.02	0.42
1:A:1023:GLU:O	1:A:1023:GLU:HG2	2.19	0.42
2:B:74:LYS:HD2	2:B:103:TYR:OH	2.20	0.42
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:PRO:O	1:C:615:ARG:HB3	2.20	0.42
1:C:717:PHE:CE1	1:C:740:ARG:HA	2.55	0.42
1:C:811:ARG:O	1:C:811:ARG:HG3	2.19	0.42
1:C:905:VAL:O	1:C:1062:GLN:HG3	2.20	0.42
1:C:916:THR:O	1:C:1076:THR:HG23	2.20	0.42
2:D:27:LEU:HD21	2:D:446:GLY:HA2	2.02	0.42
2:D:532:ARG:HD3	2:D:554:GLU:HG3	2.02	0.42
1:A:102:TYR:CG	1:A:331:GLU:HB3	2.54	0.42
1:A:437:SER:HA	1:A:463:HIS:O	2.20	0.42
1:A:614:PRO:O	1:A:615:ARG:HB3	2.19	0.42
1:A:660:LEU:HB3	1:A:713:LEU:HD21	2.01	0.42
1:A:860:LEU:HD23	1:A:861:ALA:N	2.34	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42
2:B:155:LEU:HD12	2:B:155:LEU:C	2.40	0.42
2:B:186:LEU:HD21	2:B:198:GLU:HB2	2.02	0.42
2:B:215:LEU:HD12	2:B:246:HIS:O	2.19	0.42
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.50	0.42
2:B:484:CYS:HB2	2:B:488:GLY:O	2.19	0.42
1:C:491:LEU:HD21	1:C:545:ILE:HG12	2.01	0.42
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.02	0.42
1:C:827:LEU:HD12	1:C:827:LEU:O	2.19	0.42
1:C:915:PHE:CZ	1:C:917:LYS:HB2	2.55	0.42
2:D:215:LEU:HD12	2:D:246:HIS:O	2.20	0.42
2:D:265:HIS:HB2	2:D:273:ARG:HG3	2.01	0.42
4:J:1:NAG:O3	4:J:2:NAG:C7	2.68	0.42
1:A:435:ILE:HD13	2:B:311:LEU:HB2	2.02	0.42
1:A:656:VAL:HG21	1:A:687:LEU:HD12	2.01	0.42
1:A:772:LYS:O	1:A:773:SER:CB	2.68	0.42
1:A:799:THR:HG22	1:A:845:ARG:HB3	2.02	0.42
1:A:930:HIS:O	1:A:931:VAL:C	2.58	0.42
2:B:363:PHE:HB2	2:B:388:THR:HB	2.01	0.42
1:C:484:ARG:NH1	2:D:586:GLN:HG3	2.35	0.42
1:C:1063:LEU:N	1:C:1064:PRO:CD	2.83	0.42
4:J:2:NAG:C3	4:J:3:MAN:H2	2.49	0.42
1:A:71:MET:HA	1:A:92:THR:C	2.40	0.41
1:A:327:SER:O	1:A:328:PHE:O	2.38	0.41
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.55	0.41
1:A:433:THR:HG23	1:A:464:TYR:CE1	2.55	0.41
1:A:721:GLY:O	1:A:722:LYS:HB2	2.19	0.41
1:A:944:ARG:N	1:A:1020:VAL:HG21	2.34	0.41
1:A:956:VAL:O	1:A:963:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:SER:HB2	2:B:21:CYS:SG	2.60	0.41
2:B:611:LYS:CB	2:B:667:VAL:HB	2.50	0.41
1:C:99:ARG:HG3	1:C:100:ASN:OD1	2.20	0.41
1:C:499:TRP:CZ2	2:D:284:GLN:HG3	2.55	0.41
1:C:613:ILE:HA	1:C:614:PRO:HD3	1.86	0.41
1:C:721:GLY:O	1:C:722:LYS:HB2	2.19	0.41
2:D:429:ASP:HB2	2:D:430:GLN:H	1.66	0.41
1:A:25:TYR:HB3	1:A:29:TRP:O	2.19	0.41
1:A:444:CYS:HB3	1:A:506:LEU:HD13	2.01	0.41
1:A:533:ALA:HA	1:A:554:ALA:HA	2.02	0.41
1:A:698:LEU:C	1:A:699:LEU:HD12	2.41	0.41
1:A:766:PHE:CD1	1:A:766:PHE:C	2.93	0.41
1:A:800:ILE:HD11	1:A:879:ALA:HB1	2.02	0.41
2:B:75:GLN:O	2:B:97:PHE:HA	2.19	0.41
2:B:75:GLN:CD	2:B:98:ARG:O	2.58	0.41
2:B:188:LEU:CD1	2:B:230:TRP:HA	2.50	0.41
2:B:587:LEU:N	2:B:587:LEU:CD1	2.83	0.41
1:C:71:MET:HA	1:C:92:THR:C	2.40	0.41
1:C:433:THR:HG23	1:C:464:TYR:CE1	2.55	0.41
1:C:444:CYS:HB3	1:C:506:LEU:HD13	2.02	0.41
2:D:187:LYS:HG2	2:D:188:LEU:N	2.36	0.41
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.51	0.41
2:D:484:CYS:HB2	2:D:488:GLY:O	2.20	0.41
1:A:103:LEU:HD12	2:B:156:PRO:HB3	2.01	0.41
1:A:380:ASP:O	1:A:381:MET:HB3	2.20	0.41
1:A:969:VAL:HG13	1:A:969:VAL:O	2.20	0.41
1:A:1065:GLY:O	1:A:1066:GLN:CG	2.68	0.41
1:A:1075:THR:HG23	1:A:1075:THR:O	2.20	0.41
2:B:565:ARG:HA	2:B:565:ARG:HD3	1.84	0.41
1:C:94:HIS:CD2	2:D:155:LEU:CD2	2.97	0.41
1:C:384:SER:HB2	1:C:405:ALA:HB1	2.02	0.41
1:C:477:PRO:C	1:C:479:PRO:HD3	2.41	0.41
1:C:566:GLY:O	1:C:567:GLN:C	2.59	0.41
1:C:599:VAL:O	1:C:599:VAL:CG2	2.67	0.41
1:C:1075:THR:HG23	1:C:1075:THR:O	2.20	0.41
2:D:98:ARG:HD2	2:D:384:ASN:OD1	2.21	0.41
1:A:604:VAL:CG1	1:A:742:PHE:CD2	3.03	0.41
1:A:634:ASN:HA	1:A:695:ASN:HA	2.03	0.41
2:B:27:LEU:CG	2:B:446:GLY:HA2	2.51	0.41
2:B:532:ARG:O	2:B:543:HIS:HB2	2.19	0.41
1:C:637:LEU:HD11	1:C:658:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:ILE:HD11	1:C:746:LEU:HD13	2.02	0.41
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.55	0.41
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.08	0.41
1:C:1023:GLU:O	1:C:1023:GLU:HG2	2.20	0.41
2:D:155:LEU:HB2	2:D:156:PRO:CA	2.39	0.41
2:D:155:LEU:C	2:D:155:LEU:HD12	2.41	0.41
2:D:222:ALA:HB2	2:D:294:ILE:HD12	2.02	0.41
2:D:462:GLN:CG	2:D:463:THR:N	2.84	0.41
2:D:517:ILE:HD12	2:D:518:ASN:N	2.35	0.41
2:D:611:LYS:CB	2:D:667:VAL:HB	2.51	0.41
1:A:799:THR:HG22	1:A:845:ARG:CB	2.51	0.41
1:A:915:PHE:CZ	1:A:917:LYS:HB2	2.55	0.41
1:A:916:THR:O	1:A:1076:THR:HG23	2.20	0.41
2:B:101:LYS:HG2	2:B:102:GLY:H	1.85	0.41
2:B:472:GLU:HA	2:B:475:CYS:HB3	2.02	0.41
1:C:103:LEU:HD12	2:D:156:PRO:HB3	2.02	0.41
1:C:756:HIS:O	1:C:756:HIS:CG	2.74	0.41
1:C:915:PHE:CD1	1:C:1074:THR:CG2	3.03	0.41
2:D:75:GLN:CD	2:D:98:ARG:O	2.59	0.41
2:D:438:HIS:CE1	2:D:460:GLU:CB	3.04	0.41
2:D:599:PRO:HB2	2:D:603:TYR:HE2	1.85	0.41
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.35	0.41
2:B:505:LYS:HA	2:B:517:ILE:HG21	2.02	0.41
1:C:543:PRO:O	1:C:544:SER:HB3	2.21	0.41
1:C:649:SER:O	1:C:650:ARG:CB	2.68	0.41
1:C:671:ALA:O	1:C:672:THR:HG23	2.20	0.41
1:C:831:SER:CA	1:C:842:THR:HG22	2.50	0.41
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.20	0.41
1:C:1040:ILE:CD1	1:C:1042:GLN:HB2	2.51	0.41
1:C:1058:SER:O	1:C:1059:VAL:CB	2.67	0.41
1:C:1065:GLY:O	1:C:1066:GLN:CG	2.69	0.41
2:D:98:ARG:HD3	2:D:386:PRO:HG3	2.02	0.41
1:A:610:PRO:O	1:A:611:ALA:C	2.58	0.41
2:B:98:ARG:HD3	2:B:386:PRO:HG3	2.02	0.41
2:B:187:LYS:HG2	2:B:188:LEU:N	2.36	0.41
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.03	0.41
2:D:652:TYR:O	2:D:652:TYR:CD2	2.74	0.41
1:A:464:TYR:O	1:A:465:TYR:HB3	2.21	0.41
1:A:527:GLU:HG3	1:A:533:ALA:CB	2.50	0.41
1:A:624:VAL:HG23	1:A:625:VAL:H	1.86	0.41
1:A:717:PHE:CE1	1:A:740:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:PHE:CD1	1:A:1074:THR:CG2	3.04	0.41
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.86	0.41
1:C:492:TYR:CD2	1:C:492:TYR:O	2.74	0.41
1:C:533:ALA:HA	1:C:554:ALA:HA	2.03	0.41
1:C:713:LEU:C	1:C:713:LEU:HD23	2.41	0.41
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.36	0.41
2:D:74:LYS:NZ	2:D:103:TYR:HE2	2.18	0.41
2:D:161:HIS:HA	2:D:162:PRO:HA	1.81	0.41
2:D:176:CYS:HB2	2:D:204:ILE:O	2.21	0.41
1:A:328:PHE:HB2	1:A:354:PHE:O	2.21	0.41
1:A:404:GLY:O	1:A:406:PRO:HD3	2.21	0.41
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.56	0.41
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.84	0.41
1:A:586:GLY:HA2	1:A:591:VAL:HG23	2.03	0.41
1:A:599:VAL:O	1:A:599:VAL:CG2	2.68	0.41
1:A:713:LEU:C	1:A:713:LEU:HD23	2.41	0.41
1:A:831:SER:CA	1:A:842:THR:HG22	2.50	0.41
1:A:849:LEU:HA	2:B:482:ILE:HG22	2.03	0.41
1:A:946:LEU:HD12	1:A:946:LEU:O	2.21	0.41
2:B:302:SER:HB3	2:B:322:GLU:CG	2.51	0.41
2:B:305:VAL:HG13	2:B:306:LYS:HG3	2.02	0.41
1:C:374:MET:SD	1:C:417:PHE:CE2	3.14	0.41
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.50	0.41
1:C:444:CYS:HB2	1:C:506:LEU:HD12	2.03	0.41
1:C:648:GLY:O	1:C:649:SER:O	2.39	0.41
1:C:698:LEU:C	1:C:699:LEU:HD12	2.42	0.41
1:C:776:VAL:HG12	1:C:867:PRO:O	2.21	0.41
1:C:918:TYR:C	2:D:643:ARG:HH22	2.24	0.41
1:C:941:LEU:N	1:C:941:LEU:CD1	2.84	0.41
1:C:975:PRO:HG2	1:C:977:LEU:HD11	2.02	0.41
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.51	0.41
2:D:293:ASN:OD1	2:D:412:THR:HG22	2.21	0.41
1:A:4:ASP:OD2	1:A:597:ARG:NH2	2.54	0.41
1:A:823:ARG:NH1	1:A:825:LEU:O	2.54	0.41
2:B:265:HIS:HB2	2:B:273:ARG:HG3	2.02	0.41
2:B:352:LEU:HD22	2:B:358:VAL:HG23	2.03	0.41
1:C:402:VAL:HG22	1:C:416:ILE:HG23	2.03	0.41
2:D:110:LEU:CD1	2:D:218:MET:SD	3.09	0.41
2:D:169:CYS:HA	2:D:170:PRO:HD3	1.84	0.41
2:D:181:ALA:HB3	2:D:271:TYR:CE2	2.56	0.41
2:D:260:ASN:OD1	2:D:260:ASN:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HD12	1:A:487:CYS:SG	2.61	0.40
1:A:907:THR:HG21	1:A:1053:ILE:HD13	2.03	0.40
1:C:363:TYR:CD1	1:C:369:PRO:HB3	2.56	0.40
1:C:507:THR:HG21	1:C:570:SER:HA	2.03	0.40
1:C:593:LEU:C	1:C:594:LEU:HD12	2.41	0.40
1:C:824:SER:N	1:C:825:LEU:HG	2.34	0.40
1:C:930:HIS:O	1:C:931:VAL:C	2.58	0.40
2:D:230:TRP:CE3	2:D:235:ARG:HD3	2.57	0.40
2:D:368:VAL:HG11	2:D:370:HIS:ND1	2.36	0.40
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.50	0.40
1:A:543:PRO:O	1:A:544:SER:HB3	2.21	0.40
1:C:121:VAL:O	1:C:121:VAL:CG1	2.69	0.40
1:C:648:GLY:O	1:C:649:SER:C	2.60	0.40
1:C:660:LEU:HB3	1:C:713:LEU:HD21	2.02	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
1:C:934:HIS:ND1	1:C:1074:THR:HB	2.35	0.40
2:D:256:ILE:HG21	2:D:275:ASN:O	2.22	0.40
2:D:587:LEU:N	2:D:587:LEU:CD1	2.84	0.40
2:D:654:LEU:HD13	2:D:665:ILE:CG1	2.51	0.40
1:A:103:LEU:HD21	2:B:155:LEU:CD2	2.52	0.40
1:A:637:LEU:HD11	1:A:658:LEU:HD21	2.03	0.40
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.21	0.40
2:B:230:TRP:CE3	2:B:235:ARG:HD3	2.56	0.40
2:B:372:ASN:O	2:B:373:GLN:HG3	2.22	0.40
1:C:438:TYR:CD1	2:D:247:PHE:HE1	2.39	0.40
1:C:604:VAL:CG1	1:C:742:PHE:CD2	3.02	0.40
1:C:799:THR:HG22	1:C:845:ARG:CB	2.51	0.40
1:C:800:ILE:HD11	1:C:879:ALA:HB1	2.03	0.40
1:C:956:VAL:O	1:C:963:VAL:HG23	2.21	0.40
1:A:638:TYR:HB3	1:A:691:ALA:HA	2.03	0.40
1:A:756:HIS:O	1:A:756:HIS:CG	2.74	0.40
1:A:757:ILE:O	1:A:758:CYS:HB2	2.22	0.40
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.52	0.40
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.03	0.40
1:A:714:ARG:C	1:A:714:ARG:HD2	2.42	0.40
1:A:752:CYS:HB2	1:A:793:GLU:OE2	2.21	0.40
1:A:804:HIS:CB	1:A:808:LEU:HD11	2.52	0.40
1:A:971:HIS:N	1:A:972:PRO:HD3	2.36	0.40
1:C:43:GLN:HG2	1:C:44:THR:HG23	2.03	0.40
1:C:897:LEU:HD12	1:C:897:LEU:O	2.22	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	880/1095 (80%)	667 (76%)	192 (22%)	21 (2%)	6	35
1	C	878/1095 (80%)	664 (76%)	195 (22%)	19 (2%)	6	37
2	B	671/687 (98%)	518 (77%)	141 (21%)	12 (2%)	8	41
2	D	671/687 (98%)	512 (76%)	146 (22%)	13 (2%)	8	40
All	All	3100/3564 (87%)	2361 (76%)	674 (22%)	65 (2%)	7	38

