Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 06:05 pm GMT

PDB ID	:	2XWB
Title	:	Crystal Structure of Complement C3b in complex with Factors B and D
Authors	:	Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.
Deposited on	:	2010-11-01
Resolution	:	3.49 Å(reported)

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

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

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

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

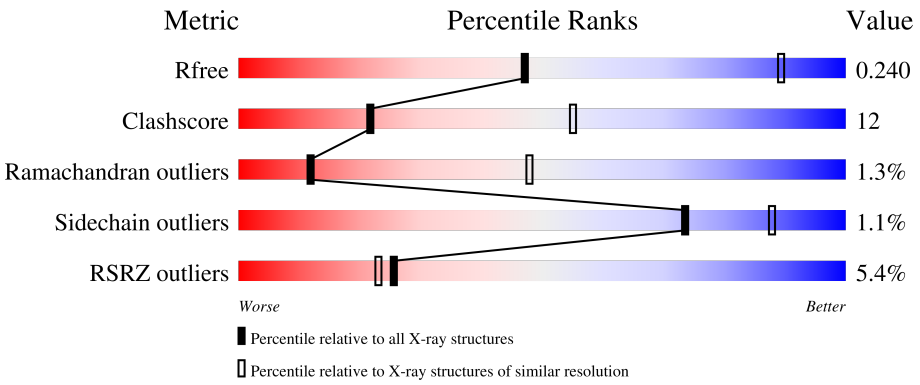
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.49 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	642	7% 70% 28%
1	C	642	13% 70% 28%
2	B	912	2% 71% 27%
2	D	912	9% 70% 28%
3	F	732	% 73% 23%

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Mol	Chain	Length	Quality of chain
3	H	732	3%, 74%, 21%
4	I	228	80%, 19%
4	J	228	78%, 21%
5	E	2	50%, 50%
5	G	2	50%, 50%
5	K	2	100%
6	L	3	33%, 67%
6	M	3	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	K	1	-	-	X	-
8	NAG	F	1747	X	-	-	-
9	GOL	J	1229	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 39285 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 COMPLEMENT C3B BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	640	4992	3179	846	952	15	0	0	0
1	C	640	4992	3179	846	952	15	0	0	0

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	901	7197	4563	1210	1386	38	0	0	0
2	D	901	7197	4563	1210	1386	38	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024
D	991	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	714	5627	3536	979	1079	33	0	0	0
3	H	711	5608	3523	976	1076	33	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	GLY	ASP	engineered mutation	UNP P00751
F	260	ASP	ASN	engineered mutation	UNP P00751

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Chain	Residue	Modelled	Actual	Comment	Reference
F	740	ALA	-	expression tag	UNP P00751
F	741	ALA	-	expression tag	UNP P00751
H	254	GLY	ASP	engineered mutation	UNP P00751
H	260	ASP	ASN	engineered mutation	UNP P00751
H	740	ALA	-	expression tag	UNP P00751
H	741	ALA	-	expression tag	UNP P00751

- Molecule 4 is a protein called COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	228	1710	1058	325	317	10	0	0	0
4	J	228	1710	1058	325	317	10	0	0	0

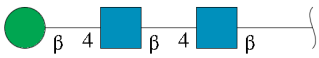
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	ALA	SER	engineered mutation	UNP P00746
J	183	ALA	SER	engineered mutation	UNP P00746

- Molecule 5 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
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0
5	G	2	28	16	2	10	0	0	0
5	K	2	28	16	2	10	0	0	0

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

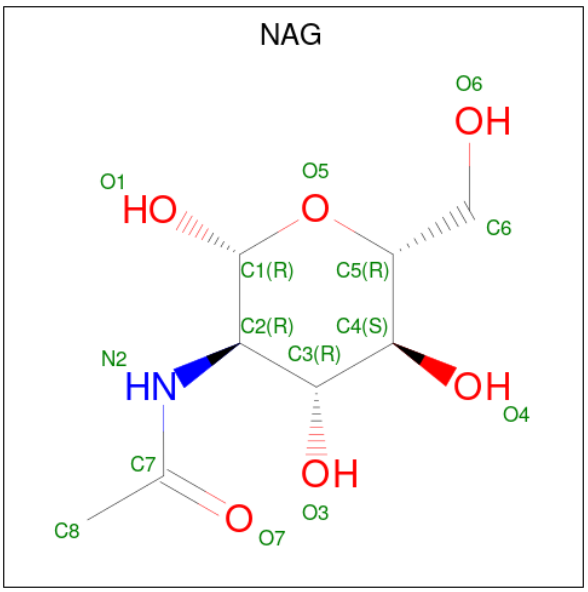


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	L	3	39	22	2	15	0	0	0
			Total	C	N	O			
6	M	3	39	22	2	15	0	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	A	1	1	1	0	0
			Total	Mg		
7	C	1	1	1	0	0
			Total	Mg		
7	F	1	1	1	0	0
			Total	Mg		
7	H	1	1	1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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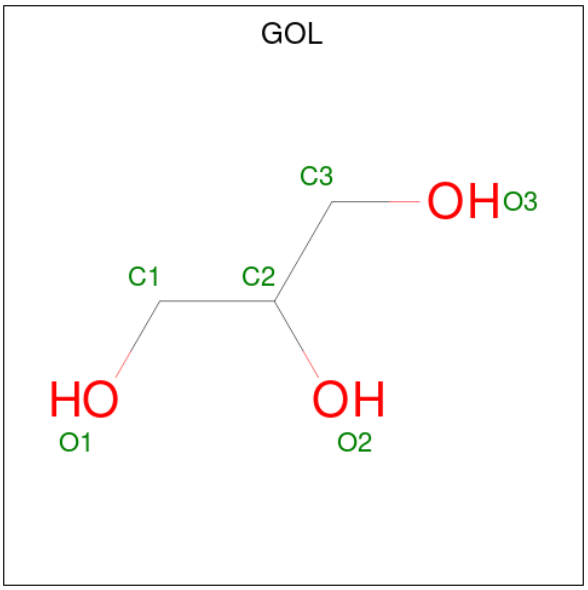
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	F	1	14	8	1	5	0	0
			Total	C	N	O		
8	F	1	14	8	1	5	0	0
			Total	C	N	O		
8	H	1	14	8	1	5	0	0
			Total	C	N	O		
8	H	1	14	8	1	5	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
9	I	1	6	3	3		0	0
			Total	C	O			
9	J	1	6	3	3		0	0

- Molecule 10 is water.

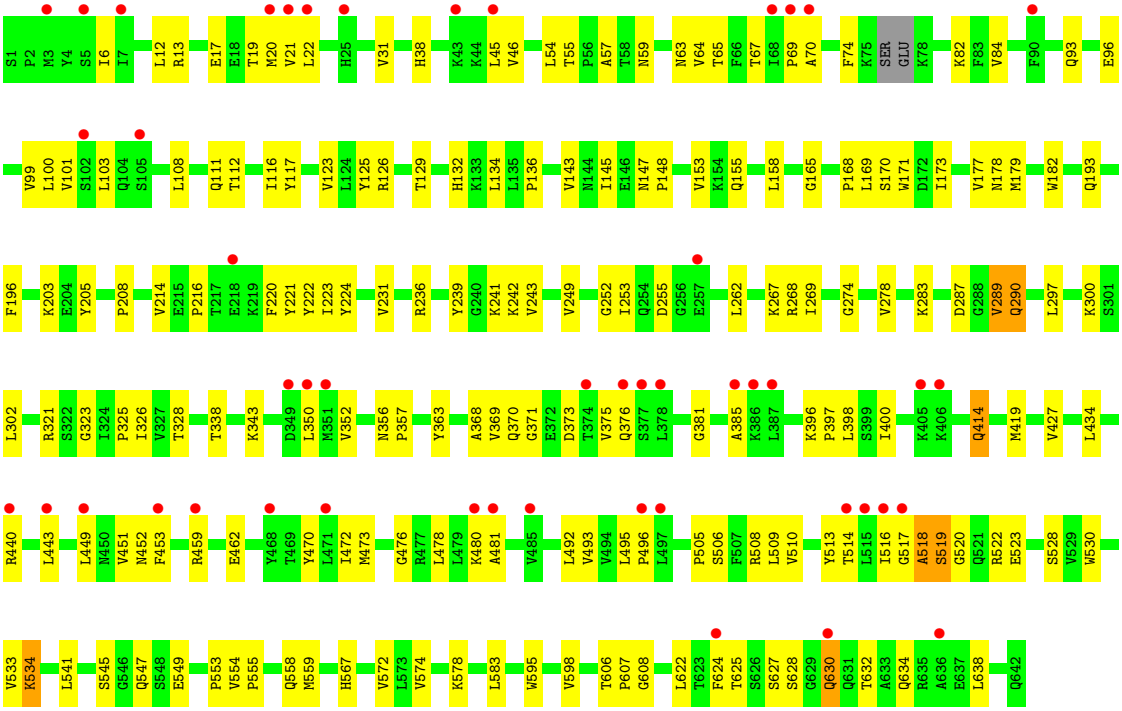
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
10	F	2	2	2		0	0
			Total	O			
10	H	2	2	2		0	0

3 Residue-property plots (i)

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

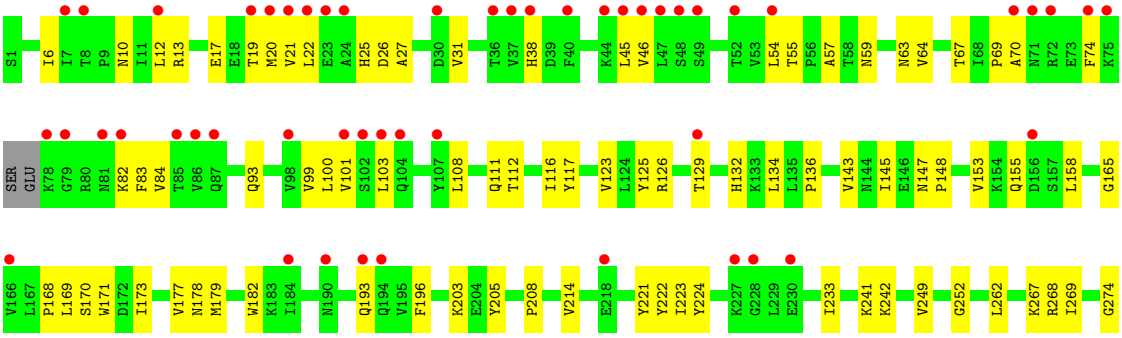
• Molecule 1: COMPLEMENT C3B BETA CHAIN

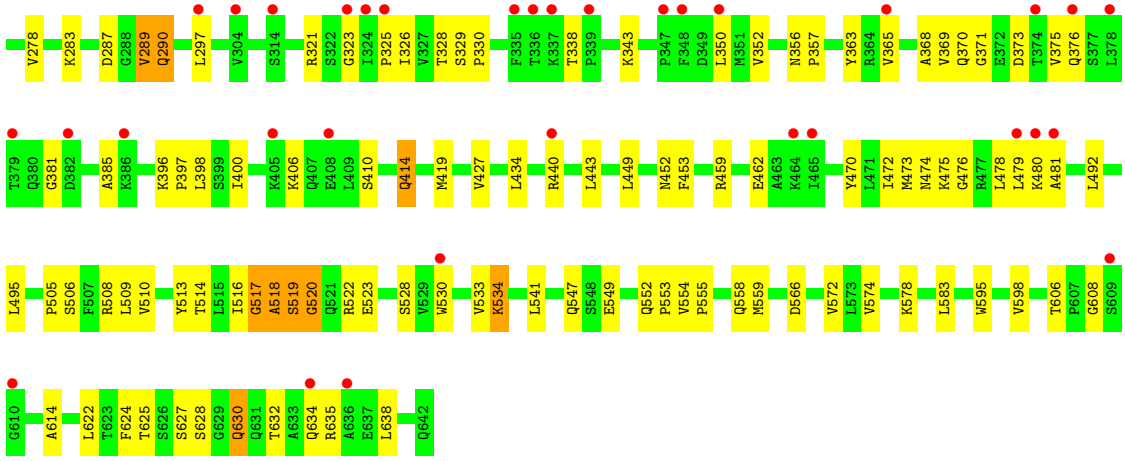
Chain A:



• Molecule 1: COMPLEMENT C3B BETA CHAIN

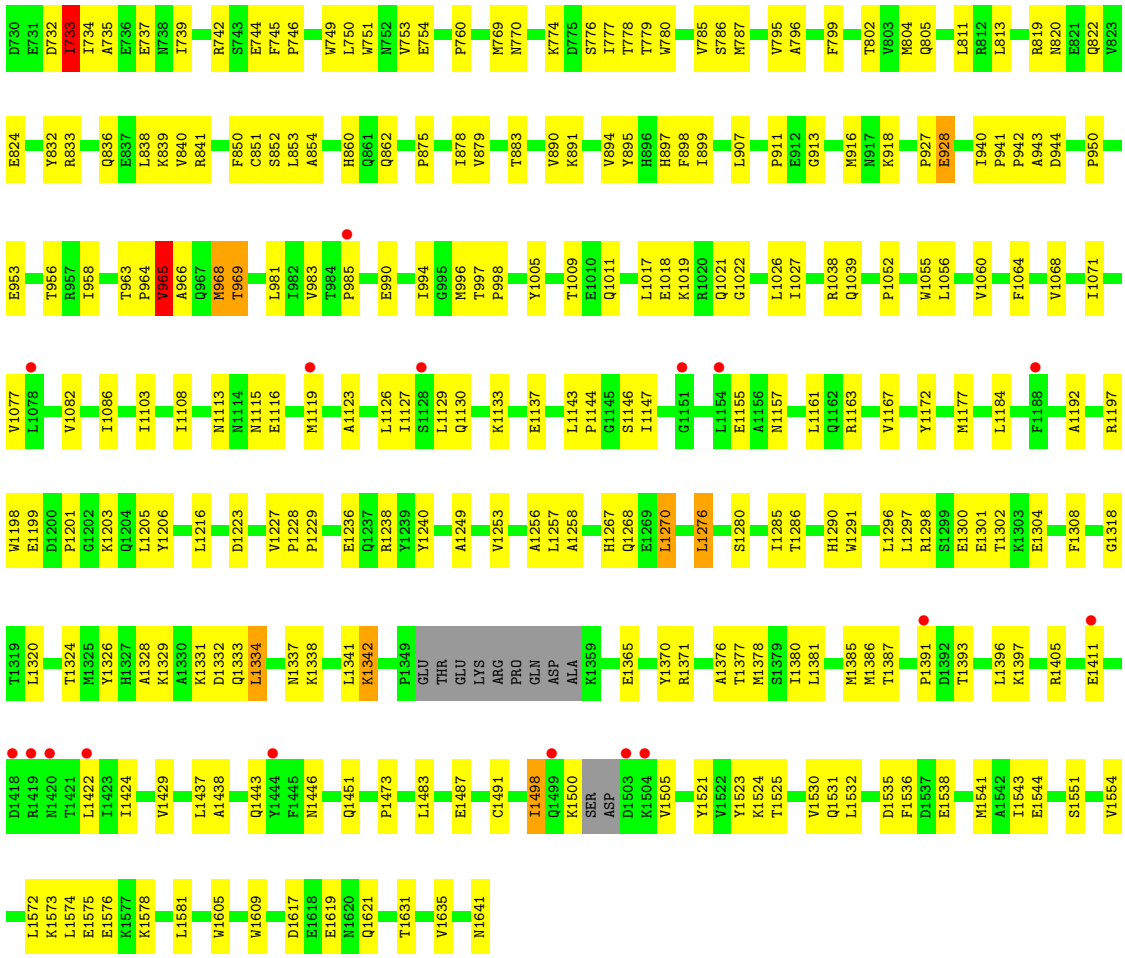
Chain C:





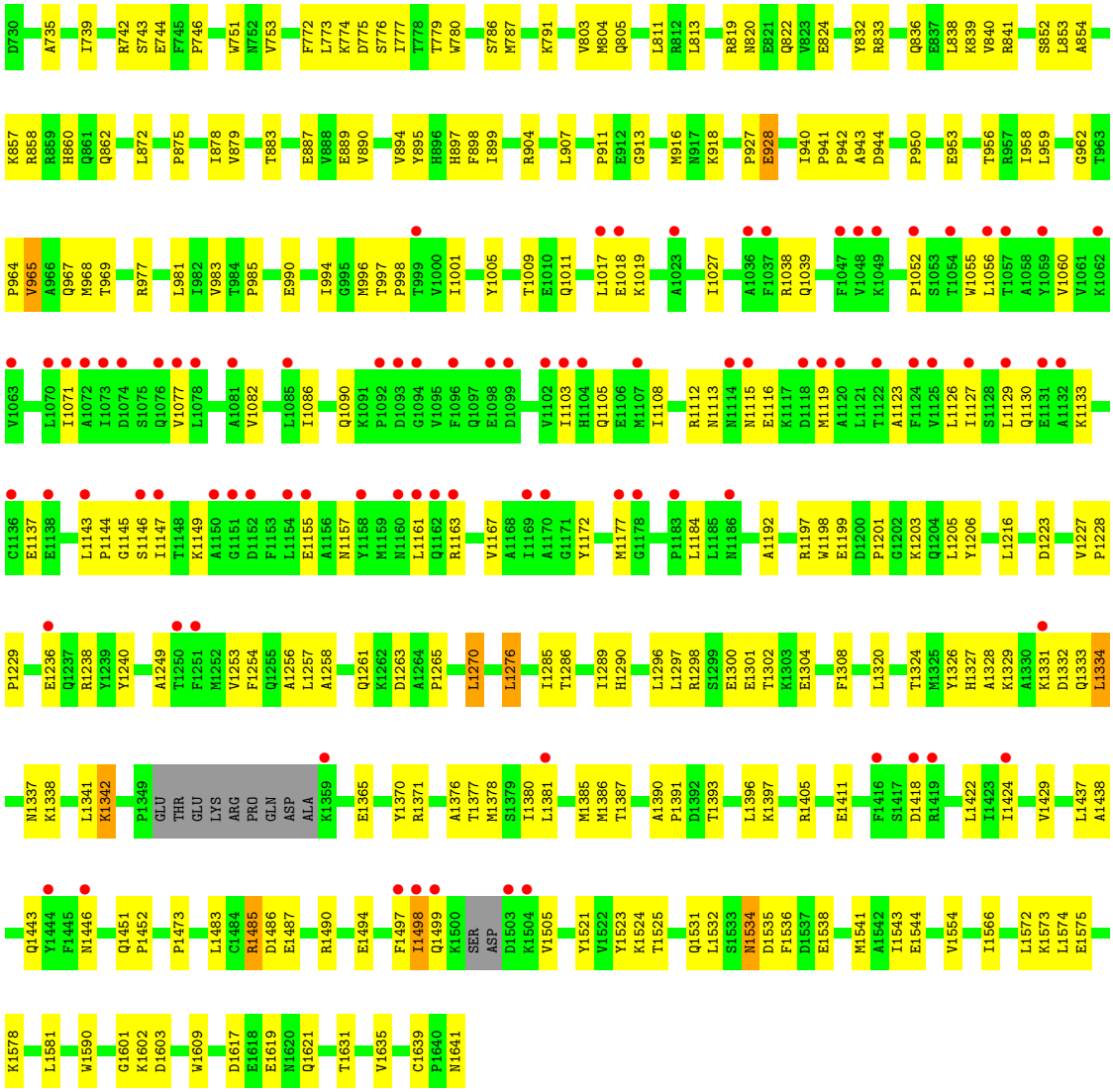
- Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain B:



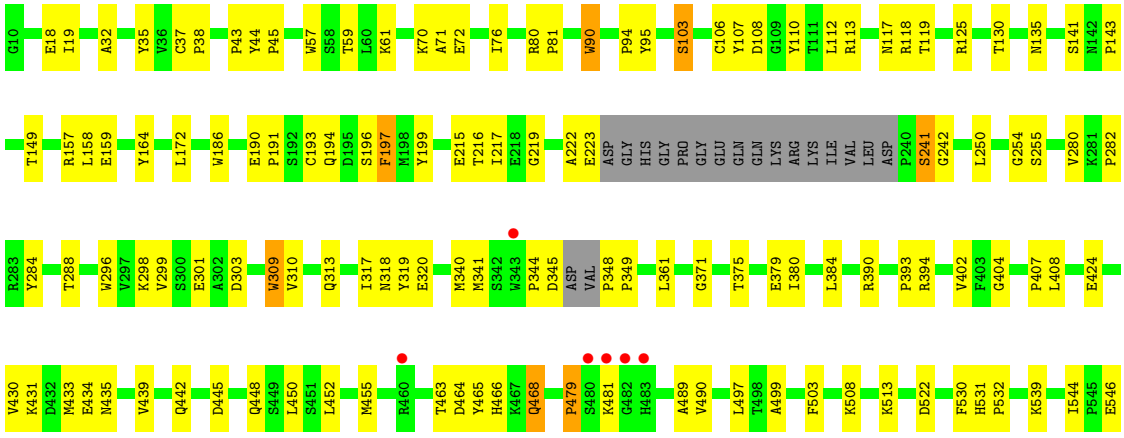
- Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

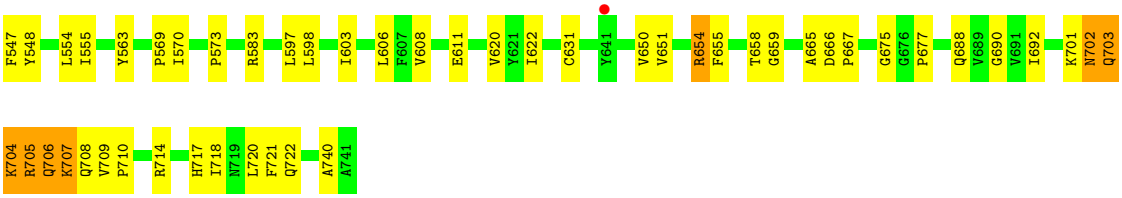
Chain D:



• Molecule 3: COMPLEMENT FACTOR B

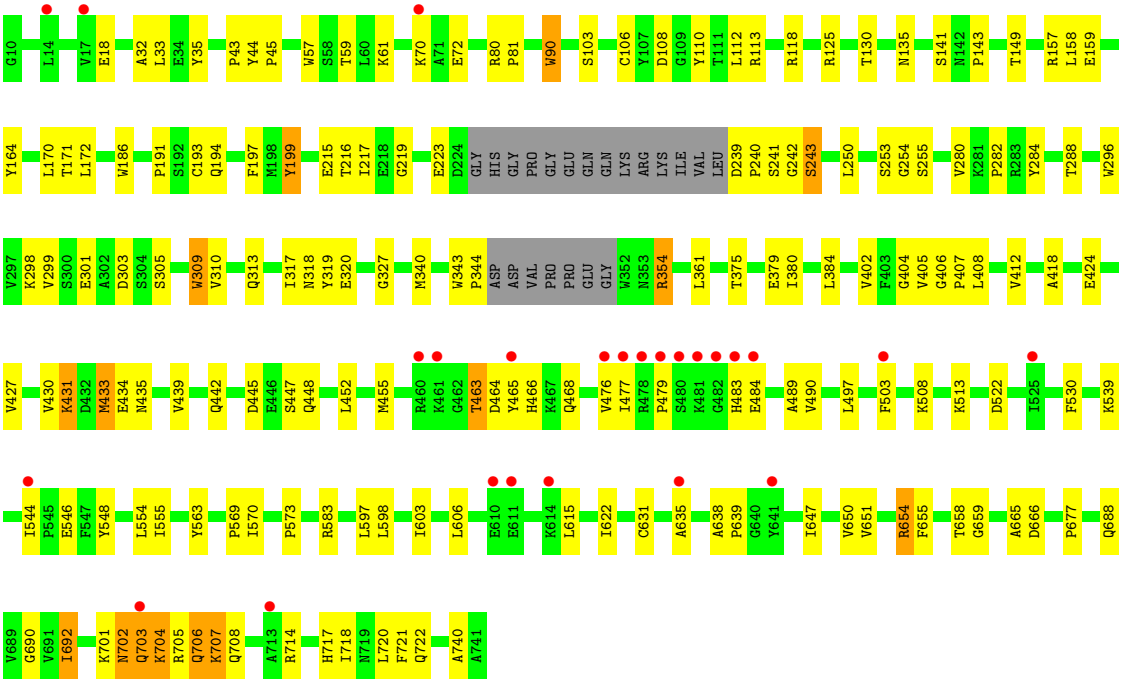
Chain F:





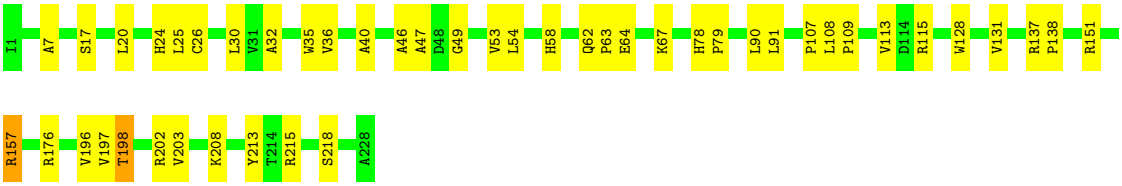
- Molecule 3: COMPLEMENT FACTOR B

Chain H:



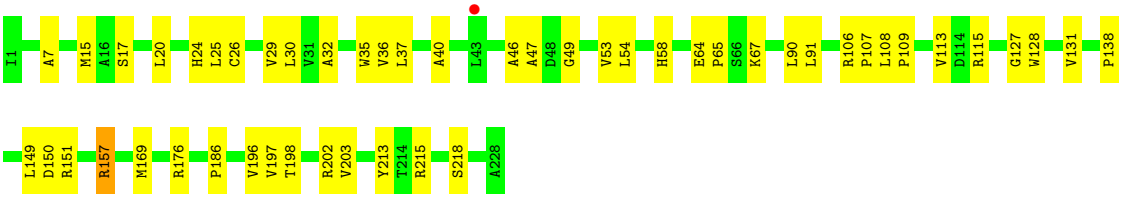
- Molecule 4: COMPLEMENT FACTOR D

Chain I:



- Molecule 4: COMPLEMENT FACTOR D

Chain J:



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

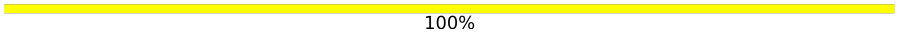
Chain E:

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

Chain G:

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

Chain K:

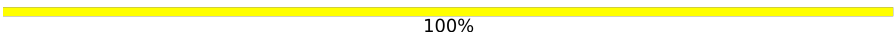


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

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

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	108.28Å 135.78Å 149.97Å 95.47° 110.69° 113.39°	Depositor
Resolution (Å)	65.95 – 3.49 67.46 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.95-3.49) 91.0 (67.46-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.189 , 0.244 0.186 , 0.240	Depositor DCC
R_{free} test set	4098 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 90.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	39285	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: MG, BMA, NAG, GOL

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	0.20	0/5092	0.37	0/6917
1	C	0.21	0/5092	0.39	0/6917
2	B	0.20	0/7340	0.36	0/9936
2	D	0.20	0/7340	0.36	0/9936
3	F	0.21	0/5754	0.37	0/7786
3	H	0.22	0/5733	0.37	0/7758
4	I	0.19	0/1745	0.36	0/2376
4	J	0.18	0/1745	0.36	0/2376
All	All	0.21	0/39841	0.37	0/54002

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	964	PRO	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	4992	0	5055	137	0
1	C	4992	0	5056	144	0
2	B	7197	0	7124	199	0
2	D	7197	0	7124	189	0
3	F	5627	0	5476	124	0
3	H	5608	0	5456	119	0
4	I	1710	0	1698	30	0
4	J	1710	0	1698	32	0
5	E	28	0	25	2	0
5	G	28	0	25	1	0
5	K	28	0	25	10	0
6	L	39	0	34	1	0
6	M	39	0	34	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	D	14	0	13	0	0
8	F	28	0	26	1	0
8	H	28	0	26	0	0
9	I	6	0	8	3	0
9	J	6	0	8	4	0
10	F	2	0	0	0	0
10	H	2	0	0	1	0
All	All	39285	0	38911	932	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 12.