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	ILE
2	B	162	PRO
2	B	598	SER
1	C	624	VAL
1	C	757	ILE
2	D	162	PRO
2	D	438	HIS
2	D	598	SER
1	A	490	VAL
1	A	624	VAL
1	A	649	SER
1	A	722	LYS
1	A	931	VAL
1	A	956	VAL
2	B	314	ILE
1	C	490	VAL
1	C	649	SER
1	C	722	LYS
1	C	931	VAL
1	C	956	VAL
2	D	314	ILE
2	D	436	LEU

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Mol	Chain	Res	Type
2	D	437	CYS
1	A	773	SER
1	A	847	ASN
1	C	773	SER
1	C	847	ASN
1	A	26	ALA
1	A	354	PHE
1	A	691	ALA
2	B	69	HIS
2	B	101	LYS
2	B	639	THR
1	C	354	PHE
1	C	558	LEU
1	C	691	ALA
2	D	435	SER
2	D	639	THR
1	A	327	SER
1	A	558	LEU
1	A	819	GLN
1	A	846	ILE
1	C	26	ALA
1	C	846	ILE
2	D	69	HIS
1	A	121	VAL
2	B	351	ALA
2	B	377	ASP
2	B	617	PHE
1	C	121	VAL
2	D	377	ASP
1	A	816	GLY
2	D	517	ILE
1	A	120	PRO
1	A	540	VAL
1	A	1059	VAL
2	B	204	ILE
2	B	517	ILE
1	C	120	PRO
1	C	1007	GLY
2	D	204	ILE
2	B	421	PRO
1	C	540	VAL
1	C	1059	VAL

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Mol	Chain	Res	Type
2	D	421	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	753/934 (81%)	742 (98%)	11 (2%)	65	81
1	C	751/934 (80%)	740 (98%)	11 (2%)	65	81
2	B	582/592 (98%)	579 (100%)	3 (0%)	88	94
2	D	582/592 (98%)	575 (99%)	7 (1%)	71	84
All	All	2668/3052 (87%)	2636 (99%)	32 (1%)	71	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	395	TRP
1	A	478	LEU
1	A	565	PHE
1	A	679	ARG
1	A	714	ARG
1	A	823	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	A	1052	GLU
2	B	467	SER
2	B	479	ASN
2	B	511	TYR
1	C	118	ARG
1	C	119	LEU
1	C	395	TRP
1	C	478	LEU
1	C	565	PHE
1	C	679	ARG

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Mol	Chain	Res	Type
1	C	714	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
1	C	1052	GLU
2	D	426	ARG
2	D	429	ASP
2	D	432	ARG
2	D	467	SER
2	D	479	ASN
2	D	489	ASP
2	D	511	TYR

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	334	GLN
1	A	434	GLN
1	A	472	GLN
1	A	692	HIS
1	A	819	GLN
2	B	159	ASN
2	B	295	GLN
1	C	124	GLN
1	C	334	GLN
1	C	434	GLN
1	C	472	GLN
1	C	692	HIS
2	D	159	ASN
2	D	295	GLN
2	D	458	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.53	0	17,19,21	0.80	0
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.61	0	17,19,21	1.09	1 (5%)
4	NAG	F	2	4	14,14,15	0.56	0	17,19,21	1.91	2 (11%)
4	MAN	F	3	4	11,11,12	0.48	0	15,15,17	1.34	2 (13%)
4	MAN	F	4	4	11,11,12	0.71	0	15,15,17	0.79	1 (6%)
4	MAN	F	5	4	11,11,12	0.68	0	15,15,17	0.70	0
5	NAG	G	1	5,1	14,14,15	0.50	0	17,19,21	1.70	2 (11%)
5	NAG	G	2	5	14,14,15	0.74	0	17,19,21	1.48	2 (11%)
5	MAN	G	3	5	11,11,12	0.80	0	15,15,17	2.62	2 (13%)
5	NAG	H	1	5,1	14,14,15	0.54	0	17,19,21	2.58	5 (29%)
5	NAG	H	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.23	2 (11%)
5	MAN	H	3	5	11,11,12	0.70	0	15,15,17	2.54	4 (26%)
3	NAG	I	1	1,3	14,14,15	0.50	0	17,19,21	0.72	0
3	NAG	I	2	3	14,14,15	0.58	0	17,19,21	1.13	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.60	0	17,19,21	1.14	2 (11%)
4	NAG	J	2	4	14,14,15	0.54	0	17,19,21	1.99	2 (11%)
4	MAN	J	3	4	11,11,12	0.45	0	15,15,17	1.32	2 (13%)
4	MAN	J	4	4	11,11,12	0.72	0	15,15,17	0.78	1 (6%)
4	MAN	J	5	4	11,11,12	0.64	0	15,15,17	0.69	0
5	NAG	K	1	5,1	14,14,15	0.59	0	17,19,21	1.41	1 (5%)
5	NAG	K	2	5	14,14,15	0.56	0	17,19,21	1.15	1 (5%)
5	MAN	K	3	5	11,11,12	0.94	0	15,15,17	1.16	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	MAN	F	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	MAN	H	3	5	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	MAN	K	3	5	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	C1-C2	2.46	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1	NAG	C1-O5-C5	9.15	124.44	112.19
5	G	3	MAN	C1-O5-C5	8.83	124.02	112.19
4	J	2	NAG	C1-O5-C5	6.85	121.36	112.19
4	F	2	NAG	C1-O5-C5	6.57	120.99	112.19
5	H	3	MAN	C1-C2-C3	-6.49	100.19	109.64
5	H	3	MAN	C1-O5-C5	-5.62	104.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	1	NAG	C1-O5-C5	4.66	118.43	112.19
5	G	3	MAN	C1-C2-C3	3.76	115.12	109.64
5	G	2	NAG	O4-C4-C3	3.60	118.87	110.38
5	G	2	NAG	C1-O5-C5	3.42	116.77	112.19
3	I	2	NAG	C1-O5-C5	3.29	116.59	112.19
5	H	3	MAN	O5-C5-C6	3.23	113.94	107.66
5	K	1	NAG	O3-C3-C2	3.10	115.85	109.40
4	F	3	MAN	O3-C3-C2	3.01	116.20	110.05
5	K	2	NAG	C1-O5-C5	2.93	116.12	112.19
4	J	3	MAN	O3-C3-C2	2.85	115.88	110.05
5	H	2	NAG	O4-C4-C5	-2.79	102.44	109.32
5	G	1	NAG	O3-C3-C2	2.76	115.13	109.40
4	J	1	NAG	O5-C1-C2	2.73	115.51	111.29
4	F	3	MAN	C2-C3-C4	-2.63	106.24	110.86
4	F	1	NAG	O5-C1-C2	2.62	115.34	111.29
4	J	3	MAN	C2-C3-C4	-2.61	106.27	110.86
3	E	2	NAG	C1-O5-C5	2.59	115.65	112.19
5	K	3	MAN	C1-C2-C3	2.48	113.26	109.64
5	H	2	NAG	C1-O5-C5	2.45	115.47	112.19
5	H	1	NAG	O5-C1-C2	2.44	115.06	111.29
5	H	3	MAN	C3-C4-C5	2.42	114.62	110.23
4	J	2	NAG	O5-C1-C2	2.36	114.95	111.29
5	H	1	NAG	C3-C4-C5	2.31	114.43	110.23
4	F	2	NAG	O5-C1-C2	2.29	114.84	111.29
5	H	1	NAG	O3-C3-C2	2.23	114.03	109.40
5	K	3	MAN	O5-C5-C6	-2.16	103.46	107.66
4	J	1	NAG	C1-O5-C5	2.12	115.03	112.19
5	H	1	NAG	O4-C4-C3	-2.04	105.56	110.38
4	F	4	MAN	C1-O5-C5	-2.03	109.46	112.19
4	J	4	MAN	C1-O5-C5	-2.00	109.50	112.19

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1
4	F	3	MAN	C1
4	J	1	NAG	C1
4	J	3	MAN	C1
5	G	3	MAN	C1
5	H	3	MAN	C1
5	K	3	MAN	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C3-C2-N2-C7
4	J	3	MAN	O5-C5-C6-O6
4	F	3	MAN	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
4	F	3	MAN	C4-C5-C6-O6
4	J	3	MAN	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C3-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	4	MAN	1	0

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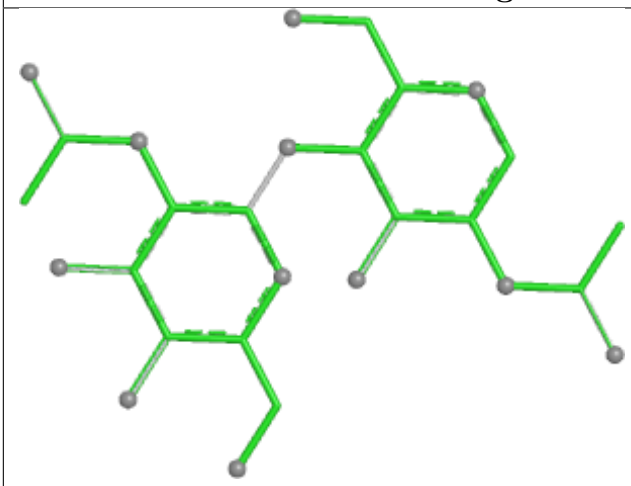
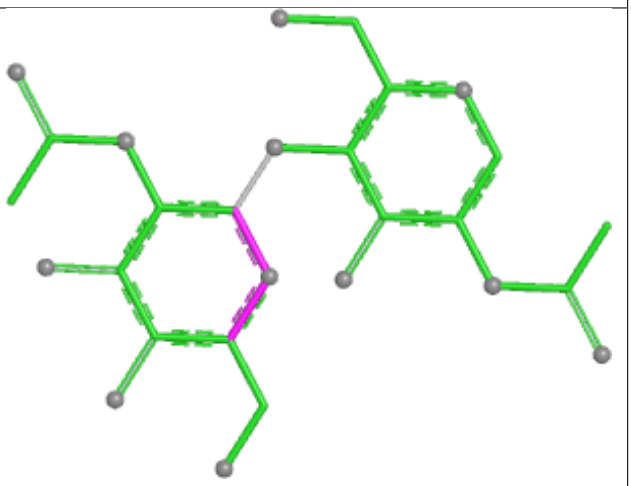
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	4	0
5	K	1	NAG	11	0
5	K	3	MAN	2	0
4	J	2	NAG	4	0
4	J	3	MAN	3	0
5	H	1	NAG	2	0
4	F	3	MAN	3	0
5	K	2	NAG	4	0
4	F	2	NAG	3	0
5	H	2	NAG	2	0
4	J	4	MAN	1	0
5	H	3	MAN	1	0
4	F	1	NAG	2	0
4	J	1	NAG	3	0
4	J	5	MAN	1	0
5	G	2	NAG	1	0