All (932) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:HD21	5:K:1:NAG:C1	1.35	1.30
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.36	1.06
1:C:69:PRO:HA	1:C:70:ALA:HB3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:ILE:HD11	2:B:841:ARG:HH21	1.32	0.94
1:A:628:SER:HB2	1:A:630:GLN:HE22	1.32	0.93
3:F:222:ALA:N	3:F:223:GLU:HA	1.82	0.93
1:C:628:SER:HB2	1:C:630:GLN:HE22	1.32	0.92
1:A:268:ARG:HH11	2:B:1378:MET:HE3	1.36	0.89
3:H:706:GLN:O	3:H:708:GLN:N	2.08	0.87
3:F:705:ARG:HG2	3:F:705:ARG:HH11	1.37	0.87
2:B:1331:LYS:HA	2:B:1332:ASP:HB2	1.56	0.87
2:B:733:ILE:HG22	2:B:895:TYR:HA	1.55	0.87
2:D:1331:LYS:HA	2:D:1332:ASP:HB2	1.58	0.86
1:C:268:ARG:HH11	2:D:1378:MET:HE3	1.40	0.86
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.41	0.84
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.42	0.84
2:D:840:VAL:HG22	2:D:894:VAL:HG12	1.58	0.83
1:C:517:GLY:O	1:C:518:ALA:O	1.97	0.83
1:C:158:LEU:HD21	1:C:169:LEU:HD21	1.60	0.81
3:H:706:GLN:O	3:H:706:GLN:HG3	1.81	0.80
1:A:158:LEU:HD21	1:A:169:LEU:HD21	1.63	0.79
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.63	0.79
2:D:1205:LEU:HD12	2:D:1249:ALA:HB2	1.65	0.78
3:H:489:ALA:HB2	3:H:677:PRO:HG3	1.64	0.78
3:F:489:ALA:HB2	3:F:677:PRO:HG3	1.65	0.78
2:B:1205:LEU:HD12	2:B:1249:ALA:HB2	1.65	0.78
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.65	0.77
3:H:539:LYS:HB3	3:H:544:ILE:HB	1.68	0.76
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.21	0.75
3:F:361:LEU:HD21	3:F:402:VAL:HG22	1.69	0.75
3:F:539:LYS:HB3	3:F:544:ILE:HB	1.67	0.75
1:C:223:ILE:H	1:C:223:ILE:HD12	1.52	0.75
3:H:361:LEU:HD21	3:H:402:VAL:HG22	1.69	0.75
1:C:168:PRO:HB3	3:H:108:ASP:HB3	1.69	0.74
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.70	0.74
3:H:705:ARG:O	3:H:707:LYS:N	2.21	0.74
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.70	0.74
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.70	0.74
1:C:443:LEU:HD21	1:C:449:LEU:HD13	1.70	0.73
4:J:150:ASP:HA	9:J:1229:GOL:H2	1.69	0.73
2:B:850:PHE:HZ	2:B:907:LEU:HD21	1.53	0.73
2:B:964:PRO:HA	2:B:965:VAL:HG12	1.71	0.73
1:A:223:ILE:HD12	1:A:223:ILE:H	1.52	0.72
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.71	0.72
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.25	0.72
1:C:100:LEU:HD21	1:C:638:LEU:HD23	1.72	0.71
3:F:143:PRO:HG3	3:F:186:TRP:CE2	2.25	0.71
2:B:1333:GLN:HA	2:B:1334:LEU:CB	2.21	0.70
3:H:508:LYS:HA	3:H:508:LYS:HE2	1.73	0.70
1:A:414:GLN:HE21	1:A:414:GLN:HA	1.56	0.70
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.57	0.70
4:J:151:ARG:H	9:J:1229:GOL:H11	1.56	0.70
3:H:430:VAL:HG11	3:H:433:MET:HE1	1.72	0.70
1:A:547:GLN:HE22	1:A:559:MET:HA	1.56	0.70
1:C:480:LYS:HA	5:K:1:NAG:H81	1.73	0.70
2:D:1333:GLN:HA	2:D:1334:LEU:CB	2.20	0.70
2:B:1103:ILE:HD12	2:B:1103:ILE:H	1.56	0.70
1:C:547:GLN:HE22	1:C:559:MET:HA	1.56	0.69
1:C:63:ASN:HD21	5:K:1:NAG:C2	2.03	0.69
1:A:443:LEU:HD21	1:A:449:LEU:HD13	1.73	0.69
2:D:858:ARG:HH22	2:D:1494:GLU:HA	1.56	0.69
3:H:143:PRO:HG3	3:H:186:TRP:CE2	2.28	0.69
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.73	0.68
3:F:508:LYS:HE2	3:F:508:LYS:HA	1.76	0.68
3:F:705:ARG:HG2	3:F:705:ARG:NH1	2.03	0.68
1:C:63:ASN:CG	5:K:1:NAG:C1	2.61	0.67
3:F:706:GLN:O	3:F:708:GLN:N	2.27	0.67
2:B:785:VAL:HG22	2:B:795:VAL:HG12	1.74	0.67
1:C:55:THR:HG22	1:C:57:ALA:H	1.59	0.67
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.76	0.67
1:C:443:LEU:HD11	1:C:449:LEU:HD22	1.76	0.67
2:D:1333:GLN:HA	2:D:1334:LEU:HB3	1.77	0.66
1:C:518:ALA:O	1:C:520:GLY:N	2.28	0.66
2:D:804:MET:HG2	2:D:805:GLN:H	1.60	0.66
3:F:464:ASP:O	3:F:465:TYR:HB2	1.95	0.66
2:B:1333:GLN:HA	2:B:1334:LEU:HB3	1.78	0.66
3:F:430:VAL:HG11	3:F:433:MET:HE1	1.78	0.66
2:D:967:GLN:HG2	2:D:968:MET:H	1.61	0.65
2:B:819:ARG:HH12	2:B:1487:GLU:HG2	1.60	0.65
2:B:819:ARG:NH1	2:B:1487:GLU:HG2	2.12	0.65
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.77	0.65
4:J:32:ALA:HB3	4:J:35:TRP:HB2	1.78	0.65
2:D:857:LYS:HD2	2:D:1602:LYS:HE2	1.79	0.65
4:I:64:GLU:HB2	4:I:67:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:64:GLU:HB2	4:J:67:LYS:HG3	1.78	0.64
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.64
2:D:927:PRO:O	2:D:928:GLU:HB2	1.98	0.64
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.32	0.64
2:B:1280:SER:HA	3:F:390:ARG:HD3	1.80	0.64
2:B:927:PRO:O	2:B:928:GLU:HB2	1.98	0.63
1:C:208:PRO:HD3	1:C:583:LEU:HD11	1.80	0.63
3:H:318:ASN:HD21	3:H:320:GLU:HG2	1.64	0.63
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.80	0.63
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.63	0.63
1:C:606:THR:HG22	1:C:608:GLY:H	1.63	0.63
4:I:32:ALA:HB3	4:I:35:TRP:HB2	1.79	0.63
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.81	0.63
2:D:1490:ARG:HD2	2:D:1590:TRP:CZ3	2.33	0.63
1:A:606:THR:HG22	1:A:608:GLY:H	1.63	0.63
2:B:819:ARG:HE	2:B:883:THR:HG23	1.63	0.63
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.81	0.63
1:A:69:PRO:HA	1:A:70:ALA:CB	2.17	0.62
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.11	0.62
1:C:19:THR:HB	1:C:478:LEU:HB2	1.80	0.62
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.82	0.62
1:C:69:PRO:HA	1:C:70:ALA:CB	2.18	0.62
1:A:19:THR:HB	1:A:478:LEU:HB2	1.81	0.62
3:H:598:LEU:HA	3:H:603:ILE:HD13	1.81	0.62
1:C:368:ALA:HB2	1:C:376:GLN:HG2	1.82	0.62
1:A:452:ASN:HB3	1:A:492:LEU:HD11	1.82	0.62
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.65	0.62
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.64	0.62
2:B:943:ALA:HB2	2:B:1324:THR:HG21	1.82	0.61
1:C:45:LEU:HD23	1:C:45:LEU:H	1.65	0.61
2:D:1531:GLN:HB2	2:D:1538:GLU:HB2	1.82	0.61
2:D:819:ARG:HE	2:D:883:THR:HG23	1.64	0.61
1:A:208:PRO:HD3	1:A:583:LEU:HD11	1.83	0.61
2:D:958:ILE:HG21	2:D:1276:LEU:HD13	1.83	0.61
3:F:705:ARG:O	3:F:707:LYS:N	2.34	0.61
1:C:452:ASN:HB3	1:C:492:LEU:HD11	1.83	0.61
3:F:299:VAL:H	3:F:340:MET:HE3	1.65	0.60
4:I:108:LEU:HD12	4:I:109:PRO:HD2	1.83	0.60
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.66	0.60
3:H:113:ARG:HH22	3:H:141:SER:HB2	1.65	0.60
1:A:45:LEU:HD23	1:A:45:LEU:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:958:ILE:HG21	2:B:1276:LEU:HD13	1.84	0.60
3:F:598:LEU:HA	3:F:603:ILE:HD13	1.83	0.60
4:J:108:LEU:HD12	4:J:109:PRO:HD2	1.82	0.60
3:H:239:ASP:CB	3:H:240:PRO:HD2	2.32	0.60
2:B:853:LEU:HB2	2:B:860:HIS:CD2	2.37	0.59
2:D:943:ALA:HB2	2:D:1324:THR:HG21	1.84	0.59
1:A:368:ALA:HB2	1:A:376:GLN:HG2	1.83	0.59
2:D:1113:ASN:HB3	2:D:1163:ARG:HH12	1.67	0.59
1:C:479:LEU:O	5:K:1:NAG:H83	2.03	0.59
2:D:853:LEU:HB2	2:D:860:HIS:CD2	2.37	0.59
1:A:396:LYS:HD2	1:A:397:PRO:HD2	1.83	0.59
3:H:442:GLN:HE22	4:J:176:ARG:HH22	1.50	0.59
1:C:126:ARG:HG3	2:D:751:TRP:CZ2	2.38	0.58
2:D:1534:ASN:O	2:D:1566:ILE:HG13	2.04	0.58
3:F:631:CYS:SG	3:F:714:ARG:HD2	2.43	0.58
3:H:318:ASN:ND2	3:H:320:GLU:HG2	2.18	0.58
2:D:1276:LEU:HG	2:D:1285:ILE:HB	1.86	0.58
2:D:811:LEU:HD22	2:D:890:VAL:HG22	1.85	0.58
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.14	0.58
1:C:6:ILE:HD11	1:C:20:MET:HG2	1.86	0.58
3:F:690:GLY:HA2	3:F:718:ILE:O	2.04	0.58
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.86	0.57
1:A:352:VAL:HB	1:A:385:ALA:HB3	1.86	0.57
1:C:396:LYS:HD2	1:C:397:PRO:HD2	1.85	0.57
2:D:1126:LEU:HD21	2:D:1177:MET:HE3	1.87	0.57
1:A:221:TYR:HD2	1:A:326:ILE:HG23	1.70	0.57
1:A:239:TYR:HB2	2:B:804:MET:HE2	1.86	0.57
2:B:1113:ASN:HB3	2:B:1163:ARG:HH12	1.69	0.57
3:H:563:TYR:CZ	3:H:569:PRO:HG3	2.40	0.57
1:C:514:THR:OG1	1:C:522:ARG:HD2	2.04	0.57
4:J:131:VAL:HG13	4:J:138:PRO:HG3	1.86	0.57
1:A:168:PRO:HB3	3:F:108:ASP:HB3	1.87	0.57
1:C:289:VAL:HG21	1:C:297:LEU:HD21	1.86	0.57
2:D:997:THR:N	2:D:998:PRO:HD2	2.20	0.57
2:B:811:LEU:HD22	2:B:890:VAL:HG22	1.86	0.57
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.86	0.57
1:A:514:THR:OG1	1:A:522:ARG:HD2	2.05	0.56
2:B:883:THR:HG21	2:B:911:PRO:HG3	1.85	0.56
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.87	0.56
3:H:622:ILE:HA	3:H:658:THR:HG22	1.87	0.56
4:I:131:VAL:HG13	4:I:138:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:ND2	5:K:1:NAG:O5	2.34	0.56
2:D:804:MET:HG2	2:D:805:GLN:N	2.19	0.56
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.86	0.56
1:A:289:VAL:HG21	1:A:297:LEU:HD21	1.87	0.56
3:H:299:VAL:H	3:H:340:MET:HE3	1.69	0.56
4:J:20:LEU:HD11	4:J:49:GLY:HA3	1.87	0.56
1:A:6:ILE:HD11	1:A:20:MET:HG2	1.87	0.56
4:I:20:LEU:HD11	4:I:49:GLY:HA3	1.87	0.56
1:C:480:LYS:HA	5:K:1:NAG:C8	2.36	0.56
3:H:690:GLY:HA2	3:H:718:ILE:O	2.06	0.56
5:E:1:NAG:C1	5:E:1:NAG:O4	2.52	0.56
2:B:1302:THR:HG22	2:B:1304:GLU:H	1.71	0.56
1:A:289:VAL:O	1:A:290:GLN:HG2	2.06	0.56
2:B:997:THR:N	2:B:998:PRO:HD2	2.20	0.56
2:B:1376:ALA:HB3	2:B:1429:VAL:HG23	1.88	0.56
1:C:134:LEU:HD11	1:C:598:VAL:HG21	1.87	0.56
2:D:1238:ARG:HG2	2:D:1240:TYR:OH	2.06	0.56
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.88	0.55
3:F:622:ILE:HA	3:F:658:THR:HG22	1.88	0.55
3:H:172:LEU:HD11	3:H:191:PRO:HB3	1.88	0.55
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.22	0.55
1:C:289:VAL:O	1:C:290:GLN:HG2	2.06	0.55
2:D:1302:THR:HG22	2:D:1304:GLU:H	1.70	0.55
2:B:1331:LYS:CA	2:B:1332:ASP:HB2	2.32	0.55
1:C:221:TYR:HD2	1:C:326:ILE:HG23	1.70	0.55
3:H:597:LEU:HD12	3:H:721:PHE:HZ	1.72	0.55
1:A:363:TYR:HD1	1:A:381:GLY:HA2	1.72	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.87	0.55
2:D:889:GLU:HB2	2:D:904:ARG:HG3	1.89	0.55
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.89	0.55
2:B:1126:LEU:HD21	2:B:1177:MET:HE3	1.89	0.55
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.89	0.55
2:D:742:ARG:HH12	2:D:777:ILE:HG13	1.72	0.55
1:C:241:LYS:HG3	2:D:832:TYR:CE1	2.42	0.55
1:C:363:TYR:HD1	1:C:381:GLY:HA2	1.72	0.55
2:D:911:PRO:HD2	2:D:1327:HIS:HE1	1.72	0.55
1:C:352:VAL:HB	1:C:385:ALA:HB3	1.88	0.54
3:F:113:ARG:HH22	3:F:141:SER:HB2	1.71	0.54
1:A:517:GLY:O	1:A:518:ALA:O	2.25	0.54
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.88	0.54
3:F:563:TYR:CZ	3:F:569:PRO:HG3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.90	0.54
2:B:1238:ARG:HG2	2:B:1240:TYR:OH	2.07	0.54
3:H:659:GLY:HA2	3:H:666:ASP:HB2	1.90	0.54
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.88	0.54
2:B:964:PRO:HA	2:B:965:VAL:CG1	2.36	0.54
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.23	0.54
3:F:172:LEU:HD11	3:F:191:PRO:HB3	1.90	0.54
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.72	0.54
2:D:956:THR:HG23	2:D:1324:THR:HG22	1.90	0.54
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.43	0.54
2:D:1376:ALA:HB3	2:D:1429:VAL:HG23	1.90	0.54
3:F:216:THR:HG22	3:F:216:THR:O	2.08	0.54
3:H:631:CYS:SG	3:H:714:ARG:HD2	2.48	0.54
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.90	0.54
2:D:1370:TYR:CD1	2:D:1376:ALA:HB2	2.43	0.54
3:F:573:PRO:HB3	3:F:721:PHE:CZ	2.43	0.54
3:F:18:GLU:HG2	3:F:70:LYS:NZ	2.23	0.54
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.90	0.53
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.43	0.53
3:F:468:GLN:HG2	3:F:608:VAL:HG21	1.88	0.53
3:H:284:TYR:HB2	3:H:310:VAL:HG21	1.90	0.53
2:B:1276:LEU:HG	2:B:1285:ILE:HB	1.89	0.53
1:C:193:GLN:CD	1:C:193:GLN:H	2.11	0.53
1:C:578:LYS:HG3	2:D:779:THR:O	2.09	0.53
3:F:284:TYR:HB2	3:F:310:VAL:HG21	1.88	0.53
1:A:193:GLN:H	1:A:193:GLN:CD	2.11	0.53
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.74	0.53
2:B:1005:TYR:HD1	2:B:1258:ALA:HB2	1.73	0.53
3:F:149:THR:HG22	3:F:193:CYS:SG	2.48	0.53
2:D:894:VAL:HG23	2:D:897:HIS:HB2	1.91	0.53
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.53
2:D:1203:LYS:HG3	2:D:1206:TYR:CE2	2.44	0.53
3:F:433:MET:C	3:F:435:ASN:H	2.13	0.53
3:H:573:PRO:HB3	3:H:721:PHE:CZ	2.43	0.53
4:J:197:VAL:HG22	4:J:213:TYR:HE2	1.73	0.53
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.90	0.53
2:B:776:SER:HB2	2:B:780:TRP:HZ2	1.72	0.53
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.91	0.53
3:F:503:PHE:CZ	3:F:555:ILE:HD11	2.43	0.53
3:F:659:GLY:HA2	3:F:666:ASP:HB2	1.91	0.53
5:K:1:NAG:O6	5:K:2:NAG:N2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:959:LEU:HD11	2:D:1297:LEU:HD22	1.91	0.53
3:H:219:GLY:HA2	3:H:455:MET:CE	2.39	0.53
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.52
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.44	0.52
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.89	0.52
3:F:348:PRO:N	3:F:349:PRO:HD3	2.24	0.52
3:F:442:GLN:HE22	4:I:176:ARG:HH22	1.58	0.52
2:B:742:ARG:NH1	2:B:777:ILE:HG13	2.24	0.52
1:C:126:ARG:HG3	2:D:751:TRP:HZ2	1.74	0.52
2:D:894:VAL:CG2	2:D:899:ILE:HB	2.40	0.52
3:H:239:ASP:HB3	3:H:240:PRO:HD2	1.92	0.52
2:B:742:ARG:HH12	2:B:777:ILE:HG13	1.74	0.52
2:B:965:VAL:HG21	2:B:1268:GLN:HE21	1.75	0.52
2:B:1572:LEU:HB3	2:B:1574:LEU:HG	1.91	0.52
2:D:950:PRO:HD3	2:D:1329:LYS:HE2	1.92	0.52
3:H:18:GLU:HG2	3:H:70:LYS:NZ	2.25	0.52
2:B:1203:LYS:HG3	2:B:1206:TYR:CE2	2.44	0.52
2:D:1525:THR:HB	2:D:1541:MET:HB3	1.92	0.52
3:F:407:PRO:HB2	3:F:408:LEU:HD22	1.91	0.52
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.44	0.52
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.10	0.52
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.10	0.52
3:H:219:GLY:HA2	3:H:455:MET:HE1	1.92	0.52
4:I:196:VAL:O	4:I:198:THR:HG22	2.09	0.52
2:D:744:GLU:C	2:D:746:PRO:HD3	2.31	0.52
3:H:503:PHE:CZ	3:H:555:ILE:HD11	2.44	0.52
4:I:24:HIS:CE1	4:I:128:TRP:HB2	2.45	0.52
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.92	0.52
2:D:1331:LYS:CA	2:D:1332:ASP:HB2	2.34	0.52
3:H:216:THR:HG22	3:H:216:THR:O	2.09	0.52
2:D:1133:LYS:O	2:D:1137:GLU:HB2	2.10	0.51
3:H:430:VAL:HG21	3:H:433:MET:CE	2.40	0.51
2:B:819:ARG:HH12	2:B:1487:GLU:CG	2.23	0.51
2:D:967:GLN:HG2	2:D:968:MET:N	2.25	0.51
4:J:24:HIS:CE1	4:J:128:TRP:HB2	2.45	0.51
1:C:84:VAL:HG13	1:C:101:VAL:HG21	1.92	0.51
1:C:223:ILE:HD13	1:C:328:THR:HG22	1.92	0.51
1:A:13:ARG:NH1	1:A:132:HIS:HB3	2.25	0.51
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.76	0.51
2:D:773:LEU:HD13	2:D:803:VAL:HG21	1.91	0.51
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1498:ILE:HA	2:D:1602:LYS:O	2.11	0.51
4:J:113:VAL:HG12	4:J:115:ARG:HG3	1.93	0.51
4:J:149:LEU:O	9:J:1229:GOL:H31	2.10	0.51
2:B:1575:GLU:HB2	2:B:1578:LYS:HD2	1.93	0.51
4:I:197:VAL:HG22	4:I:213:TYR:HE2	1.75	0.51
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.41	0.51
1:C:136:PRO:HG3	2:D:787:MET:SD	2.50	0.51
2:D:1103:ILE:HD12	2:D:1103:ILE:H	1.74	0.51
3:F:463:THR:O	3:F:466:HIS:HB2	2.11	0.51
1:A:223:ILE:HD13	1:A:328:THR:HG22	1.91	0.51
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.93	0.51
1:C:147:ASN:HA	1:C:182:TRP:CE3	2.46	0.51
3:H:242:GLY:O	3:H:243:SER:HB2	2.11	0.51
3:H:253:SER:HB3	10:H:2001:HOH:O	2.11	0.51