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

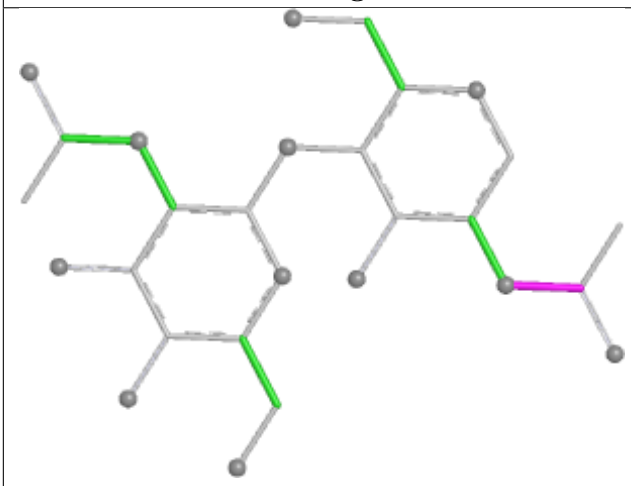
Oligosaccharide Chain E



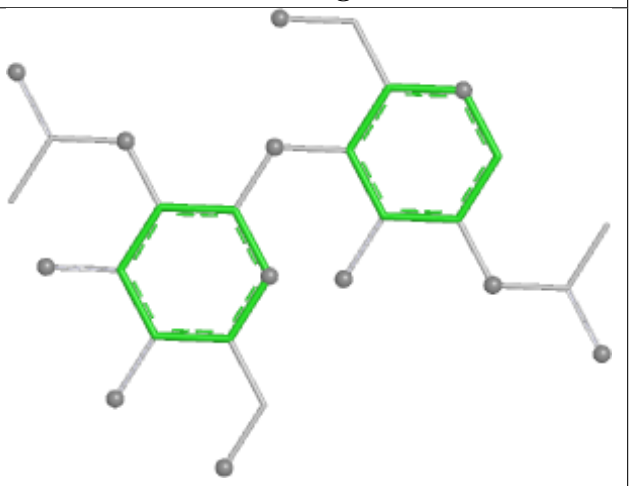
Bond lengths



Bond angles

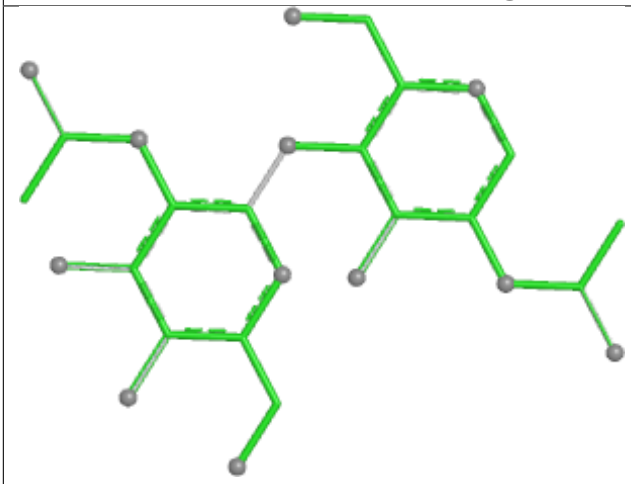


Torsions

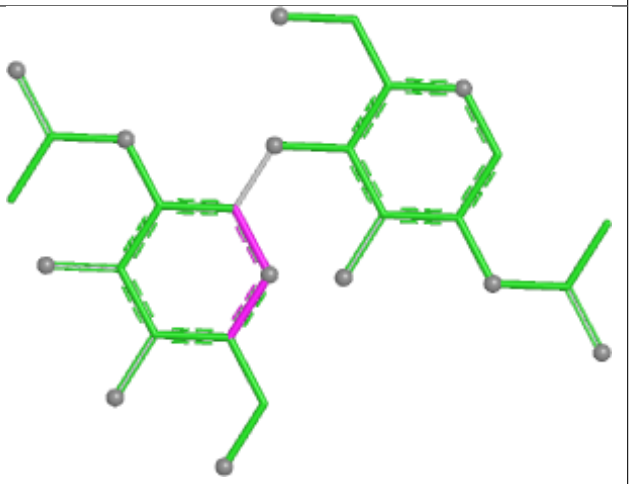


Rings

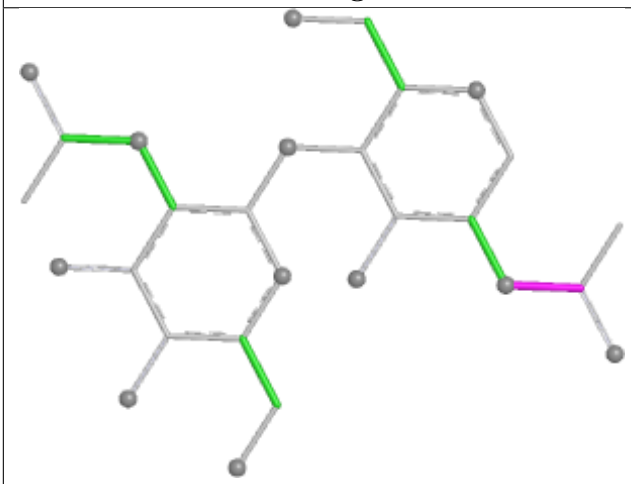
Oligosaccharide Chain I



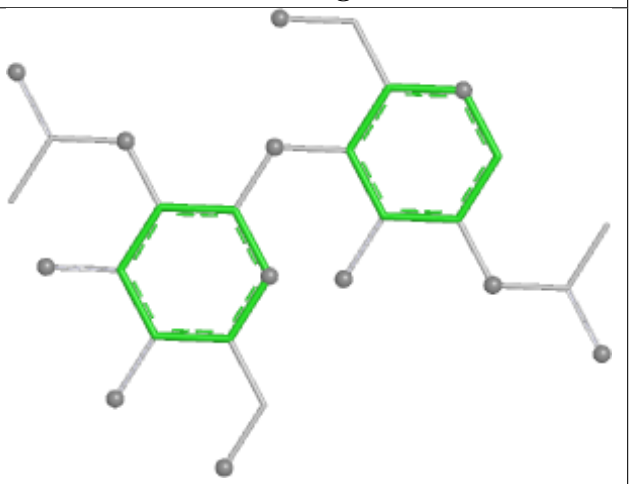
Bond lengths



Bond angles

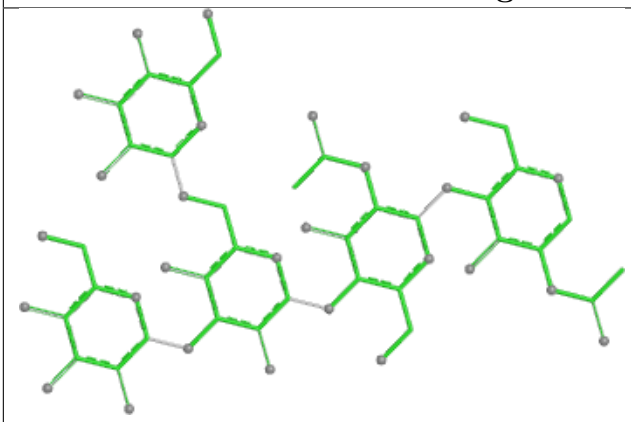


Torsions

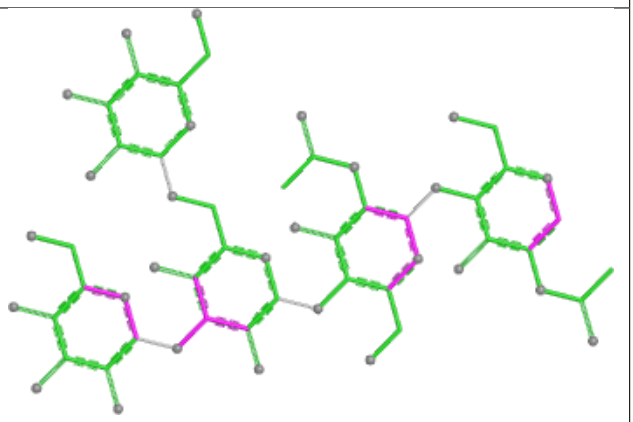


Rings

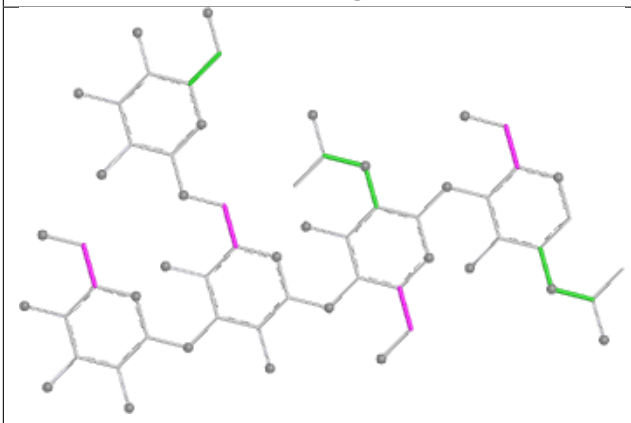
Oligosaccharide Chain F



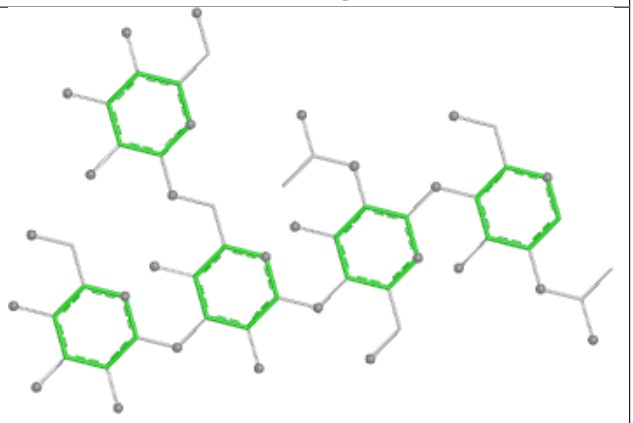
Bond lengths



Bond angles

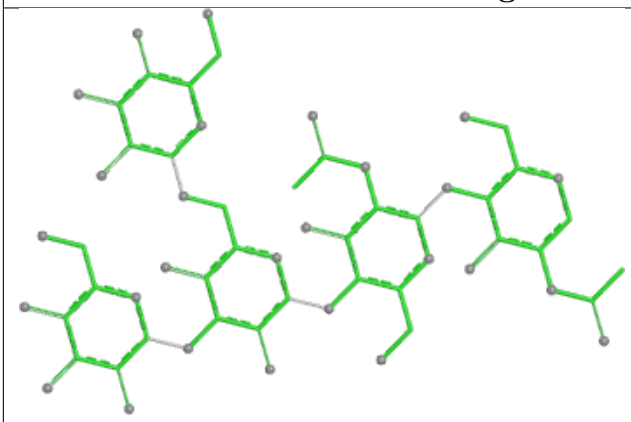


Torsions

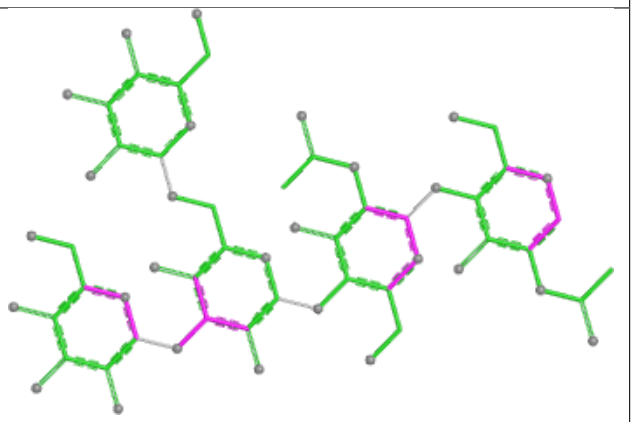


Rings

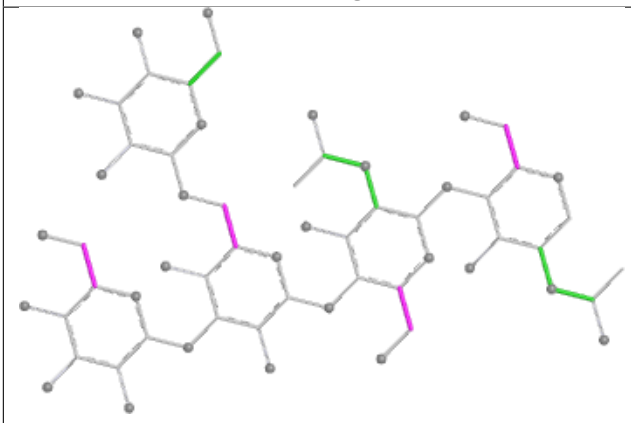
Oligosaccharide Chain J



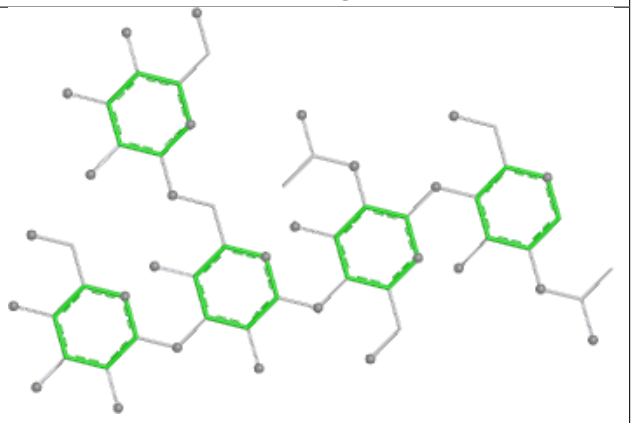
Bond lengths



Bond angles

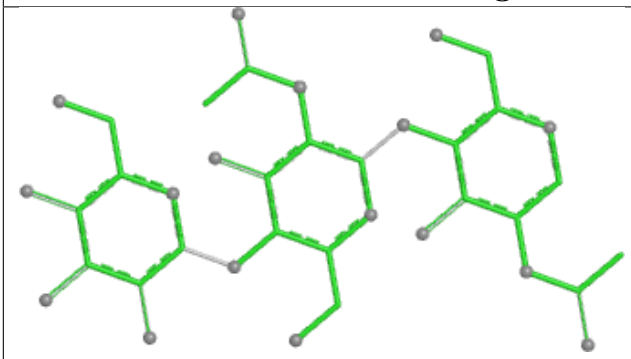


Torsions

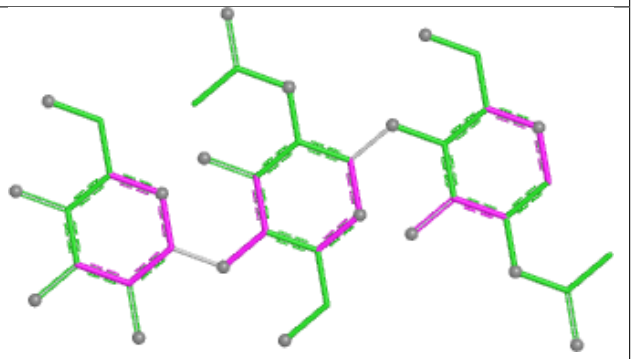


Rings

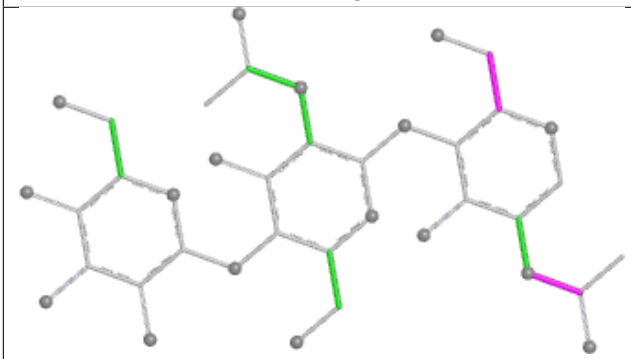
Oligosaccharide Chain G



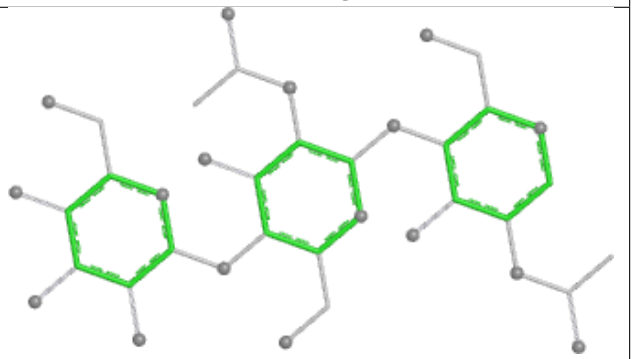
Bond lengths



Bond angles

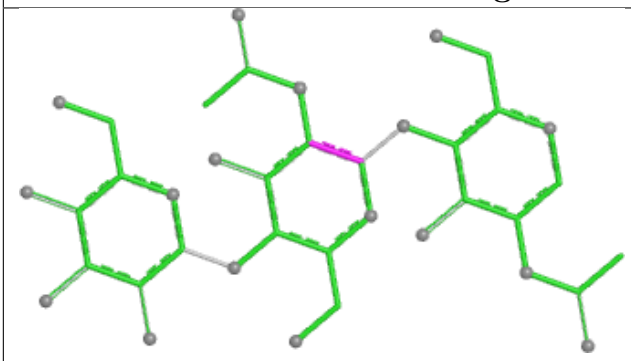


Torsions

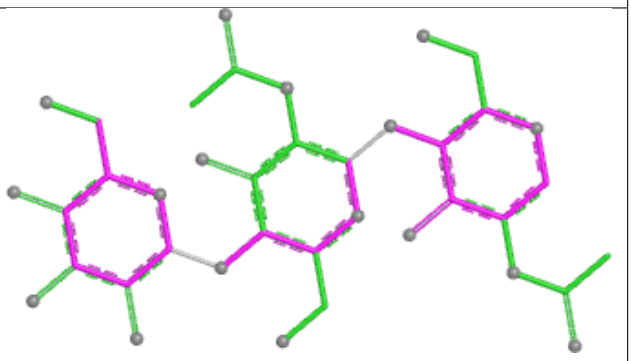


Rings

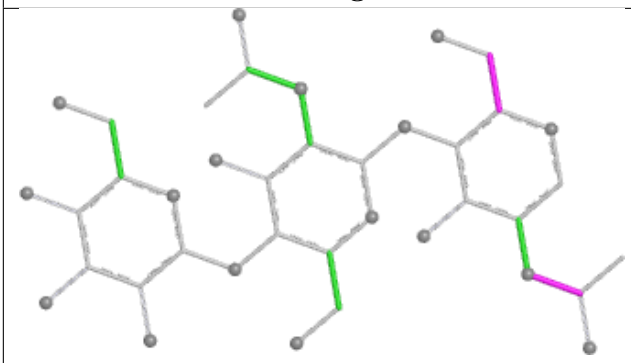
Oligosaccharide Chain H



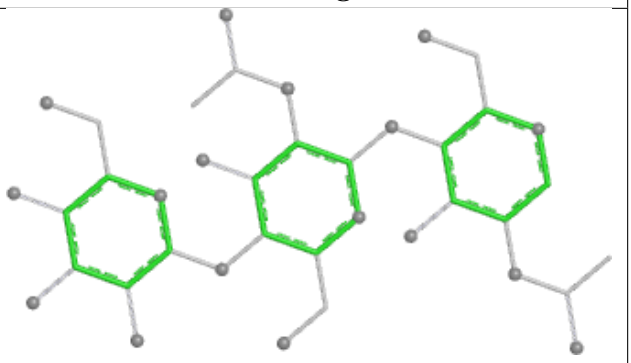
Bond lengths



Bond angles

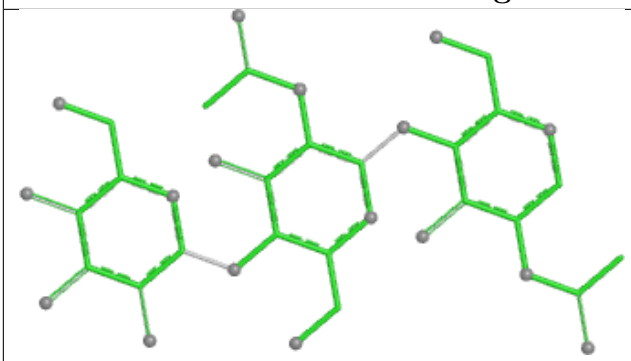


Torsions

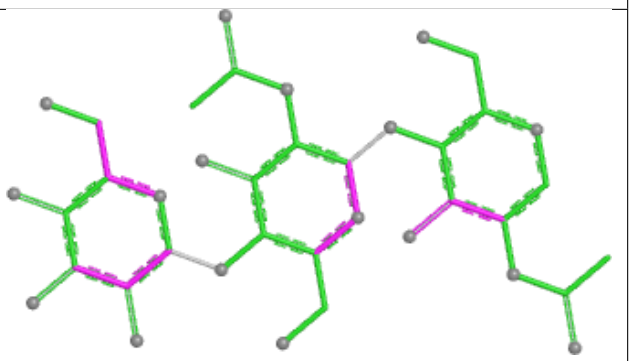


Rings

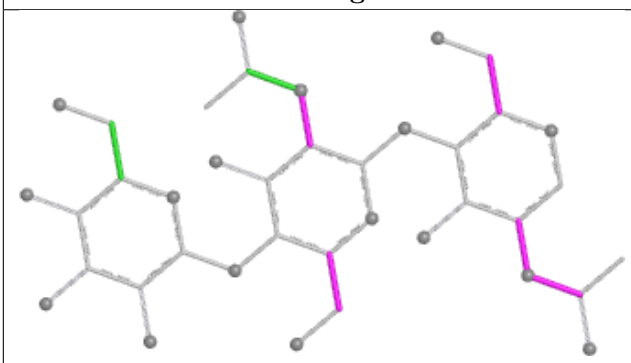
Oligosaccharide Chain K



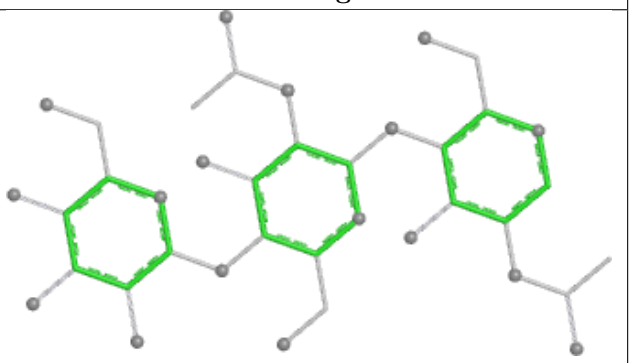
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	3678	1	14,14,15	0.51	0	17,19,21	0.69	0
6	NAG	C	3880	1	14,14,15	0.32	0	17,19,21	1.60	1 (5%)
6	NAG	D	3094	2	14,14,15	0.53	0	17,19,21	0.63	0
6	NAG	B	3094	2	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
8	MAN	C	3378	-	11,11,12	0.96	1 (9%)	15,15,17	2.11	3 (20%)
6	NAG	B	3479	2	14,14,15	4.41	14 (100%)	17,19,21	3.46	10 (58%)
6	NAG	C	3678	1	14,14,15	0.52	0	17,19,21	0.65	0
6	NAG	D	3479	2	14,14,15	4.87	13 (92%)	17,19,21	2.81	9 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
8	MAN	C	3378	-	-	2/2/19/22	0/1/1/1
6	NAG	B	3479	2	-	1/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3479	2	-	0/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3479	NAG	O5-C5	7.04	1.57	1.43
6	D	3479	NAG	C4-C5	6.74	1.67	1.53
6	B	3479	NAG	C4-C5	6.45	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3479	NAG	O7-C7	6.45	1.37	1.23
6	D	3479	NAG	O7-C7	6.41	1.37	1.23
6	D	3479	NAG	O5-C1	6.08	1.53	1.43
6	D	3479	NAG	C1-C2	5.99	1.60	1.52
6	B	3479	NAG	C4-C3	5.53	1.66	1.52
6	B	3479	NAG	C3-C2	4.97	1.62	1.52
6	D	3479	NAG	C8-C7	4.72	1.60	1.50
6	B	3479	NAG	C2-N2	4.70	1.54	1.46
6	B	3479	NAG	O5-C5	4.61	1.52	1.43
6	D	3479	NAG	C4-C3	4.31	1.63	1.52
6	B	3479	NAG	C8-C7	4.27	1.59	1.50
6	D	3479	NAG	C2-N2	4.25	1.53	1.46
6	D	3479	NAG	C7-N2	4.10	1.47	1.34
6	B	3479	NAG	C1-C2	4.00	1.57	1.52
6	D	3479	NAG	O4-C4	3.87	1.52	1.43
6	B	3479	NAG	O3-C3	3.82	1.52	1.43
6	D	3479	NAG	C3-C2	3.48	1.59	1.52
6	D	3479	NAG	C6-C5	3.45	1.63	1.51
6	B	3479	NAG	C6-C5	3.38	1.63	1.51
6	B	3479	NAG	O5-C1	2.99	1.48	1.43
6	B	3479	NAG	O4-C4	2.82	1.50	1.43
6	B	3479	NAG	C7-N2	2.67	1.43	1.34
8	C	3378	MAN	O5-C1	-2.48	1.39	1.43
6	B	3479	NAG	O6-C6	2.38	1.52	1.42
6	D	3479	NAG	O3-C3	2.31	1.48	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3479	NAG	O5-C1-C2	8.39	124.28	111.29
6	D	3479	NAG	C1-O5-C5	7.25	121.90	112.19
8	C	3378	MAN	C1-C2-C3	-5.52	101.60	109.64
6	C	3880	NAG	C1-O5-C5	5.50	119.55	112.19
8	C	3378	MAN	C1-O5-C5	-4.59	106.04	112.19
6	B	3479	NAG	O3-C3-C4	4.52	121.04	110.38
6	B	3479	NAG	C8-C7-N2	-4.26	109.06	116.12
6	B	3479	NAG	C3-C4-C5	4.11	117.69	110.23
6	B	3479	NAG	C1-O5-C5	4.06	117.62	112.19
6	D	3479	NAG	C2-N2-C7	-3.85	117.74	122.90
6	B	3479	NAG	O5-C5-C4	3.71	119.84	110.83
6	B	3479	NAG	O5-C5-C6	3.50	114.48	107.66
6	D	3479	NAG	C4-C3-C2	3.43	116.04	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	3479	NAG	O5-C5-C6	3.21	113.91	107.66
6	B	3479	NAG	C2-N2-C7	-3.15	118.68	122.90
8	C	3378	MAN	C3-C4-C5	3.09	115.84	110.23
6	D	3479	NAG	O4-C4-C3	3.08	117.64	110.38
6	D	3479	NAG	O5-C1-C2	3.00	115.93	111.29
6	B	3479	NAG	O4-C4-C3	2.78	116.94	110.38
6	B	3094	NAG	C1-O5-C5	2.49	115.52	112.19
6	D	3479	NAG	O7-C7-C8	-2.32	117.92	122.05
6	D	3479	NAG	C3-C4-C5	2.27	114.36	110.23
6	D	3479	NAG	O5-C5-C4	2.24	116.27	110.83
6	B	3479	NAG	O7-C7-C8	2.02	125.65	122.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3880	NAG	C8-C7-N2-C2
6	C	3880	NAG	O7-C7-N2-C2
8	C	3378	MAN	O5-C5-C6-O6
8	C	3378	MAN	C4-C5-C6-O6
6	C	3880	NAG	O5-C5-C6-O6
6	B	3479	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3378	MAN	1	0
6	B	3479	NAG	1	0
6	D	3479	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	884/1095 (80%)	0.13	36 (4%)	37	27	106, 204, 303, 383	0
1	C	882/1095 (80%)	0.09	33 (3%)	41	30	112, 207, 304, 400	0
2	B	673/687 (97%)	0.40	72 (10%)	6	5	133, 256, 325, 426	2 (0%)
2	D	673/687 (97%)	0.52	90 (13%)	3	3	144, 258, 332, 424	2 (0%)
All	All	3112/3564 (87%)	0.26	231 (7%)	14	10	106, 233, 318, 426	4 (0%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	92	ALA	11.4
2	D	433	ASP	10.6
2	B	470	GLU	8.9
2	D	432	ARG	8.6
2	B	323	LEU	7.9
2	B	161	HIS	7.6
2	B	67	GLU	7.1
1	A	396	LYS	7.1
2	B	72	GLY	7.0
2	B	469	GLN	7.0
1	A	482	TRP	6.8
2	B	92	ALA	6.8
1	C	482	TRP	6.6
2	B	73	GLN	6.5
2	D	32	PRO	6.3
1	C	108	PHE	6.2
2	D	391	VAL	6.1
2	D	429	ASP	6.1
2	D	91	ALA	5.8
2	D	161	HIS	5.7
2	D	95	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	1045	VAL	5.5
2	D	35	PRO	5.4
2	D	430	GLN	5.3
1	C	33	GLY	5.2
2	D	236	LEU	5.2
1	A	726	ALA	5.1
2	B	414	ILE	5.1
1	C	1078	LEU	5.0
2	B	160	THR	5.0
1	A	483	ARG	4.9
2	D	107	LEU	4.7
2	D	669	GLU	4.7
2	B	32	PRO	4.6
2	D	435	SER	4.5
1	A	124	GLN	4.4
1	A	326	SER	4.3
1	C	624	VAL	4.3
2	B	629	GLN	4.3
2	D	393	VAL	4.3
1	A	102	TYR	4.3
2	D	49	ARG	4.2
2	D	33	GLY	4.2
1	C	102	TYR	4.1
1	A	918	TYR	4.1
1	C	74	GLY	4.0
2	D	106	ASP	3.9
2	B	446	GLY	3.9
1	A	87	LEU	3.9
2	B	35	PRO	3.9
1	C	623	GLN	3.8
1	A	335	GLU	3.8
2	B	429	ASP	3.7
1	A	108	PHE	3.7
2	D	389	PHE	3.7
1	C	396	LYS	3.7