2:B:1530:VAL:HG23	2:B:1576:GLU:HG2	1.92	0.51
1:C:13:ARG:NH1	1:C:132:HIS:HB3	2.26	0.51
3:H:250:LEU:HB3	3:H:288:THR:HG22	1.92	0.51
3:H:407:PRO:HB2	3:H:408:LEU:HD22	1.93	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.46	0.51
2:B:950:PRO:HD3	2:B:1329:LYS:HE2	1.93	0.51
2:D:1572:LEU:HB3	2:D:1574:LEU:HG	1.92	0.51
3:H:298:LYS:HZ2	3:H:340:MET:HA	1.77	0.51
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.93	0.50
2:D:1498:ILE:HG12	2:D:1603:ASP:HA	1.93	0.50
4:I:113:VAL:HG12	4:I:115:ARG:HG3	1.92	0.50
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.47	0.50
2:D:1532:LEU:O	2:D:1532:LEU:HD12	2.11	0.50
1:C:241:LYS:HE2	2:D:804:MET:HE1	1.93	0.50
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.46	0.50
2:B:1133:LYS:O	2:B:1137:GLU:HB2	2.12	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.30	0.50
2:D:1113:ASN:HB3	2:D:1163:ARG:NH1	2.26	0.50
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.47	0.50
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.12	0.50
1:A:470:TYR:HB2	1:A:509:LEU:HD21	1.94	0.50
2:D:1017:LEU:C	2:D:1019:LYS:H	2.15	0.50
2:D:1286:THR:HG22	3:H:665:ALA:HB3	1.93	0.50
4:J:196:VAL:O	4:J:198:THR:HG22	2.12	0.50
3:H:424:GLU:OE2	3:H:583:ARG:HD3	2.11	0.50
1:A:96:GLU:OE2	2:B:1021:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.47	0.50
3:H:303:ASP:HB3	3:H:309:TRP:CD1	2.47	0.50
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.93	0.49
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.27	0.49
2:D:743:SER:HB3	2:D:904:ARG:NH1	2.27	0.49
3:H:433:MET:C	3:H:435:ASN:H	2.15	0.49
2:B:833:ARG:HD3	2:B:836:GLN:HE21	1.76	0.49
3:F:303:ASP:HB3	3:F:309:TRP:CD1	2.47	0.49
3:H:298:LYS:HB3	3:H:301:GLU:HG3	1.94	0.49
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.47	0.49
2:B:746:PRO:HG2	2:B:774:LYS:HE3	1.94	0.49
1:C:126:ARG:CZ	1:C:572:VAL:HB	2.43	0.49
2:D:1535:ASP:O	2:D:1536:PHE:HB2	2.12	0.49
3:F:298:LYS:HB3	3:F:301:GLU:HG3	1.94	0.49
1:C:153:VAL:HG12	2:D:1297:LEU:HD12	1.94	0.49
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.43	0.49
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	1.94	0.49
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.93	0.49
3:H:570:ILE:HD13	3:H:688:GLN:HB2	1.94	0.49
4:I:157:ARG:HD3	4:I:157:ARG:C	2.32	0.49
2:B:735:ALA:HB1	2:B:737:GLU:OE1	2.12	0.49
1:C:6:ILE:HD11	1:C:20:MET:CG	2.42	0.49
3:F:296:TRP:CE2	3:F:317:ILE:HG22	2.47	0.49
4:I:40:ALA:HA	4:I:91:LEU:HB2	1.95	0.49
2:B:751:TRP:HB3	3:F:107:TYR:CD1	2.48	0.49
3:H:149:THR:HG22	3:H:193:CYS:SG	2.53	0.49
4:J:29:VAL:HB	4:J:186:PRO:HG3	1.95	0.49
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.94	0.49
2:D:1381:LEU:HB2	2:D:1424:ILE:O	2.13	0.49
3:F:424:GLU:OE2	3:F:583:ARG:HD3	2.12	0.49
4:I:25:LEU:HG	4:I:26:CYS:SG	2.52	0.49
2:B:1381:LEU:HB2	2:B:1424:ILE:O	2.13	0.49
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.94	0.49
3:F:597:LEU:HD12	3:F:721:PHE:HZ	1.76	0.49
4:J:40:ALA:HA	4:J:91:LEU:HB2	1.94	0.49
1:A:136:PRO:HG3	2:B:787:MET:SD	2.53	0.48
2:B:850:PHE:CZ	2:B:907:LEU:HD21	2.42	0.48
2:D:1285:ILE:HG21	2:D:1300:GLU:HG3	1.95	0.48
3:F:570:ILE:HD13	3:F:688:GLN:HB2	1.96	0.48
3:H:118:ARG:NH1	3:H:130:THR:HA	2.29	0.48
3:H:430:VAL:HG21	3:H:433:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1119:MET:HG3	2:D:1161:LEU:HD21	1.95	0.48
3:H:476:VAL:HB	3:H:484:GLU:HB3	1.95	0.48
1:A:478:LEU:HD21	1:A:622:LEU:HD21	1.94	0.48
1:A:624:PHE:H	1:A:632:THR:CG2	2.27	0.48
2:B:940:ILE:HD12	2:B:1308:PHE:CE2	2.49	0.48
2:B:1113:ASN:HB3	2:B:1163:ARG:NH1	2.27	0.48
3:H:158:LEU:O	3:H:159:GLU:HB2	2.13	0.48
4:I:36:VAL:HG21	4:I:53:VAL:HG11	1.95	0.48
3:F:241:SER:CB	3:F:242:GLY:HA3	2.43	0.48
1:A:242:LYS:HB3	1:A:274:GLY:HA3	1.96	0.48
1:A:369:VAL:HG12	1:A:371:GLY:H	1.79	0.48
1:A:624:PHE:H	1:A:632:THR:HG21	1.78	0.48
2:B:744:GLU:C	2:B:746:PRO:HD3	2.34	0.48
2:B:1331:LYS:HA	2:B:1332:ASP:CB	2.26	0.48
3:F:250:LEU:HB3	3:F:288:THR:HG22	1.95	0.48
6:L:1:NAG:H61	6:L:2:NAG:HN2	1.79	0.48
1:A:323:GLY:O	1:A:325:PRO:HD3	2.13	0.48
2:B:927:PRO:O	2:B:928:GLU:CB	2.62	0.48
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.14	0.48
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.94	0.48
2:B:1017:LEU:C	2:B:1019:LYS:H	2.17	0.48
2:B:1103:ILE:HD12	2:B:1103:ILE:N	2.27	0.48
2:B:1301:GLU:HG2	3:F:157:ARG:NH1	2.29	0.48
1:C:6:ILE:HG22	1:C:625:THR:O	2.13	0.48
2:D:907:LEU:HD23	2:D:907:LEU:H	1.78	0.48
2:D:985:PRO:HG3	2:D:996:MET:HA	1.96	0.48
2:D:990:GLU:O	2:D:994:ILE:HG13	2.14	0.48
2:D:1197:ARG:HE	2:D:1199:GLU:CD	2.17	0.48
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.49	0.47
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.96	0.47
1:C:470:TYR:HB2	1:C:509:LEU:HD21	1.96	0.47
2:D:883:THR:HG21	2:D:911:PRO:HG3	1.96	0.47
3:H:706:GLN:O	3:H:706:GLN:CG	2.55	0.47
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.49	0.47
2:B:968:MET:O	2:B:969:THR:HB	2.14	0.47
1:C:148:PRO:HD3	1:C:182:TRP:CE2	2.49	0.47
1:C:177:VAL:HG22	1:C:178:ASN:N	2.29	0.47
1:C:242:LYS:HB3	1:C:274:GLY:HA3	1.96	0.47
2:D:916:MET:HG3	2:D:1328:ALA:CB	2.44	0.47
2:D:1005:TYR:HD1	2:D:1258:ALA:HB2	1.79	0.47
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:433:MET:HG3	3:F:434:GLU:N	2.29	0.47
1:C:45:LEU:HB2	1:C:46:VAL:HB	1.97	0.47
2:D:1543:ILE:HD12	2:D:1554:VAL:HG21	1.95	0.47
1:A:177:VAL:HG22	1:A:178:ASN:N	2.29	0.47
1:A:179:MET:HG3	1:A:203:LYS:HA	1.96	0.47
2:B:732:ASP:O	2:B:733:ILE:HG12	2.15	0.47
2:B:1483:LEU:HD11	2:B:1536:PHE:HB3	1.95	0.47
1:C:624:PHE:H	1:C:632:THR:HG21	1.79	0.47
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.15	0.47
3:H:296:TRP:CE2	3:H:317:ILE:HG22	2.50	0.47
4:J:36:VAL:HG21	4:J:53:VAL:HG11	1.96	0.47
2:B:1581:LEU:HB2	2:B:1609:TRP:HE3	1.79	0.47
1:C:630:GLN:H	1:C:630:GLN:NE2	2.13	0.47
2:D:918:LYS:NZ	2:D:944:ASP:HB3	2.29	0.47
2:D:927:PRO:O	2:D:928:GLU:CB	2.62	0.47
1:A:6:ILE:HD11	1:A:20:MET:CG	2.43	0.47
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.96	0.47
1:A:578:LYS:HG3	2:B:779:THR:O	2.15	0.47
2:B:940:ILE:HD11	2:B:1320:LEU:HD21	1.97	0.47
1:C:624:PHE:H	1:C:632:THR:CG2	2.28	0.47
2:D:1263:ASP:O	2:D:1265:PRO:HD3	2.14	0.47
3:F:404:GLY:O	3:F:430:VAL:HG22	2.14	0.47
3:H:703:GLN:O	3:H:704:LYS:HB2	2.14	0.47
4:J:157:ARG:HD3	4:J:157:ARG:C	2.34	0.47
1:A:177:VAL:HG22	1:A:178:ASN:H	1.80	0.47
1:A:268:ARG:NH1	2:B:1378:MET:HE3	2.18	0.47
2:B:739:ILE:HB	2:B:891:LYS:HD3	1.95	0.47
2:B:965:VAL:O	2:B:965:VAL:HG13	2.13	0.47
1:C:323:GLY:O	1:C:325:PRO:HD3	2.13	0.47
2:D:1443:GLN:HE21	2:D:1446:ASN:HA	1.79	0.47
3:F:118:ARG:NH1	3:F:130:THR:HA	2.30	0.47
3:F:701:LYS:O	3:F:702:ASN:C	2.53	0.47
4:J:197:VAL:HG22	4:J:213:TYR:CE2	2.50	0.47
2:B:966:ALA:HA	2:B:1267:HIS:HA	1.97	0.47
2:B:1119:MET:HG3	2:B:1161:LEU:HD21	1.96	0.47
3:F:344:PRO:O	3:F:345:ASP:HB2	2.15	0.47
3:H:435:ASN:O	3:H:439:VAL:HG23	2.14	0.47
4:J:215:ARG:NH1	4:J:218:SER:HB2	2.30	0.47
2:B:1531:GLN:HB2	2:B:1538:GLU:HB2	1.95	0.47
1:C:179:MET:HG3	1:C:203:LYS:HA	1.97	0.47
1:C:369:VAL:HG12	1:C:371:GLY:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:822:GLN:HA	2:D:879:VAL:HG22	1.97	0.47
2:D:1575:GLU:HB2	2:D:1578:LYS:HD2	1.96	0.47
3:F:654:ARG:HG3	3:F:722:GLN:HB3	1.97	0.47
3:H:254:GLY:HA2	3:H:319:TYR:OH	2.14	0.47
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.97	0.47
2:B:804:MET:HG2	2:B:805:GLN:N	2.30	0.47
2:D:894:VAL:HG22	2:D:899:ILE:HB	1.97	0.47
2:D:1581:LEU:HB2	2:D:1609:TRP:HE3	1.80	0.47
3:H:59:THR:HG23	3:H:61:LYS:HG2	1.96	0.47
3:H:433:MET:O	3:H:434:GLU:HB2	2.15	0.47
2:B:1285:ILE:HG21	2:B:1300:GLU:HG3	1.98	0.46
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.96	0.46
2:D:872:LEU:HD13	2:D:1418:ASP:HB3	1.96	0.46
3:F:158:LEU:O	3:F:159:GLU:HB2	2.14	0.46
3:F:503:PHE:HB2	3:F:530:PHE:HZ	1.80	0.46
3:H:433:MET:HG3	3:H:434:GLU:N	2.30	0.46
4:I:151:ARG:H	9:I:1229:GOL:H11	1.80	0.46
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.15	0.46
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.14	0.46
3:H:44:TYR:HB3	3:H:72:GLU:O	2.15	0.46
1:A:6:ILE:HG22	1:A:625:THR:O	2.15	0.46
1:A:45:LEU:HB2	1:A:46:VAL:HB	1.97	0.46
1:A:453:PHE:HE1	1:A:495:LEU:HB2	1.80	0.46
2:B:822:GLN:HA	2:B:879:VAL:HG22	1.97	0.46
2:B:985:PRO:HG3	2:B:996:MET:HA	1.97	0.46
3:F:215:GLU:C	3:F:217:ILE:H	2.19	0.46
4:J:169:MET:HB2	9:J:1229:GOL:O3	2.15	0.46
2:B:1119:MET:SD	2:B:1157:ASN:HB2	2.55	0.46
2:D:916:MET:HG3	2:D:1328:ALA:HB3	1.98	0.46
2:D:1341:LEU:C	2:D:1342:LYS:HD3	2.36	0.46
3:H:375:THR:O	3:H:379:GLU:HG3	2.15	0.46
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.46
1:A:583:LEU:N	1:A:583:LEU:HD12	2.31	0.46
1:A:630:GLN:NE2	1:A:630:GLN:H	2.13	0.46
1:C:112:THR:HG22	1:C:125:TYR:HB3	1.98	0.46
2:D:965:VAL:HG22	2:D:965:VAL:O	2.15	0.46
2:D:1119:MET:SD	2:D:1157:ASN:HB2	2.55	0.46
3:F:59:THR:HG23	3:F:61:LYS:HG2	1.96	0.46
3:F:435:ASN:O	3:F:439:VAL:HG23	2.16	0.46
3:H:215:GLU:C	3:H:217:ILE:H	2.19	0.46
1:A:12:LEU:HG	1:A:99:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1197:ARG:HE	2:B:1199:GLU:CD	2.19	0.46
1:C:31:VAL:HG13	1:C:54:LEU:HB2	1.97	0.46
2:D:833:ARG:HD3	2:D:836:GLN:HE21	1.80	0.46
3:F:309:TRP:HZ3	3:F:313:GLN:CD	2.18	0.46
3:H:464:ASP:C	3:H:466:HIS:H	2.19	0.46
3:H:688:GLN:HG2	3:H:720:LEU:HD11	1.98	0.46
4:I:197:VAL:HG22	4:I:213:TYR:CE2	2.51	0.46
4:J:25:LEU:HG	4:J:26:CYS:SG	2.55	0.46
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.98	0.46
1:C:558:GLN:HG2	2:D:772:PHE:CE2	2.51	0.46
2:D:940:ILE:HD11	2:D:1320:LEU:HD21	1.98	0.46
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.81	0.46
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.56	0.46
2:D:940:ILE:HD12	2:D:1308:PHE:CE2	2.50	0.46
2:D:1385:MET:HE2	2:D:1385:MET:HA	1.98	0.46
2:D:1639:CYS:O	3:H:327:GLY:HA2	2.16	0.46
2:B:894:VAL:HG22	2:B:899:ILE:HB	1.98	0.46
2:B:913:GLY:O	2:B:1331:LYS:HE3	2.16	0.46
1:C:74:PHE:C	1:C:82:LYS:HZ3	2.20	0.46
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.97	0.46
1:C:223:ILE:HD12	1:C:223:ILE:N	2.25	0.46
3:H:404:GLY:O	3:H:430:VAL:HG22	2.15	0.46
3:H:503:PHE:HB2	3:H:530:PHE:HZ	1.81	0.46
2:B:1525:THR:HB	2:B:1541:MET:HB3	1.97	0.45
3:F:95:TYR:HE2	8:F:1743:NAG:HN2	1.65	0.45
3:F:164:TYR:CD1	3:F:191:PRO:HG2	2.52	0.45
3:H:171:THR:HG23	3:H:412:VAL:HG22	1.99	0.45
1:A:223:ILE:HD12	1:A:223:ILE:N	2.26	0.45
1:A:268:ARG:HD3	2:B:1378:MET:CE	2.47	0.45
1:A:628:SER:HB2	1:A:630:GLN:NE2	2.16	0.45
2:B:918:LYS:NZ	2:B:944:ASP:HB3	2.31	0.45
2:B:1443:GLN:HE21	2:B:1446:ASN:HA	1.80	0.45
1:A:45:LEU:HA	1:A:46:VAL:HA	1.72	0.45
1:A:112:THR:HG22	1:A:125:TYR:HB3	1.98	0.45
1:A:356:ASN:HB3	1:A:357:PRO:HD2	1.97	0.45
1:C:614:ALA:HB1	1:C:632:THR:HA	1.99	0.45
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.45
3:H:606:LEU:C	3:H:606:LEU:HD12	2.37	0.45
3:H:654:ARG:HG3	3:H:722:GLN:HB3	1.98	0.45
4:I:215:ARG:NH1	4:I:218:SER:HB2	2.31	0.45
1:C:177:VAL:HG22	1:C:178:ASN:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD22	1:C:400:ILE:HD11	1.98	0.45
2:D:742:ARG:NH1	2:D:777:ILE:HG13	2.32	0.45
3:F:430:VAL:HG21	3:F:433:MET:CE	2.46	0.45
3:H:464:ASP:HB2	3:H:615:LEU:HD12	1.98	0.45
2:B:1286:THR:HG22	3:F:665:ALA:HB3	1.99	0.45
1:C:222:TYR:HE2	1:C:224:TYR:HB2	1.82	0.45
1:C:453:PHE:HE1	1:C:495:LEU:HB2	1.82	0.45
1:C:541:LEU:HD22	2:D:786:SER:CB	2.46	0.45
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.82	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.15	0.45
3:F:655:PHE:HA	3:F:717:HIS:O	2.16	0.45
3:F:703:GLN:O	3:F:704:LYS:HB2	2.15	0.45
1:A:222:TYR:HE2	1:A:224:TYR:HB2	1.81	0.45
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.97	0.45
2:B:1017:LEU:O	2:B:1018:GLU:HB3	2.16	0.45
2:D:1163:ARG:O	2:D:1167:VAL:HG23	2.17	0.45
2:B:733:ILE:HD11	2:B:841:ARG:NH2	2.15	0.45
2:B:819:ARG:HE	2:B:883:THR:CG2	2.27	0.45
2:B:990:GLU:O	2:B:994:ILE:HG13	2.17	0.45
2:B:1333:GLN:HB3	2:B:1334:LEU:C	2.37	0.45
2:D:852:SER:HB3	2:D:878:ILE:HG22	1.98	0.45
3:H:477:ILE:HG13	3:H:483:HIS:CE1	2.51	0.45
3:H:544:ILE:HD13	3:H:650:VAL:HG12	1.98	0.45
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.17	0.45
2:B:1236:GLU:HA	2:B:1238:ARG:NH2	2.31	0.45
2:B:1581:LEU:HB2	2:B:1609:TRP:CE3	2.52	0.45
1:C:223:ILE:H	1:C:223:ILE:CD1	2.26	0.45
2:D:1105:GLN:O	2:D:1112:ARG:HD2	2.16	0.45
3:F:318:ASN:ND2	3:F:320:GLU:HG2	2.31	0.45
3:H:170:LEU:HD23	3:H:193:CYS:HB3	1.98	0.45
3:H:452:LEU:HD12	3:H:455:MET:HG3	1.99	0.45
5:K:1:NAG:O6	5:K:2:NAG:C1	2.64	0.45
2:B:907:LEU:HD23	2:B:907:LEU:H	1.82	0.45
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.45
2:D:1497:PHE:HA	2:D:1601:GLY:O	2.15	0.45
2:D:1631:THR:O	2:D:1635:VAL:HG23	2.17	0.45
3:F:345:ASP:O	3:F:348:PRO:HD2	2.16	0.45
3:F:688:GLN:HG2	3:F:720:LEU:HD11	1.99	0.45
2:B:840:VAL:HG12	2:B:841:ARG:N	2.33	0.44
2:B:854:ALA:HB2	2:B:860:HIS:HB3	1.99	0.44
2:B:1341:LEU:C	2:B:1342:LYS:HD3	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1641:ASN:OXT	3:F:255:SER:HB3	2.17	0.44
1:C:6:ILE:HD12	1:C:21:VAL:O	2.17	0.44
2:D:819:ARG:HE	2:D:883:THR:CG2	2.28	0.44
2:D:918:LYS:HZ3	2:D:944:ASP:HB3	1.82	0.44
2:D:1301:GLU:HG2	3:H:157:ARG:NH1	2.32	0.44
3:F:125:ARG:HH21	3:F:194:GLN:HE22	1.65	0.44
3:F:606:LEU:C	3:F:606:LEU:HD12	2.38	0.44
3:H:309:TRP:HZ3	3:H:313:GLN:CD	2.21	0.44
1:A:74:PHE:C	1:A:82:LYS:HZ3	2.20	0.44
1:C:63:ASN:HD22	5:K:1:NAG:C1	2.06	0.44
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.99	0.44
2:D:1483:LEU:HB3	2:D:1490:ARG:HG2	2.00	0.44
2:D:1581:LEU:HB2	2:D:1609:TRP:CE3	2.53	0.44
3:F:375:THR:O	3:F:379:GLU:HG3	2.17	0.44
3:H:32:ALA:HA	3:H:57:TRP:HZ3	1.83	0.44
3:H:199:TYR:CE1	3:H:431:LYS:HD3	2.51	0.44
3:H:655:PHE:HA	3:H:717:HIS:O	2.16	0.44
4:I:17:SER:HB3	4:I:54:LEU:HB3	1.98	0.44
2:B:833:ARG:HD2	2:B:838:LEU:HD21	1.99	0.44
2:B:916:MET:HG3	2:B:1328:ALA:CB	2.47	0.44
2:B:1551:SER:HB3	3:F:371:GLY:HA3	1.99	0.44
1:C:518:ALA:O	1:C:519:SER:C	2.54	0.44
2:D:1333:GLN:HB3	2:D:1334:LEU:C	2.37	0.44
3:F:110:TYR:CE1	3:F:135:ASN:HB3	2.52	0.44
3:F:544:ILE:HD13	3:F:650:VAL:HG12	1.98	0.44
3:F:546:GLU:HB3	3:F:548:TYR:CE1	2.52	0.44
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.82	0.44
2:D:1103:ILE:HD12	2:D:1103:ILE:N	2.31	0.44
2:D:1365:GLU:HA	2:D:1438:ALA:HB2	1.99	0.44
3:F:433:MET:O	3:F:434:GLU:HB2	2.17	0.44
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.99	0.44
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.98	0.44
1:C:583:LEU:N	1:C:583:LEU:HD12	2.33	0.44
2:D:941:PRO:HA	2:D:942:PRO:HD3	1.90	0.44
3:F:513:LYS:HB3	3:F:522:ASP:HB3	1.99	0.44
2:B:964:PRO:HA	2:B:965:VAL:CB	2.47	0.44
2:B:1276:LEU:HD23	2:B:1276:LEU:H	1.83	0.44
1:C:338:THR:HG21	1:C:419:MET:HE1	2.00	0.44
2:D:1017:LEU:O	2:D:1018:GLU:HB3	2.17	0.44
1:A:116:ILE:HG12	1:A:205:TYR:CE2	2.52	0.44
1:A:398:LEU:HD22	1:A:400:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:ILE:HG13	2:B:734:ILE:N	2.31	0.44