1	A	1078	LEU	3.7
2	B	66	GLN	3.7
2	D	160	THR	3.7
2	D	189	THR	3.7
1	A	125	GLU	3.7
2	D	206	GLY	3.5
1	A	1044	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	667	VAL	3.5
2	B	391	VAL	3.5
2	D	629	GLN	3.5
2	D	607	ALA	3.5
2	B	331	VAL	3.4
2	B	39	ARG	3.4
2	D	431	SER	3.4
2	B	330	VAL	3.4
2	D	320	VAL	3.4
1	C	117	GLN	3.4
2	D	618	GLY	3.4
2	B	335	LYS	3.4
2	D	407	ARG	3.4
2	B	622	SER	3.4
2	D	668	ASP	3.4
2	D	179	PRO	3.3
2	D	235	ARG	3.3
1	C	106	LEU	3.3
2	B	296	PRO	3.3
2	D	379	ASP	3.3
2	D	272	LYS	3.3
1	C	124	GLN	3.3
2	D	93	PHE	3.2
2	B	358	VAL	3.2
2	D	634	PRO	3.2
1	A	592	LEU	3.2
2	D	104	PRO	3.2
2	B	1	GLN	3.1
1	C	973	GLN	3.1
2	D	65	THR	3.1
1	C	594	LEU	3.1
2	B	91	ALA	3.1
2	B	377	ASP	3.0
2	D	425	CYS	3.1
2	B	40	CYS	3.0
2	D	642	GLU	3.0
2	B	345	VAL	3.0
2	D	69	HIS	3.0
2	B	180	PHE	3.0
1	A	594	LEU	3.0
2	D	72	GLY	3.0
2	B	430	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	26	LYS	2.9
1	C	918	TYR	2.9
2	D	237	LEU	2.9
2	B	416	THR	2.9
2	D	48	MET	2.9
2	B	55	ASP	2.9
2	D	399	ILE	2.8
2	B	407	ARG	2.8
2	D	369	THR	2.8
2	B	395	ALA	2.8
1	C	483	ARG	2.8
2	D	632	ASN	2.8
2	B	81	VAL	2.8
1	C	95	HIS	2.8
2	D	613	GLU	2.8
2	D	231	ARG	2.8
2	D	144	ILE	2.7
2	D	56	ILE	2.7
2	B	351	ALA	2.7
2	D	97	PHE	2.7
2	D	651	ALA	2.7
2	B	389	PHE	2.7
2	D	414	ILE	2.7
1	C	87	LEU	2.6
1	A	33	GLY	2.6
2	B	433	ASP	2.6
1	C	68	ALA	2.6
2	D	8	VAL	2.6
1	A	817	GLN	2.6
2	D	67	GLU	2.6
1	A	394	LEU	2.6
2	D	105	ILE	2.6
2	D	427	CYS	2.6
1	C	335	GLU	2.6
2	B	636	LYS	2.6
2	B	664	LEU	2.6
2	D	630	LEU	2.6
2	D	195	PHE	2.6
2	B	322	GLU	2.5
2	D	641	LYS	2.5
2	D	318	SER	2.5
1	C	592	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	628	LEU	2.5
2	B	56	ILE	2.5
2	B	665	ILE	2.5
1	A	361	PHE	2.5
1	A	88	ALA	2.5
1	A	118	ARG	2.5
2	B	321	GLY	2.5
1	C	121	VAL	2.5
2	B	393	VAL	2.5
2	B	267	GLU	2.4
1	C	88	ALA	2.4
2	D	287	HIS	2.4
2	B	97	PHE	2.4
1	C	725	LEU	2.4
2	B	320	VAL	2.4
1	C	120	PRO	2.4
2	D	133	ARG	2.4
1	C	625	VAL	2.4
1	A	106	LEU	2.4
2	D	207	ASN	2.3
1	C	481	GLY	2.3
2	D	76	LEU	2.3
2	D	610	LEU	2.3
2	D	404	PHE	2.3
2	D	428	ARG	2.3
2	B	431	SER	2.3
2	D	377	ASP	2.3
2	B	298	PHE	2.3
2	B	333	LEU	2.3
2	B	443	LEU	2.3
1	A	339	ALA	2.3
1	C	10	ALA	2.3
2	B	237	LEU	2.2
2	B	334	ILE	2.2
2	B	93	PHE	2.2
1	A	104	THR	2.2
2	B	33	GLY	2.2
2	B	611	LYS	2.2
1	A	409	GLN	2.2
2	B	272	LYS	2.2
1	A	919	LEU	2.2
1	C	104	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	113	LEU	2.2
1	C	125	GLU	2.2
2	B	227	GLU	2.2
2	D	386	PRO	2.2
2	D	413	ASP	2.2
1	A	347	VAL	2.2
2	D	469	GLN	2.2
1	A	722	LYS	2.2
2	D	62	LEU	2.2
2	D	443	LEU	2.2
2	D	387	ILE	2.2
2	D	335	LYS	2.2
2	B	329	ASN	2.1
2	D	561	LEU	2.1
2	D	298	PHE	2.1
2	B	328	SER	2.1
1	A	127	PRO	2.1
1	A	110	LEU	2.1
1	A	821	GLN	2.1
2	B	206	GLY	2.1
2	D	344	ARG	2.1
2	D	178	PRO	2.1
2	D	64	GLU	2.1
1	C	480	ARG	2.1
2	D	390	GLN	2.1
2	B	207	ASN	2.1
1	C	9	THR	2.1
2	D	66	GLN	2.1
1	A	363	TYR	2.1
2	D	416	THR	2.1
2	D	173	GLU	2.1
2	B	607	ALA	2.0
2	B	384	ASN	2.0
2	D	205	SER	2.0
2	D	115	TYR	2.0
2	B	48	MET	2.0
1	C	1045	VAL	2.0
2	B	185	VAL	2.0
1	A	480	ARG	2.0
1	A	1047	VAL	2.0
2	D	94	ASN	2.0
2	D	227	GLU	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)