1:C:356:ASN:HB3	1:C:357:PRO:HD2	1.99	0.44
2:D:840:VAL:HG12	2:D:841:ARG:N	2.32	0.44
3:F:298:LYS:HZ2	3:F:340:MET:HA	1.83	0.44
1:A:338:THR:HG21	1:A:419:MET:HE1	1.99	0.44
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.88	0.44
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.99	0.44
2:B:1333:GLN:CD	2:B:1333:GLN:H	2.21	0.44
2:B:1365:GLU:HA	2:B:1438:ALA:HB2	2.00	0.44
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.33	0.44
1:C:329:SER:HA	1:C:330:PRO:HD3	1.84	0.44
1:C:400:ILE:N	1:C:400:ILE:HD12	2.33	0.44
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.32	0.44
2:D:1236:GLU:HA	2:D:1238:ARG:NH2	2.33	0.44
2:D:1380:ILE:N	2:D:1380:ILE:HD12	2.32	0.44
2:B:804:MET:HG2	2:B:805:GLN:H	1.83	0.44
2:B:918:LYS:HE3	2:B:1326:TYR:OH	2.18	0.44
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.52	0.44
2:D:1333:GLN:H	2:D:1333:GLN:CD	2.21	0.44
2:B:1296:LEU:O	2:B:1298:ARG:HG3	2.18	0.43
2:B:1535:ASP:OD1	2:B:1535:ASP:N	2.50	0.43
1:C:111:GLN:O	1:C:125:TYR:HA	2.17	0.43
1:C:129:THR:OG1	1:C:165:GLY:HA2	2.18	0.43
2:D:819:ARG:NH1	2:D:1487:GLU:HG2	2.33	0.43
2:D:1331:LYS:HA	2:D:1332:ASP:CB	2.28	0.43
3:F:222:ALA:N	3:F:223:GLU:CA	2.66	0.43
3:F:479:PRO:C	3:F:481:LYS:H	2.21	0.43
3:H:106:CYS:SG	3:H:112:LEU:HB2	2.58	0.43
3:H:463:THR:OG1	3:H:464:ASP:N	2.51	0.43
3:H:635:ALA:HB3	3:H:647:ILE:HD11	2.00	0.43
1:A:17:GLU:HG2	1:A:67:THR:OG1	2.18	0.43
2:B:1338:LYS:HD2	2:B:1338:LYS:N	2.33	0.43
1:C:343:LYS:N	1:C:343:LYS:HD2	2.33	0.43
1:C:533:VAL:HG12	1:C:534:LYS:N	2.33	0.43
2:D:918:LYS:HE3	2:D:1326:TYR:OH	2.19	0.43
2:D:1386:MET:SD	2:D:1473:PRO:HD3	2.57	0.43
3:F:106:CYS:SG	3:F:112:LEU:HB2	2.58	0.43
3:H:380:ILE:O	3:H:384:LEU:HG	2.18	0.43
3:H:513:LYS:HB3	3:H:522:ASP:HB3	1.99	0.43
3:H:701:LYS:O	3:H:702:ASN:C	2.55	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:C	1:A:375:VAL:H	2.21	0.43
2:B:1337:ASN:HB3	2:B:1338:LYS:H	1.63	0.43
1:C:116:ILE:HG12	1:C:205:TYR:CE2	2.53	0.43
2:D:854:ALA:HB2	2:D:860:HIS:HB3	2.00	0.43
3:H:463:THR:O	3:H:466:HIS:HB2	2.17	0.43
1:A:255:ASP:HB2	1:A:300:LYS:HG2	2.00	0.43
1:A:553:PRO:HD2	2:B:802:THR:O	2.19	0.43
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.43
1:C:12:LEU:HG	1:C:99:VAL:HG11	2.00	0.43
1:C:283:LYS:O	1:C:287:ASP:HB2	2.18	0.43
2:D:913:GLY:O	2:D:1331:LYS:HE3	2.18	0.43
3:H:240:PRO:HA	3:H:241:SER:HA	1.52	0.43
1:A:283:LYS:O	1:A:287:ASP:HB2	2.18	0.43
2:B:1039:GLN:OE1	2:B:1052:PRO:HG3	2.19	0.43
2:D:833:ARG:HD2	2:D:838:LEU:HD21	2.00	0.43
2:D:1001:ILE:HG13	2:D:1254:PHE:HB2	1.99	0.43
2:D:1039:GLN:OE1	2:D:1052:PRO:HG3	2.19	0.43
3:H:433:MET:CG	3:H:434:GLU:N	2.82	0.43
3:H:433:MET:CG	3:H:434:GLU:H	2.31	0.43
4:J:202:ARG:HB3	4:J:203:VAL:H	1.62	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.53	0.43
1:A:145:ILE:O	1:A:153:VAL:HG22	2.18	0.43
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.53	0.43
2:D:1498:ILE:HG22	2:D:1499:GLN:HG2	2.00	0.43
3:F:35:TYR:HB2	3:F:43:PRO:HB3	1.99	0.43
3:F:380:ILE:O	3:F:384:LEU:HG	2.18	0.43
3:F:433:MET:CG	3:F:434:GLU:N	2.82	0.43
3:F:433:MET:CG	3:F:434:GLU:H	2.31	0.43
4:I:7:ALA:O	4:I:58:HIS:HE1	2.02	0.43
4:I:30:LEU:O	4:I:107:PRO:HA	2.19	0.43
1:A:269:ILE:HD13	1:A:278:VAL:HB	2.01	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.18	0.43
2:D:1145:GLY:O	2:D:1149:LYS:HG2	2.19	0.43
2:D:1390:ALA:HA	2:D:1391:PRO:HD3	1.90	0.43
2:D:1536:PHE:H	2:D:1566:ILE:HG12	1.83	0.43
3:F:450:LEU:HD12	3:F:450:LEU:HA	1.93	0.43
3:H:110:TYR:CE1	3:H:135:ASN:HB3	2.54	0.43
4:J:40:ALA:HB2	4:J:90:LEU:O	2.18	0.43
1:A:63:ASN:HB3	5:E:1:NAG:O5	2.18	0.43
2:B:785:VAL:HG13	2:B:795:VAL:HG12	1.99	0.43
2:B:819:ARG:O	2:B:820:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.54	0.43
2:B:1631:THR:O	2:B:1635:VAL:HG23	2.19	0.43
3:F:19:ILE:HG13	3:F:71:ALA:C	2.39	0.43
1:A:103:LEU:HD22	1:A:103:LEU:N	2.34	0.43
1:A:158:LEU:HD22	1:A:169:LEU:HD11	2.01	0.43
1:C:123:VAL:O	1:C:170:SER:HA	2.19	0.43
1:C:269:ILE:HD13	1:C:278:VAL:HB	2.00	0.43
1:C:373:ASP:C	1:C:375:VAL:H	2.22	0.43
1:C:552:GLN:HA	1:C:553:PRO:HD3	1.92	0.43
1:C:566:ASP:OD2	2:D:791:LYS:HG3	2.19	0.43
3:F:143:PRO:HG3	3:F:186:TRP:NE1	2.34	0.43
3:H:35:TYR:HB2	3:H:43:PRO:HB3	2.00	0.43
3:H:447:SER:O	4:I:208:LYS:HE2	2.18	0.43
3:H:650:VAL:HG23	3:H:651:VAL:HG23	2.01	0.43
1:A:19:THR:HA	1:A:65:THR:HG22	2.01	0.43
1:A:400:ILE:N	1:A:400:ILE:HD12	2.33	0.43
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.89	0.43
2:B:964:PRO:HB3	2:B:1291:TRP:CZ3	2.54	0.43
2:B:1380:ILE:N	2:B:1380:ILE:HD12	2.34	0.43
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	2.01	0.43
2:D:1115:ASN:O	2:D:1116:GLU:HB2	2.19	0.43
3:F:219:GLY:HA2	3:F:455:MET:CE	2.49	0.43
3:F:299:VAL:H	3:F:340:MET:CE	2.29	0.43
3:F:490:VAL:O	3:F:569:PRO:HA	2.19	0.43
3:H:692:ILE:HA	3:H:717:HIS:ND1	2.34	0.43
2:B:839:LYS:O	2:B:895:TYR:HD1	2.02	0.42
2:B:1531:GLN:C	2:B:1532:LEU:HD12	2.39	0.42
2:D:1155:GLU:HG3	2:D:1184:LEU:HD21	2.00	0.42
2:D:1338:LYS:N	2:D:1338:LYS:HD2	2.34	0.42
2:D:1490:ARG:HD2	2:D:1590:TRP:CE3	2.54	0.42
3:F:80:ARG:HA	3:F:81:PRO:HD3	1.94	0.42
1:A:123:VAL:O	1:A:170:SER:HA	2.19	0.42
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.01	0.42
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.92	0.42
2:B:963:THR:HG22	2:B:1318:GLY:HA2	2.01	0.42
2:B:1064:PHE:O	2:B:1068:VAL:HG13	2.19	0.42
2:B:1115:ASN:O	2:B:1116:GLU:HB2	2.19	0.42
2:B:1155:GLU:HG3	2:B:1184:LEU:HD21	2.01	0.42
2:B:1498:ILE:HD12	2:B:1605:TRP:HB2	2.00	0.42
1:C:10:ASN:CB	1:C:635:ARG:HH11	2.33	0.42
1:C:171:TRP:CZ3	1:C:173:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:811:LEU:HG	2:D:813:LEU:HD13	2.01	0.42
2:D:839:LYS:O	2:D:895:TYR:HD1	2.01	0.42
3:F:341:MET:SD	3:F:380:ILE:HG23	2.59	0.42
3:H:80:ARG:HA	3:H:81:PRO:HD3	1.94	0.42
3:H:280:VAL:O	3:H:282:PRO:HD3	2.19	0.42
1:A:241:LYS:HG3	2:B:832:TYR:CE1	2.54	0.42
1:A:533:VAL:HG12	1:A:534:LYS:N	2.34	0.42
2:B:1276:LEU:HD23	2:B:1276:LEU:N	2.34	0.42
2:D:959:LEU:HD21	2:D:1297:LEU:CD2	2.49	0.42
2:D:1337:ASN:HB3	2:D:1338:LYS:H	1.63	0.42
3:F:44:TYR:HB3	3:F:72:GLU:O	2.19	0.42
3:F:90:TRP:CD1	3:F:90:TRP:N	2.85	0.42
3:H:113:ARG:NH2	3:H:141:SER:HB2	2.30	0.42
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.55	0.42
1:C:38:HIS:HD2	1:C:45:LEU:HB3	1.85	0.42
1:C:578:LYS:HD3	2:D:779:THR:HB	2.01	0.42
2:D:1411:GLU:HG2	2:D:1422:LEU:HD12	2.00	0.42
3:F:44:TYR:CD1	3:F:45:PRO:HA	2.55	0.42
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	2.01	0.42
1:C:145:ILE:O	1:C:153:VAL:HG22	2.19	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
2:D:1387:THR:HG23	2:D:1387:THR:O	2.19	0.42
2:D:1485:ARG:O	2:D:1486:ASP:HB2	2.20	0.42
3:F:113:ARG:NH2	3:F:141:SER:HB2	2.33	0.42
1:A:129:THR:OG1	1:A:165:GLY:HA2	2.20	0.42
1:A:414:GLN:HA	1:A:414:GLN:NE2	2.29	0.42
2:B:754:GLU:HG3	2:B:769:MET:SD	2.59	0.42
2:B:916:MET:HG3	2:B:1328:ALA:HB3	2.01	0.42
2:B:1253:VAL:O	2:B:1257:LEU:HG	2.20	0.42
2:B:1405:ARG:HE	2:B:1437:LEU:HD22	1.84	0.42
1:C:25:HIS:HA	1:C:26:ASP:HA	1.51	0.42
2:D:977:ARG:HD2	2:D:1240:TYR:CE2	2.55	0.42
2:D:1296:LEU:O	2:D:1298:ARG:HG3	2.18	0.42
3:F:701:LYS:O	3:F:703:GLN:N	2.52	0.42
2:B:1524:LYS:O	2:B:1544:GLU:HB2	2.19	0.42
1:C:459:ARG:HA	1:C:462:GLU:HG2	2.02	0.42
1:C:547:GLN:NE2	1:C:559:MET:HA	2.29	0.42
3:F:497:LEU:HA	3:F:554:LEU:HD23	2.02	0.42
4:J:54:LEU:HD21	4:J:67:LYS:HE3	2.01	0.42
1:C:440:ARG:HA	1:C:440:ARG:HD2	1.92	0.42
2:D:1009:THR:HG22	2:D:1261:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1391:PRO:HB2	2:D:1396:LEU:HD11	2.02	0.42
3:F:280:VAL:O	3:F:282:PRO:HD3	2.20	0.42
3:H:250:LEU:O	3:H:288:THR:HA	2.20	0.42
3:H:490:VAL:O	3:H:569:PRO:HA	2.20	0.42
1:A:541:LEU:HD22	2:B:786:SER:CB	2.49	0.42
1:A:545:SER:HB2	2:B:799:PHE:HZ	1.84	0.42
1:A:606:THR:HA	1:A:607:PRO:HD3	1.94	0.42
2:B:1297:LEU:HD12	2:B:1297:LEU:HA	1.68	0.42
2:B:1500:LYS:HE3	2:B:1500:LYS:HB2	1.93	0.42
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.30	0.42
2:D:1086:ILE:HG23	2:D:1146:SER:HB2	2.00	0.42
2:D:1270:LEU:O	2:D:1290:HIS:HA	2.20	0.42
3:F:32:ALA:HA	3:F:57:TRP:HZ3	1.84	0.42
3:F:650:VAL:HG23	3:F:651:VAL:HG23	2.02	0.42
4:J:64:GLU:HA	4:J:65:PRO:HD3	1.89	0.42
1:A:470:TYR:HA	1:A:510:VAL:O	2.20	0.42
1:A:510:VAL:HG21	1:A:622:LEU:HD12	2.01	0.42
2:B:941:PRO:HA	2:B:942:PRO:HD3	1.90	0.42
2:B:1086:ILE:HG23	2:B:1146:SER:HB2	2.02	0.42
2:D:811:LEU:HG	2:D:813:LEU:CD1	2.50	0.42
2:D:968:MET:O	2:D:969:THR:HB	2.20	0.42
2:D:981:LEU:HB3	2:D:998:PRO:O	2.20	0.42
2:D:1451:GLN:HA	2:D:1452:PRO:HD3	1.95	0.42
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.55	0.42
3:F:445:ASP:O	3:F:448:GLN:HG2	2.20	0.42
3:H:546:GLU:HB3	3:H:548:TYR:CE1	2.55	0.42
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.50	0.41
1:C:103:LEU:N	1:C:103:LEU:HD22	2.34	0.41
2:D:1405:ARG:HE	2:D:1437:LEU:HD22	1.85	0.41
3:H:164:TYR:CD1	3:H:191:PRO:HG2	2.55	0.41
4:I:78:HIS:HA	4:I:79:PRO:HD3	1.89	0.41
4:J:7:ALA:O	4:J:58:HIS:HE1	2.03	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.34	0.41
2:B:1342:LYS:HD3	2:B:1342:LYS:N	2.35	0.41
1:C:93:GLN:HE21	1:C:627:SER:HB2	1.84	0.41
1:C:510:VAL:HG21	1:C:622:LEU:HD12	2.02	0.41
3:F:37:CYS:HA	3:F:38:PRO:HD3	1.93	0.41
3:H:706:GLN:C	3:H:708:GLN:H	2.10	0.41
1:A:112:THR:HB	1:A:117:TYR:OH	2.20	0.41
1:A:220:PHE:CD1	1:A:357:PRO:HG2	2.55	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:HA	1:C:406:LYS:HE2	2.02	0.41
1:C:459:ARG:HA	1:C:462:GLU:CG	2.50	0.41
2:D:1276:LEU:HD23	2:D:1276:LEU:N	2.36	0.41
3:F:158:LEU:HG	3:F:159:GLU:HG3	2.03	0.41
3:H:90:TRP:CD1	3:H:90:TRP:N	2.87	0.41
4:J:30:LEU:O	4:J:107:PRO:HA	2.20	0.41
1:A:31:VAL:CG1	1:A:54:LEU:HB2	2.50	0.41
1:A:236:ARG:HA	1:A:243:VAL:HG23	2.02	0.41
2:B:735:ALA:C	2:B:737:GLU:H	2.23	0.41
2:B:916:MET:HE2	2:B:916:MET:HA	2.02	0.41
2:B:981:LEU:HB3	2:B:998:PRO:O	2.20	0.41
1:C:143:VAL:O	1:C:155:GLN:HA	2.20	0.41
2:D:819:ARG:O	2:D:820:ASN:HB2	2.21	0.41
2:D:1524:LYS:O	2:D:1544:GLU:HB2	2.20	0.41
3:F:499:ALA:HB2	3:F:675:GLY:HA2	2.02	0.41
3:H:44:TYR:CD1	3:H:45:PRO:HA	2.56	0.41
4:I:202:ARG:HB3	4:I:203:VAL:H	1.62	0.41
2:B:1391:PRO:HB2	2:B:1396:LEU:HD11	2.03	0.41
1:C:480:LYS:HG2	1:C:481:ALA:N	2.35	0.41
2:D:1143:LEU:O	2:D:1147:ILE:HG13	2.20	0.41
3:H:497:LEU:HA	3:H:554:LEU:HD23	2.02	0.41
4:J:17:SER:HB3	4:J:54:LEU:HB3	2.02	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.84	0.41
2:B:1060:VAL:HG13	2:B:1064:PHE:CE1	2.56	0.41
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.50	0.41
1:C:470:TYR:HA	1:C:510:VAL:O	2.20	0.41
3:F:219:GLY:HA2	3:F:455:MET:HE1	2.03	0.41
3:F:531:HIS:HA	3:F:532:PRO:HD3	1.98	0.41
4:J:106:ARG:HA	4:J:107:PRO:HD3	1.91	0.41
2:B:1387:THR:HG23	2:B:1387:THR:O	2.21	0.41
1:C:17:GLU:HG2	1:C:67:THR:OG1	2.21	0.41
1:C:112:THR:HB	1:C:117:TYR:OH	2.21	0.41
1:C:233:ILE:HG13	1:C:269:ILE:HD11	2.03	0.41
2:D:983:VAL:O	2:D:985:PRO:HD3	2.20	0.41
3:H:282:PRO:O	3:H:305:SER:HA	2.21	0.41
3:H:418:ALA:HB3	3:H:427:VAL:HG22	2.02	0.41
3:H:445:ASP:O	3:H:448:GLN:HG2	2.21	0.41
4:I:151:ARG:HB2	9:I:1229:GOL:H12	2.02	0.41
1:A:451:VAL:HB	1:A:495:LEU:HB3	2.03	0.41
2:B:811:LEU:HG	2:B:813:LEU:HD13	2.03	0.41
2:B:1270:LEU:O	2:B:1290:HIS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1617:ASP:C	2:B:1619:GLU:H	2.24	0.41
1:C:31:VAL:CG1	1:C:54:LEU:HB2	2.51	0.41
1:C:83:PHE:CD2	1:C:100:LEU:HA	2.55	0.41
3:F:393:PRO:O	3:F:394:ARG:HB2	2.21	0.41
4:I:62:GLN:HA	4:I:63:PRO:HD3	1.85	0.41
4:J:37:LEU:HD11	4:J:90:LEU:HD22	2.02	0.41
2:B:745:PHE:N	2:B:746:PRO:HD3	2.36	0.41
2:B:1005:TYR:CD1	2:B:1258:ALA:HB2	2.53	0.41
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.20	0.41
2:D:1641:ASN:OXT	3:H:255:SER:HB3	2.20	0.41
3:F:76:ILE:HG23	3:F:197:PHE:CE1	2.55	0.41
3:F:94:PRO:HB2	3:F:95:TYR:CD1	2.56	0.41
3:F:103:SER:HB3	3:F:117:ASN:OD1	2.21	0.41
3:F:196:SER:O	3:F:197:PHE:HB3	2.21	0.41
3:F:452:LEU:HD12	3:F:455:MET:HG3	2.02	0.41
3:F:620:VAL:HG12	3:F:667:PRO:HD2	2.03	0.41
3:F:706:GLN:C	3:F:708:GLN:H	2.23	0.41
3:H:299:VAL:HG22	3:H:340:MET:HE3	2.02	0.41
3:H:343:TRP:HE3	3:H:344:PRO:HD2	1.86	0.41
3:H:405:VAL:HG23	3:H:406:GLY:N	2.36	0.41
4:J:15:MET:CE	4:J:127:GLY:HA2	2.51	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
1:C:158:LEU:HD22	1:C:169:LEU:HD11	2.02	0.41
3:F:299:VAL:HG22	3:F:340:MET:HE3	2.03	0.41
3:F:539:LYS:HG3	3:F:547:PHE:CD1	2.56	0.41
1:A:38:HIS:HD2	1:A:45:LEU:HB3	1.85	0.40
1:A:216:PRO:HA	1:A:231:VAL:HA	2.02	0.40
2:B:983:VAL:O	2:B:985:PRO:HD3	2.21	0.40
2:B:1022:GLY:O	2:B:1026:LEU:HG	2.21	0.40
2:B:1378:MET:HB3	2:B:1378:MET:HE2	1.93	0.40
2:D:1253:VAL:O	2:D:1257:LEU:HG	2.21	0.40
2:D:1342:LYS:HD3	2:D:1342:LYS:N	2.36	0.40
2:D:1617:ASP:C	2:D:1619:GLU:H	2.24	0.40
3:F:190:GLU:HA	3:F:191:PRO:HD3	1.81	0.40
3:H:125:ARG:HH21	3:H:194:GLN:HE22	1.69	0.40
1:A:480:LYS:HG2	1:A:481:ALA:N	2.36	0.40
2:D:1276:LEU:HD23	2:D:1276:LEU:H	1.85	0.40
3:F:318:ASN:HD21	3:F:320:GLU:HG2	1.86	0.40
3:H:33:LEU:HD12	3:H:33:LEU:C	2.41	0.40
3:H:354:ARG:C	3:H:354:ARG:HD2	2.42	0.40
4:I:137:ARG:HA	4:I:138:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:HG12	1:A:302:LEU:CD2	2.52	0.40
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.51	0.40
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.03	0.40
1:C:410:SER:O	1:C:414:GLN:HG2	2.22	0.40
1:C:474:ASN:ND2	1:C:475:LYS:HG3	2.36	0.40
2:D:1086:ILE:HA	2:D:1090:GLN:NE2	2.37	0.40
3:F:309:TRP:HZ3	3:F:313:GLN:CG	2.35	0.40
3:H:143:PRO:HB2	3:H:164:TYR:OH	2.20	0.40
3:H:464:ASP:O	3:H:465:TYR:HB2	2.21	0.40
5:G:2:NAG:HN2	5:G:2:NAG:H5	1.85	0.40
1:C:45:LEU:HA	1:C:46:VAL:HA	1.72	0.40
1:C:249:VAL:HG13	1:C:267:LYS:HB2	2.03	0.40
3:F:119:THR:HB	4:I:115:ARG:NH1	2.36	0.40
3:F:254:GLY:HA2	3:F:319:TYR:OH	2.21	0.40
1:A:143:VAL:O	1:A:155:GLN:HA	2.22	0.40
2:B:1143:LEU:O	2:B:1147:ILE:HG13	2.22	0.40
2:D:735:ALA:O	2:D:739:ILE:HG13	2.22	0.40
2:D:962:GLY:HA3	2:D:1289:ILE:HG21	2.03	0.40
3:F:408:LEU:HD22	3:F:408:LEU:N	2.37	0.40
3:F:709:VAL:HA	3:F:710:PRO:HD3	1.93	0.40
3:H:408:LEU:HD22	3:H:408:LEU:N	2.36	0.40
3:H:503:PHE:HB2	3:H:530:PHE:CZ	2.56	0.40
3:H:638:ALA:HA	3:H:639:PRO:HD3	1.97	0.40
4:I:40:ALA:HB2	4:I:90:LEU:O	2.21	0.40
4:I:54:LEU:HD21	4:I:67:LYS:HE3	2.03	0.40
4:I:151:ARG:N	9:I:1229:GOL:H11	2.37	0.40
4:J:15:MET:HE1	4:J:127:GLY:HA2	2.04	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	636/642 (99%)	569 (90%)	59 (9%)	8 (1%)	12	48
1	C	636/642 (99%)	565 (89%)	61 (10%)	10 (2%)	9	43
2	B	895/912 (98%)	802 (90%)	83 (9%)	10 (1%)	14	52
2	D	895/912 (98%)	795 (89%)	92 (10%)	8 (1%)	17	56
3	F	708/732 (97%)	642 (91%)	55 (8%)	11 (2%)	9	43
3	H	705/732 (96%)	637 (90%)	54 (8%)	14 (2%)	7	39
4	I	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	17	56
4	J	226/228 (99%)	199 (88%)	25 (11%)	2 (1%)	17	56
All	All	4927/5028 (98%)	4410 (90%)	452 (9%)	65 (1%)	12	48