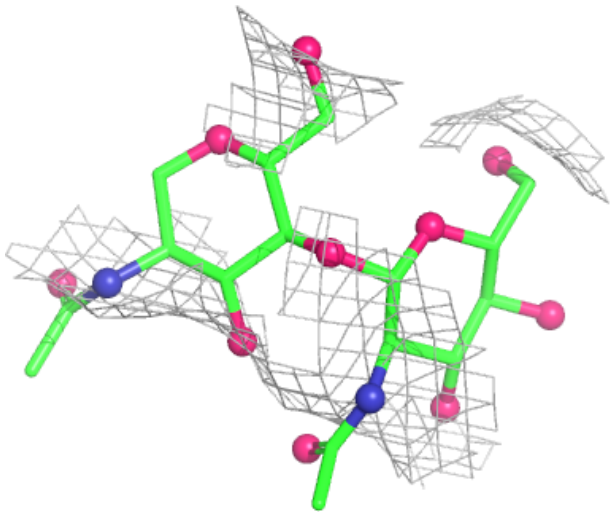
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

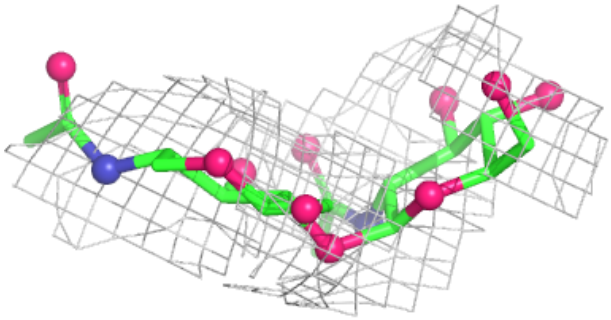
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	F	4	11/12	0.21	0.49	278,313,361,364	0
4	MAN	F	3	11/12	0.27	0.32	221,338,359,359	0
4	MAN	J	5	11/12	0.40	0.31	233,301,351,351	0
5	MAN	H	3	11/12	0.43	0.57	310,353,388,410	0
5	MAN	G	3	11/12	0.44	0.20	295,349,390,420	0
3	NAG	E	2	14/15	0.55	0.28	222,255,345,354	0
4	MAN	J	4	11/12	0.56	0.27	217,294,356,376	0
4	MAN	J	3	11/12	0.57	0.31	271,326,353,354	0
3	NAG	I	2	14/15	0.62	0.42	228,295,376,376	0
4	MAN	F	5	11/12	0.69	0.26	241,288,357,366	0
4	NAG	J	2	14/15	0.71	0.29	205,297,391,446	0
4	NAG	F	2	14/15	0.72	0.31	273,293,381,415	0
5	MAN	K	3	11/12	0.73	0.14	313,359,401,410	0
3	NAG	E	1	14/15	0.75	0.32	209,289,325,337	0
5	NAG	H	2	14/15	0.78	0.37	252,291,337,341	0
4	NAG	F	1	14/15	0.80	0.27	181,314,385,389	0
5	NAG	G	2	14/15	0.81	0.22	225,292,336,341	0
4	NAG	J	1	14/15	0.82	0.30	230,326,381,388	0
3	NAG	I	1	14/15	0.82	0.22	219,245,283,285	0
5	NAG	K	2	14/15	0.85	0.22	237,294,351,395	0
5	NAG	H	1	14/15	0.91	0.19	197,234,285,285	0
5	NAG	G	1	14/15	0.93	0.19	84,247,290,297	0
5	NAG	K	1	14/15	0.94	0.18	90,220,322,330	0

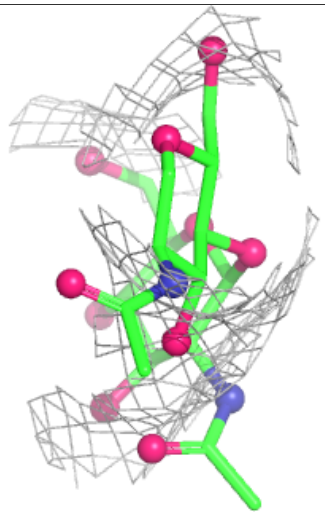
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

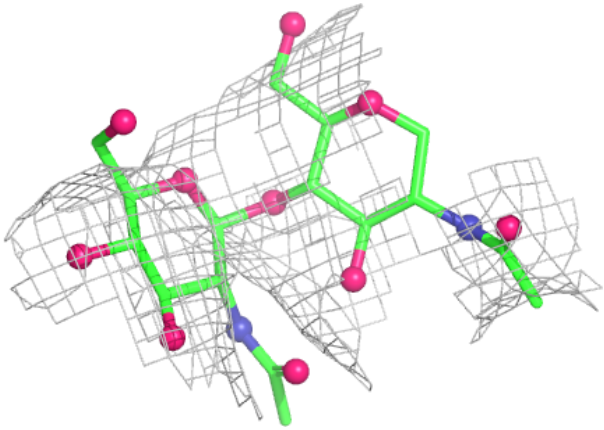


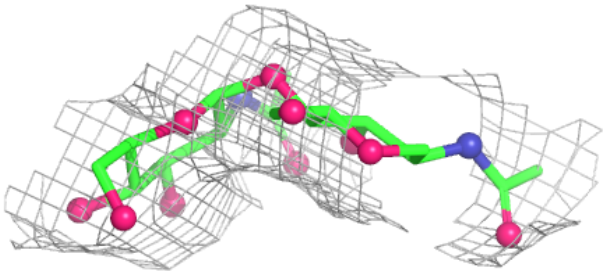


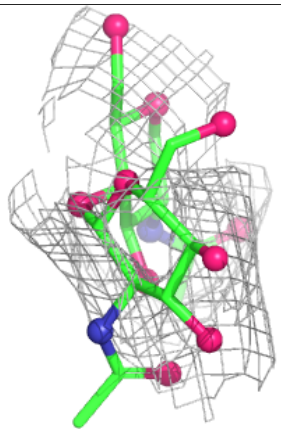


Electron density around Chain I:

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

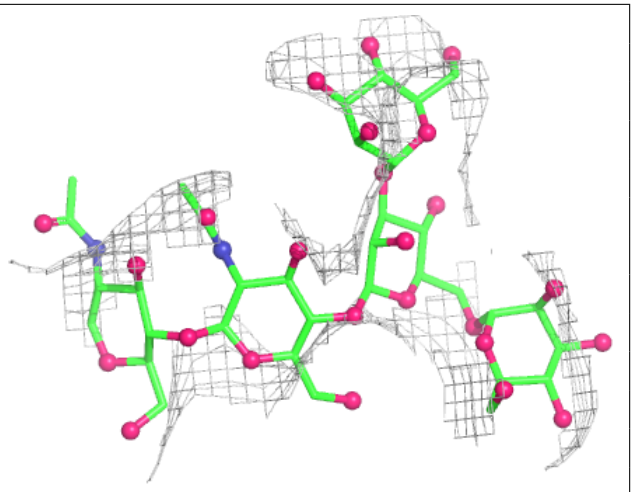


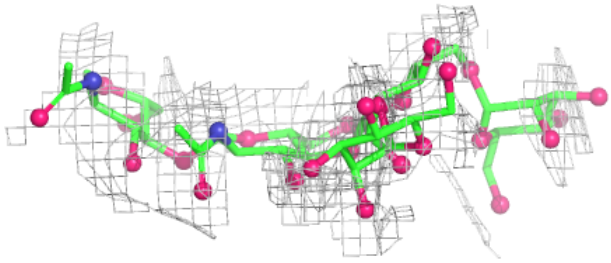


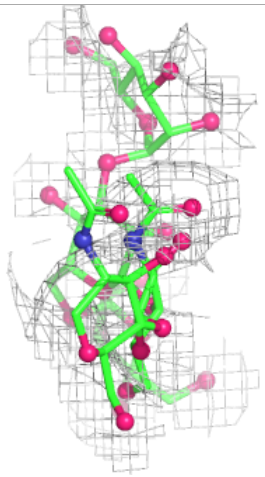


Electron density around Chain F:

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

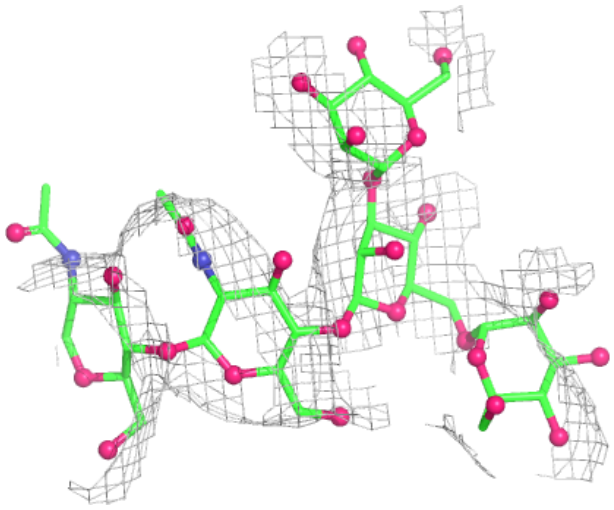


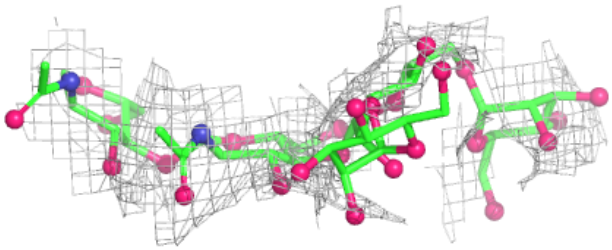


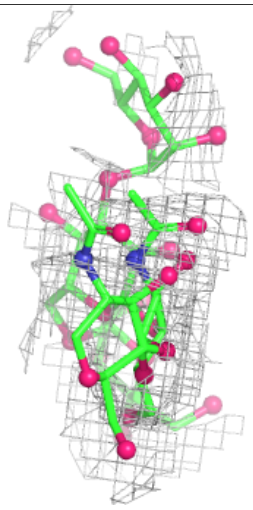


Electron density around Chain J:

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

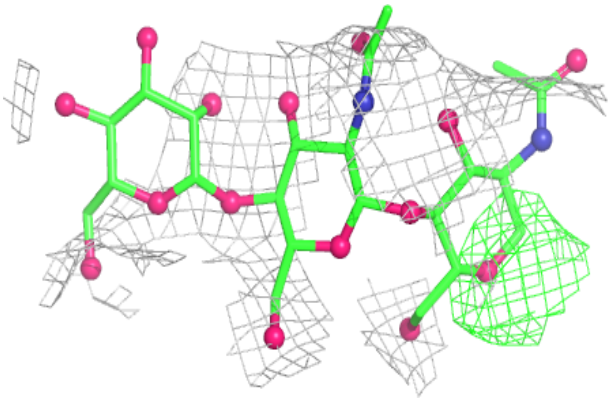


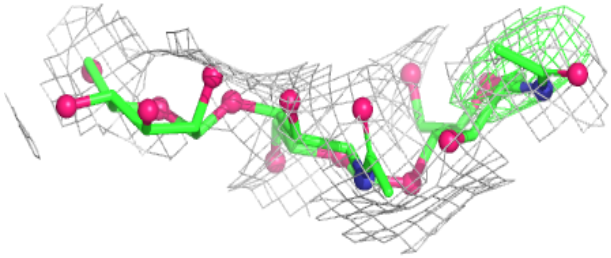


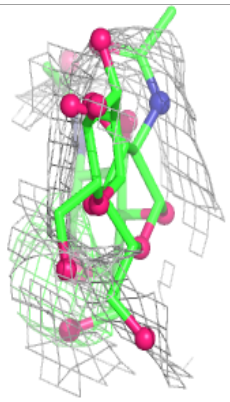


Electron density around Chain G:

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

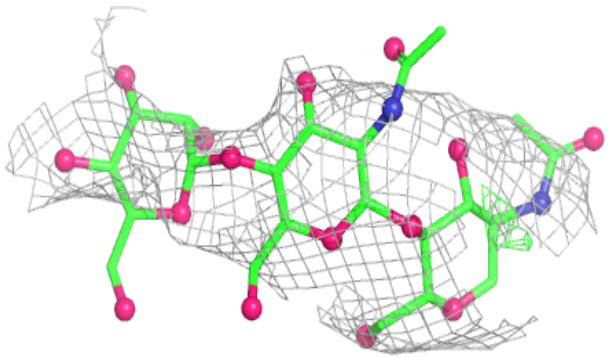


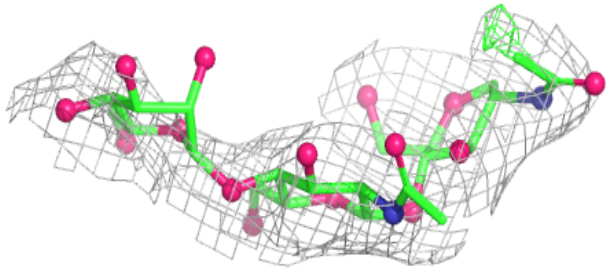


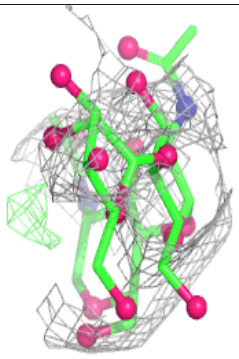


Electron density around Chain H:

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

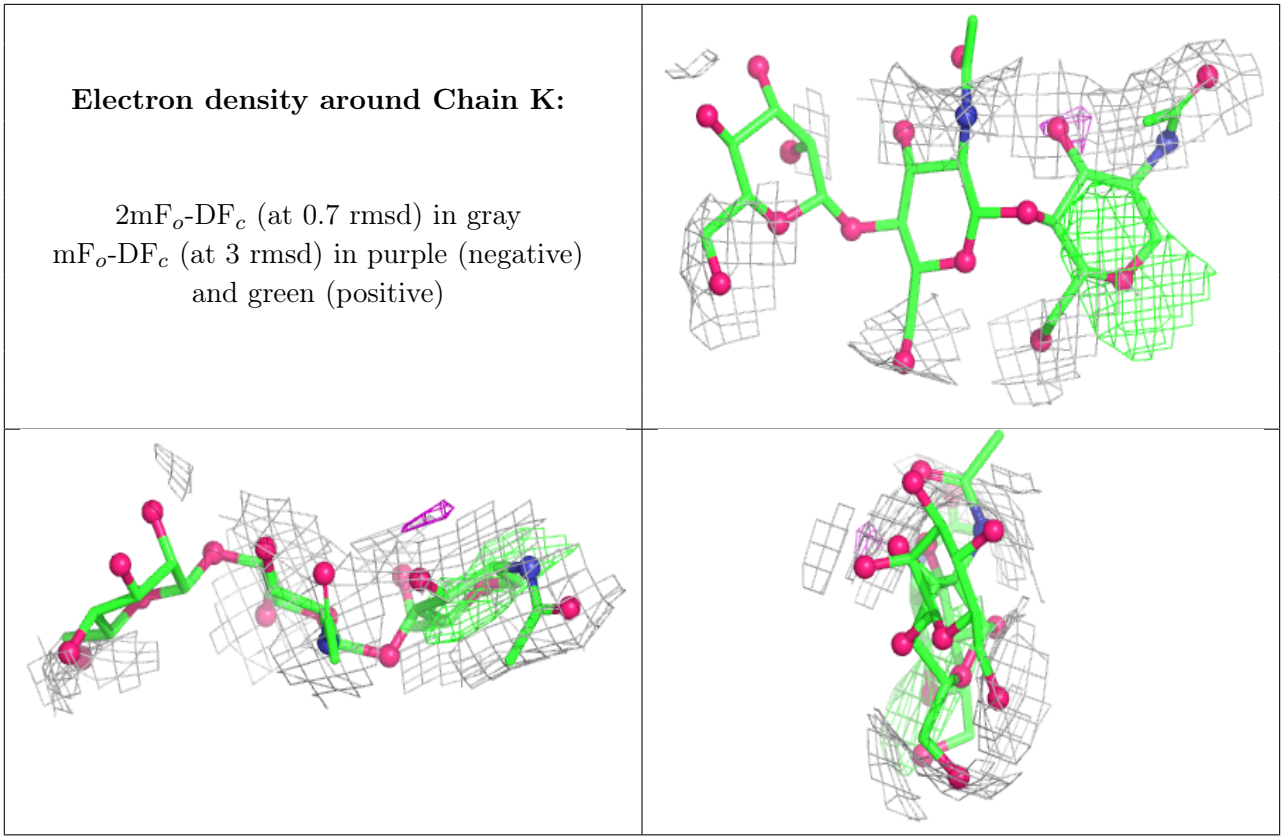






Electron density around Chain K:

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



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
8	MAN	C	3378	11/12	0.37	0.52	241,288,352,362	0
7	CA	B	2002	1/1	0.50	0.22	608,608,608,608	0
7	CA	A	2007	1/1	0.61	0.14	240,240,240,240	0
7	CA	C	2005	1/1	0.65	0.16	215,215,215,215	0
7	CA	C	2007	1/1	0.67	0.14	237,237,237,237	0
6	NAG	D	3094	14/15	0.73	0.42	254,283,315,325	0
7	CA	A	2005	1/1	0.74	0.11	193,193,193,193	0
7	CA	D	2002	1/1	0.76	0.08	594,594,594,594	0
6	NAG	B	3094	14/15	0.79	0.36	232,281,317,341	0
6	NAG	D	3479	14/15	0.80	0.27	191,259,284,291	0
6	NAG	B	3479	14/15	0.82	0.23	213,256,300,333	0
6	NAG	A	3678	14/15	0.86	0.25	167,304,342,378	0
6	NAG	C	3880	14/15	0.87	0.27	136,198,243,253	0
7	CA	C	2006	1/1	0.90	0.18	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	C	3678	14/15	0.90	0.22	177,279,379,392	0
7	CA	A	2006	1/1	0.95	0.17	143,143,143,143	0

6.5 Other polymers (i)

There are no such residues in this entry.