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	VAL
1	A	518	ALA
2	B	733	ILE
2	B	965	VAL
2	B	1498	ILE
1	C	289	VAL
1	C	518	ALA
1	C	519	SER
2	D	1498	ILE
3	F	197	PHE
3	F	702	ASN
3	F	706	GLN
3	F	707	LYS
3	H	197	PHE
3	H	702	ASN
3	H	706	GLN
3	H	707	LYS
1	A	290	GLN
1	A	534	LYS
2	B	968	MET
2	B	1377	THR
2	B	1505	VAL
1	C	290	GLN
1	C	534	LYS
2	D	928	GLU
2	D	965	VAL
2	D	1377	THR

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Mol	Chain	Res	Type
2	D	1505	VAL
3	F	199	TYR
3	F	704	LYS
3	F	740	ALA
3	H	199	TYR
3	H	463	THR
3	H	704	LYS
3	H	740	ALA
1	A	519	SER
1	A	549	GLU
2	B	928	GLU
1	C	517	GLY
1	C	549	GLU
2	D	774	LYS
2	D	1534	ASN
3	F	431	LYS
3	F	703	GLN
3	H	431	LYS
3	H	703	GLN
4	I	46	ALA
4	I	47	ALA
4	J	46	ALA
4	J	47	ALA
1	A	574	VAL
2	B	778	THR
2	B	969	THR
1	C	574	VAL
3	F	479	PRO
3	H	433	MET
1	C	27	ALA
3	H	223	GLU
3	H	479	PRO
2	D	1201	PRO
3	H	692	ILE
2	B	1201	PRO
1	C	520	GLY
1	A	520	GLY
3	F	692	ILE

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	564/566 (100%)	557 (99%)	7 (1%)	71	87
1	C	564/566 (100%)	558 (99%)	6 (1%)	73	88
2	B	797/807 (99%)	788 (99%)	9 (1%)	73	88
2	D	797/807 (99%)	789 (99%)	8 (1%)	76	88
3	F	620/635 (98%)	612 (99%)	8 (1%)	69	86
3	H	618/635 (97%)	611 (99%)	7 (1%)	73	88
4	I	181/181 (100%)	179 (99%)	2 (1%)	73	88
4	J	181/181 (100%)	180 (99%)	1 (1%)	86	94
All	All	4322/4378 (99%)	4274 (99%)	48 (1%)	73	88

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	370	GLN
1	A	414	GLN
1	A	516	ILE
1	A	519	SER
1	A	630	GLN
1	A	634	GLN
2	B	733	ILE
2	B	898	PHE
2	B	953	GLU
2	B	965	VAL
2	B	1270	LEU
2	B	1276	LEU
2	B	1334	LEU
2	B	1342	LYS
2	B	1573	LYS
1	C	59	ASN
1	C	370	GLN
1	C	414	GLN

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Mol	Chain	Res	Type
1	C	516	ILE
1	C	630	GLN
1	C	634	GLN
2	D	898	PHE
2	D	953	GLU
2	D	1270	LEU
2	D	1276	LEU
2	D	1334	LEU
2	D	1342	LYS
2	D	1485	ARG
2	D	1573	LYS
3	F	90	TRP
3	F	103	SER
3	F	241	SER
3	F	309	TRP
3	F	468	GLN
3	F	611	GLU
3	F	654	ARG
3	F	705	ARG
3	H	90	TRP
3	H	103	SER
3	H	243	SER
3	H	309	TRP
3	H	354	ARG
3	H	468	GLN
3	H	654	ARG
4	I	157	ARG
4	I	198	THR
4	J	157	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	59	ASN
1	A	104	GLN
1	A	132	HIS
1	A	311	HIS
1	A	370	GLN
1	A	414	GLN
1	A	558	GLN
1	A	587	ASN

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Mol	Chain	Res	Type
1	A	630	GLN
1	A	634	GLN
2	B	770	ASN
2	B	836	GLN
2	B	860	HIS
2	B	1090	GLN
2	B	1130	GLN
2	B	1176	GLN
2	B	1268	GLN
2	B	1545	GLN
1	C	38	HIS
1	C	59	ASN
1	C	63	ASN
1	C	104	GLN
1	C	132	HIS
1	C	311	HIS
1	C	356	ASN
1	C	370	GLN
1	C	414	GLN
1	C	558	GLN
1	C	587	ASN
1	C	630	GLN
1	C	634	GLN
2	D	770	ASN
2	D	836	GLN
2	D	860	HIS
2	D	1090	GLN
2	D	1130	GLN
2	D	1176	GLN
2	D	1267	HIS
2	D	1545	GLN
3	F	63	GLN
3	F	194	GLN
3	F	357	HIS
3	F	423	ASN
3	F	591	GLN
3	H	63	GLN
3	H	194	GLN
3	H	318	ASN
3	H	357	HIS
3	H	483	HIS
3	H	591	GLN

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Mol	Chain	Res	Type
4	I	10	HIS
4	J	10	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	1	5,1	14,14,15	0.51	0	17,19,21	1.36	2 (11%)
5	NAG	E	2	5	14,14,15	0.58	0	17,19,21	1.29	2 (11%)
5	NAG	G	1	5,2	14,14,15	0.55	0	17,19,21	0.60	0
5	NAG	G	2	5	14,14,15	0.54	0	17,19,21	0.72	0
5	NAG	K	1	5,1	14,14,15	0.57	0	17,19,21	0.67	0
5	NAG	K	2	5	14,14,15	0.57	0	17,19,21	0.67	0
6	NAG	L	1	6,3	14,14,15	0.61	0	17,19,21	1.41	3 (17%)
6	NAG	L	2	6	14,14,15	0.61	0	17,19,21	1.37	2 (11%)
6	BMA	L	3	6	11,11,12	0.27	0	15,15,17	0.63	0
6	NAG	M	1	6,3	14,14,15	0.47	0	17,19,21	1.91	5 (29%)
6	NAG	M	2	6	14,14,15	0.52	0	17,19,21	1.75	5 (29%)
6	BMA	M	3	6	11,11,12	1.68	2 (18%)	15,15,17	3.70	11 (73%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	NAG	M	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	3	BMA	C2-C3	3.41	1.57	1.52
6	M	3	BMA	C4-C3	3.11	1.60	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	3	BMA	O5-C5-C6	7.33	118.69	107.20
6	M	3	BMA	O2-C2-C1	5.04	119.47	109.15
6	M	3	BMA	O3-C3-C4	4.79	121.42	110.35
6	M	3	BMA	O4-C4-C5	4.75	121.09	109.30
6	M	3	BMA	O2-C2-C3	4.57	119.29	110.14
6	M	3	BMA	O3-C3-C2	4.49	118.59	109.99
6	M	1	NAG	C2-N2-C7	4.44	129.22	122.90
6	M	1	NAG	C1-O5-C5	3.84	117.40	112.19
5	E	2	NAG	C1-O5-C5	-3.49	107.47	112.19
6	M	3	BMA	O4-C4-C3	3.42	118.26	110.35
6	L	1	NAG	C1-O5-C5	3.34	116.71	112.19
5	E	1	NAG	C1-O5-C5	3.16	116.48	112.19
6	L	2	NAG	O5-C1-C2	-3.14	106.32	111.29
6	L	1	NAG	O5-C1-C2	3.11	116.19	111.29
6	M	3	BMA	O6-C6-C5	2.85	121.08	111.29
6	M	2	NAG	O3-C3-C2	2.81	115.28	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	2	NAG	O5-C1-C2	-2.79	106.88	111.29
5	E	1	NAG	O5-C1-C2	2.77	115.66	111.29
6	M	3	BMA	C3-C4-C5	2.72	115.09	110.24
6	M	1	NAG	C1-C2-N2	-2.68	105.91	110.49
6	M	1	NAG	C6-C5-C4	-2.47	107.22	113.00
6	L	2	NAG	C3-C4-C5	2.47	114.64	110.24
6	M	2	NAG	C6-C5-C4	-2.35	107.49	113.00
5	E	2	NAG	O5-C5-C6	2.35	110.89	107.20
6	M	2	NAG	C4-C3-C2	-2.31	107.64	111.02
6	M	2	NAG	C2-N2-C7	2.29	126.16	122.90
6	M	3	BMA	C1-O5-C5	2.24	115.22	112.19
6	L	1	NAG	C2-N2-C7	-2.10	119.91	122.90
6	M	3	BMA	O5-C1-C2	2.05	113.93	110.77
6	M	1	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O7-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
6	L	3	BMA	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6

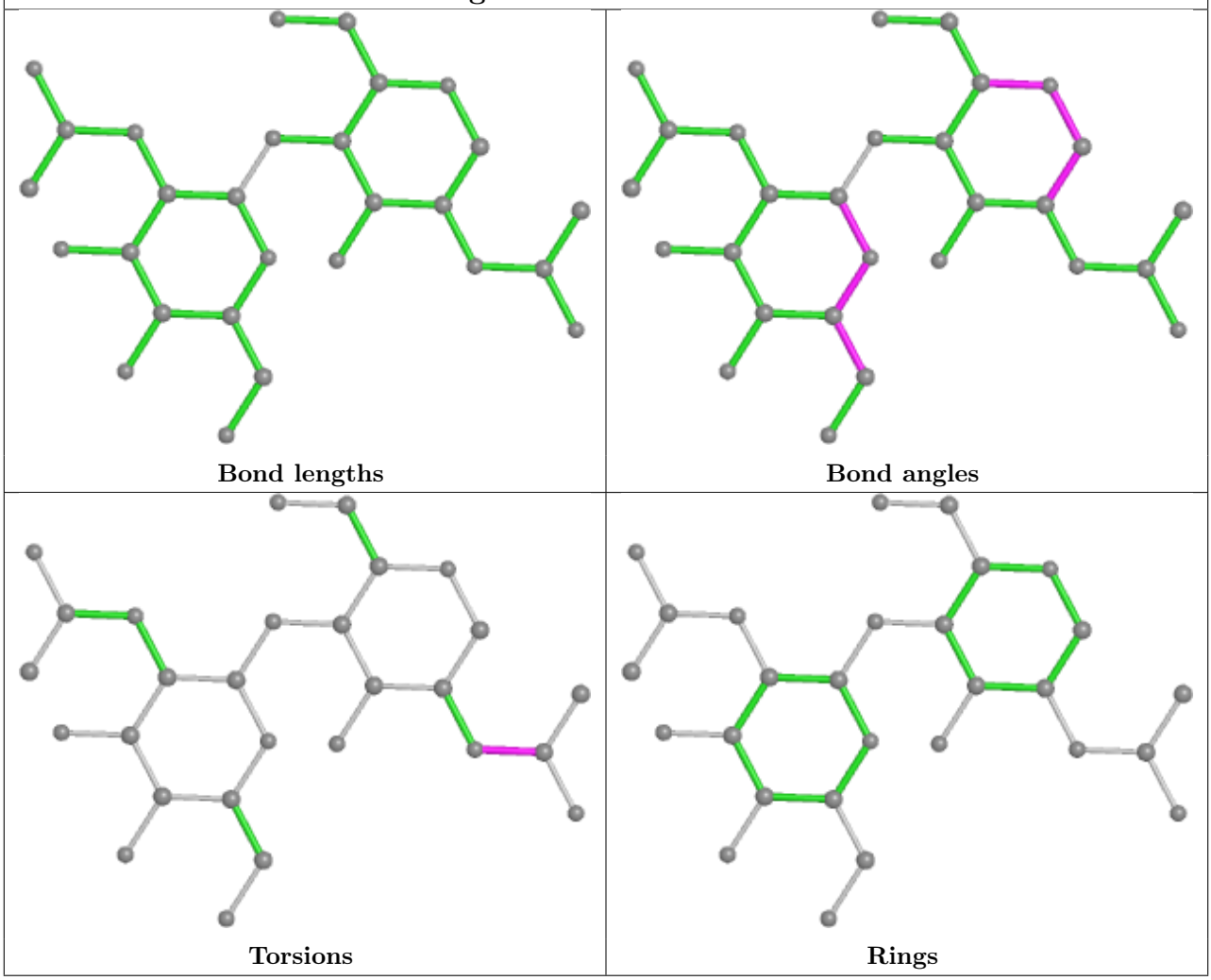
There are no ring outliers.

6 monomers are involved in 14 short contacts:

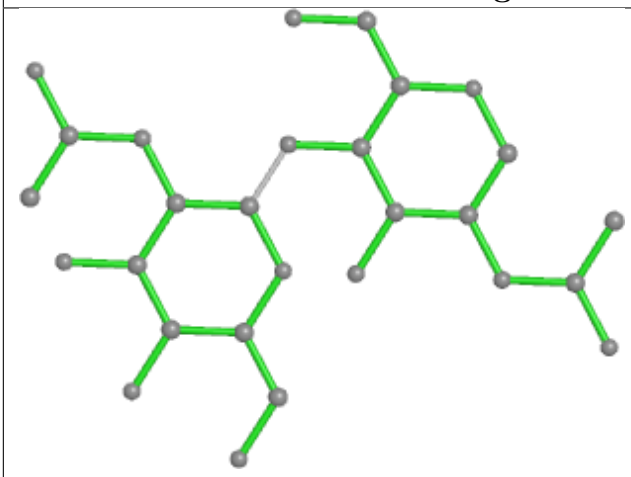
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
5	K	2	NAG	2	0
5	K	1	NAG	10	0
5	G	2	NAG	1	0
6	L	2	NAG	1	0
6	L	1	NAG	1	0

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

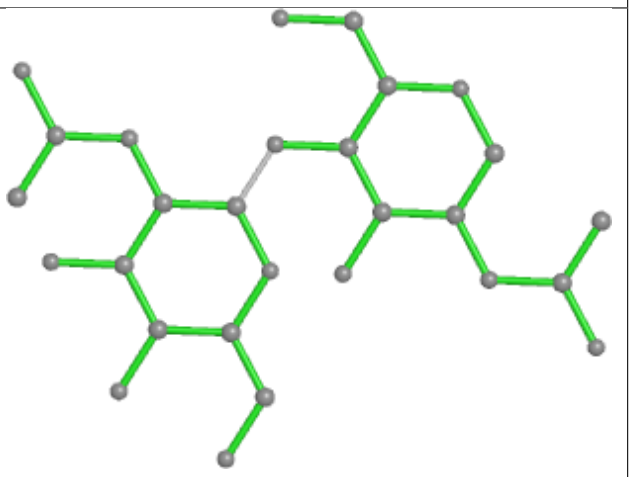
Oligosaccharide Chain E



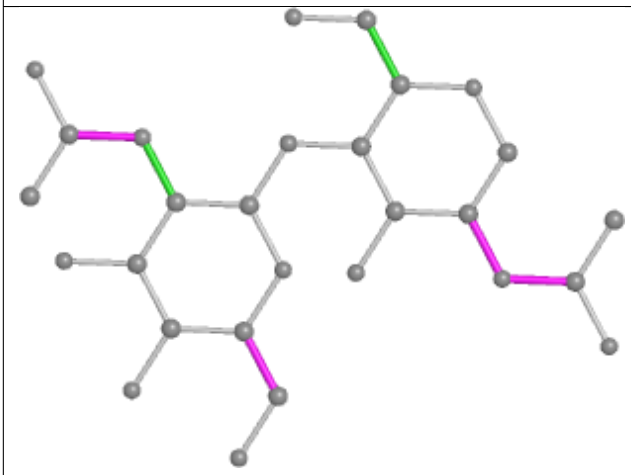
Oligosaccharide Chain G



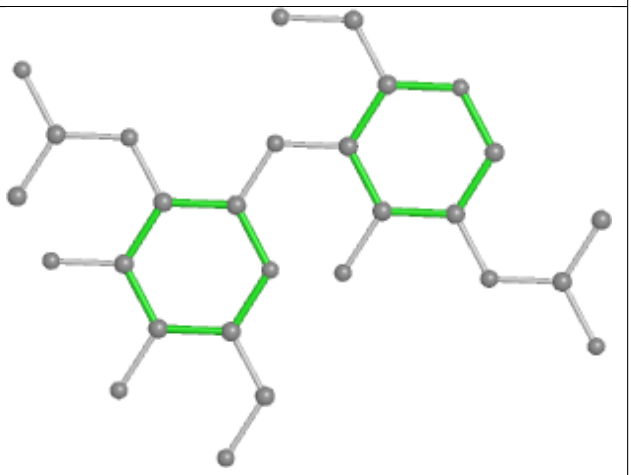
Bond lengths



Bond angles

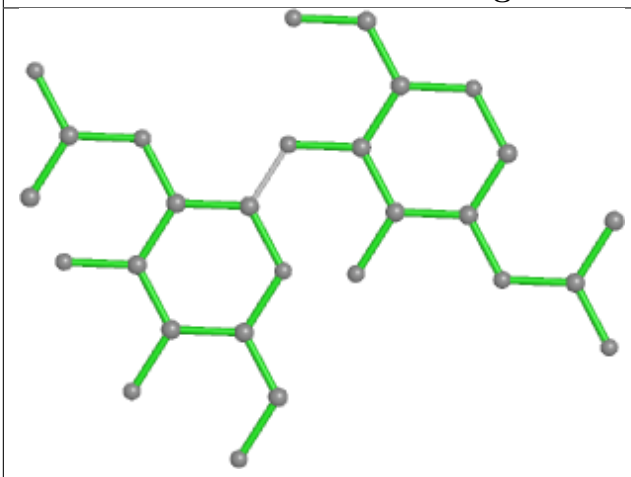


Torsions

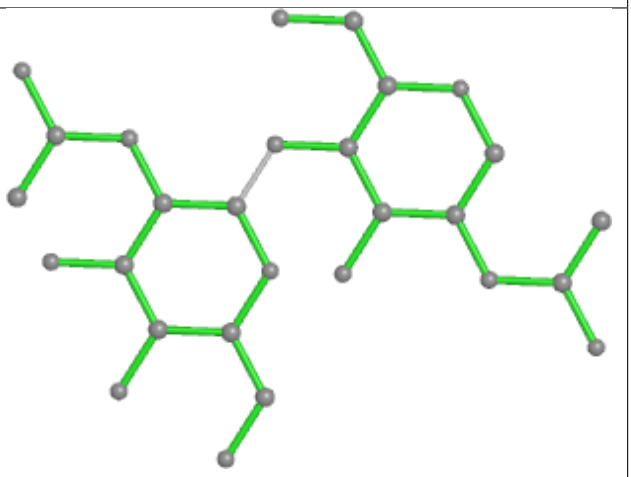


Rings

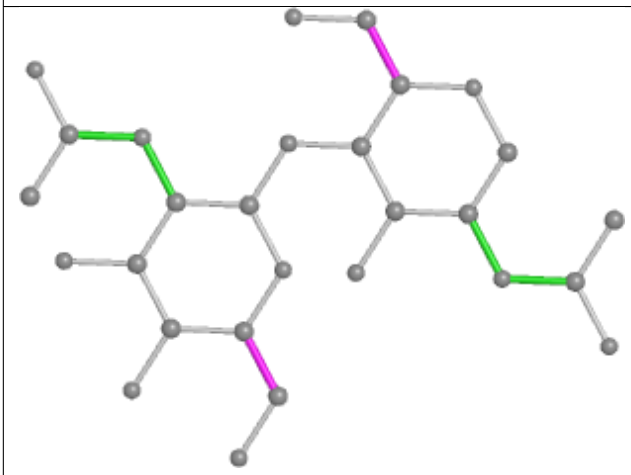
Oligosaccharide Chain K



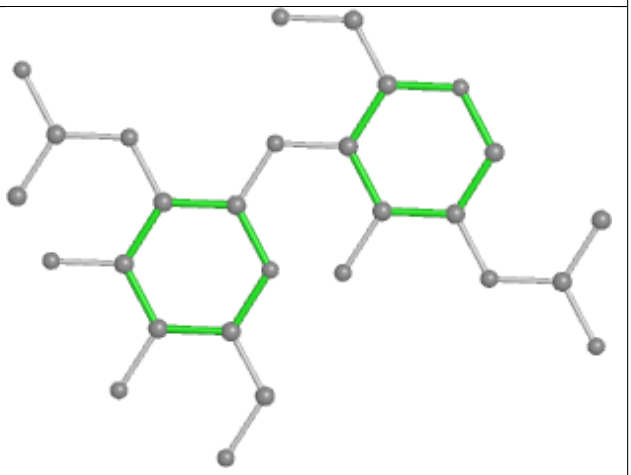
Bond lengths



Bond angles

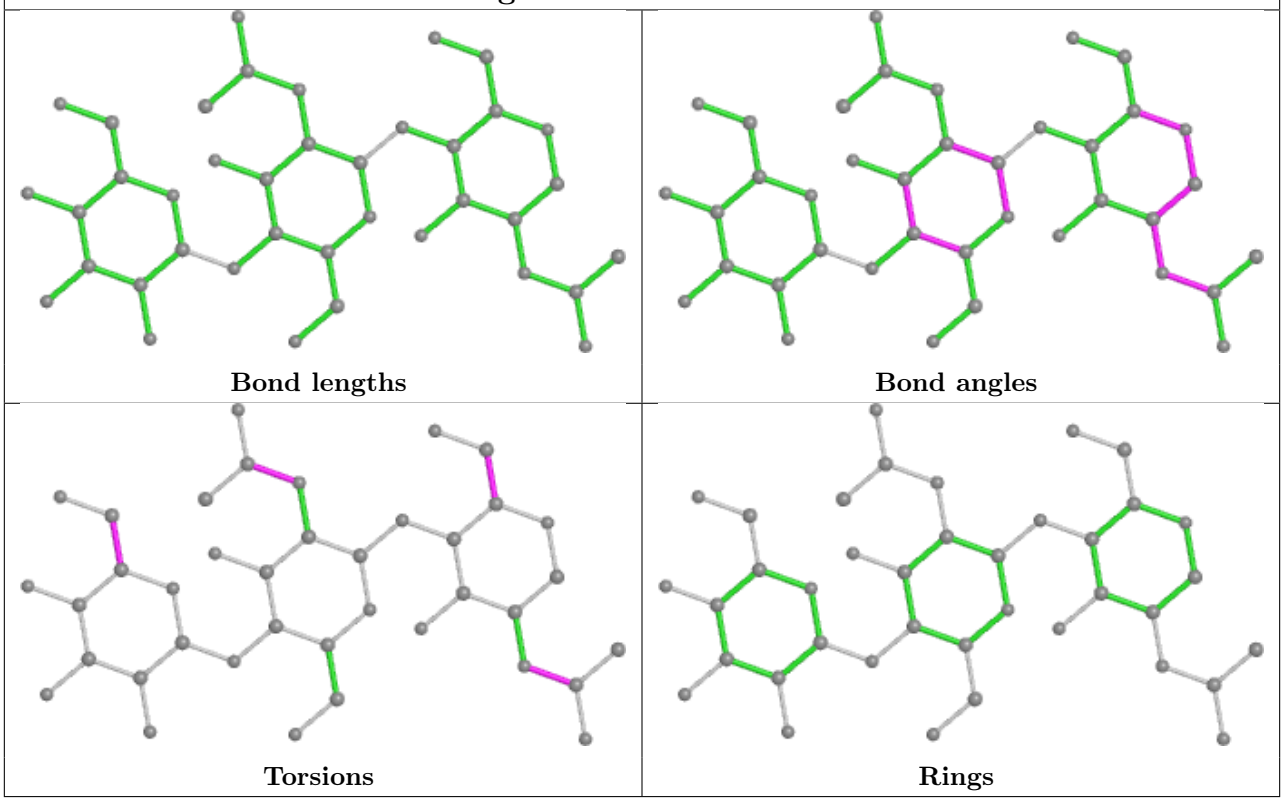


Torsions

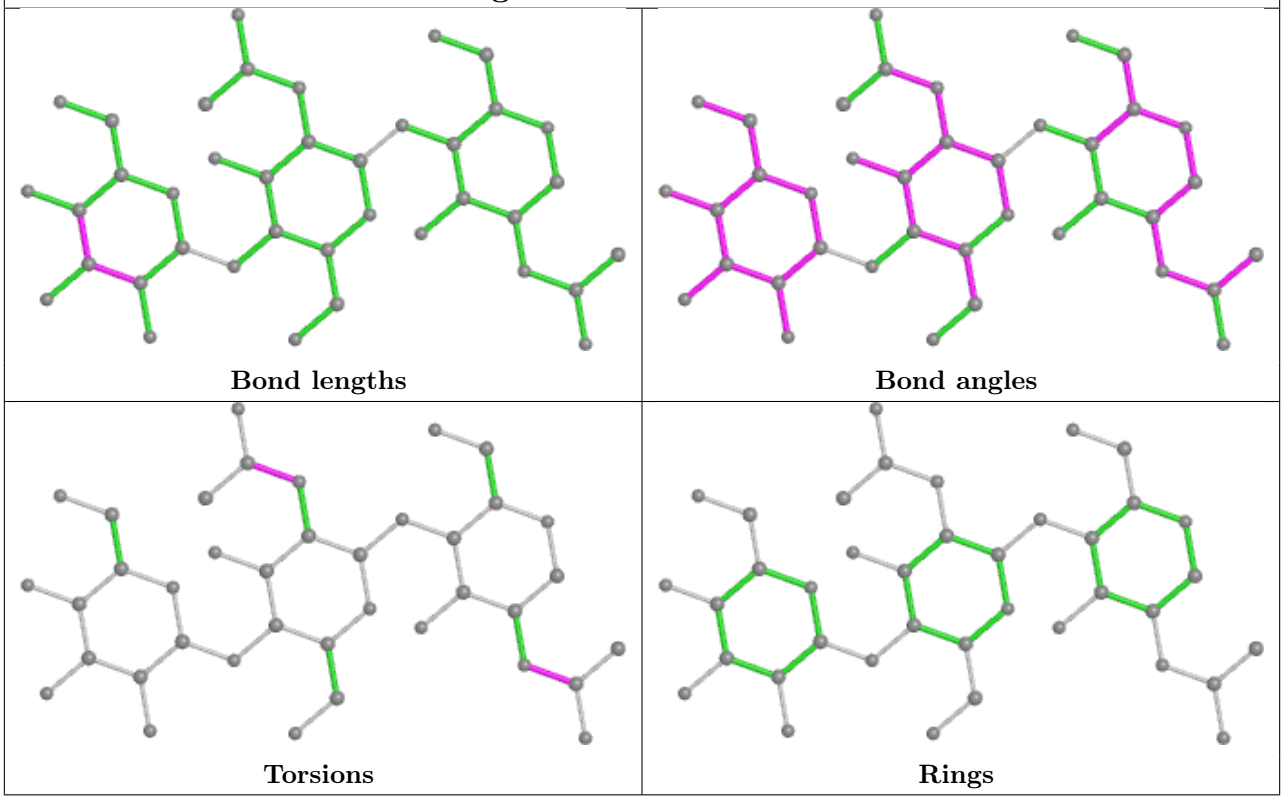


Rings

Oligosaccharide Chain L



Oligosaccharide Chain M



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
8	NAG	F	1747	3	14,14,15	0.58	0	17,19,21	0.67	0
8	NAG	H	1747	3	14,14,15	0.50	0	17,19,21	0.80	0
8	NAG	H	1743	3	14,14,15	0.53	0	17,19,21	0.62	0
9	GOL	J	1229	-	5,5,5	0.37	0	5,5,5	0.31	0
9	GOL	I	1229	-	5,5,5	0.37	0	5,5,5	0.17	0
8	NAG	F	1743	3	14,14,15	0.54	0	17,19,21	0.61	0
8	NAG	D	2642	2	14,14,15	0.56	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	1747	3	1/1/5/7	1/6/23/26	0/1/1/1
8	NAG	H	1747	3	-	1/6/23/26	0/1/1/1
8	NAG	H	1743	3	-	3/6/23/26	0/1/1/1
9	GOL	J	1229	-	-	2/4/4/4	-
9	GOL	I	1229	-	-	2/4/4/4	-
8	NAG	F	1743	3	-	2/6/23/26	0/1/1/1
8	NAG	D	2642	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	1747	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	2642	NAG	C3-C2-N2-C7
8	D	2642	NAG	C8-C7-N2-C2
8	D	2642	NAG	O7-C7-N2-C2
8	F	1743	NAG	C8-C7-N2-C2
8	F	1743	NAG	O7-C7-N2-C2
8	H	1743	NAG	C3-C2-N2-C7
8	H	1743	NAG	C8-C7-N2-C2
8	H	1743	NAG	O7-C7-N2-C2
9	I	1229	GOL	C1-C2-C3-O3
9	J	1229	GOL	C1-C2-C3-O3
9	J	1229	GOL	O2-C2-C3-O3
8	F	1747	NAG	O5-C5-C6-O6
9	I	1229	GOL	O2-C2-C3-O3
8	H	1747	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1229	GOL	4	0
9	I	1229	GOL	3	0
8	F	1743	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	640/642 (99%)	0.40	48 (7%) 14 14	58, 134, 189, 278	0
1	C	640/642 (99%)	0.70	84 (13%) 3 4	67, 134, 189, 281	0
2	B	901/912 (98%)	0.15	17 (1%) 66 61	60, 122, 203, 330	0
2	D	901/912 (98%)	0.34	86 (9%) 8 8	60, 125, 205, 328	0
3	F	714/732 (97%)	0.01	7 (0%) 82 77	37, 82, 154, 272	0
3	H	711/732 (97%)	0.14	25 (3%) 44 39	37, 84, 153, 222	0
4	I	228/228 (100%)	-0.21	0 100 100	46, 79, 125, 218	0
4	J	228/228 (100%)	-0.18	1 (0%) 92 90	42, 79, 125, 220	0
All	All	4963/5028 (98%)	0.23	268 (5%) 25 23	37, 109, 189, 330	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1151	GLY	8.5
2	D	1073	ILE	8.4
3	F	482	GLY	7.6
2	D	1154	LEU	6.9
1	C	636	ALA	6.5
2	D	1136	CYS	6.1
1	C	78	LYS	5.8
2	D	1503	ASP	5.8
1	C	74	PHE	5.8
1	C	46	VAL	5.8
1	A	378	LEU	5.7
1	C	45	LEU	5.7
1	C	47	LEU	5.6
1	C	337	LYS	5.6
1	A	69	PRO	5.6
2	D	1118	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	102	SER	5.4
2	D	1115	ASN	5.3
2	D	1092	PRO	5.3
3	F	480	SER	5.2
2	B	1499	GLN	5.2
2	D	1093	ASP	5.0
1	C	103	LEU	4.9
2	D	1057	THR	4.9
1	C	48	SER	4.9
1	A	70	ALA	4.9
2	D	1074	ASP	4.9
2	D	1169	ILE	4.8
3	H	480	SER	4.8
2	D	1499	GLN	4.7
1	C	20	MET	4.6
1	C	408	GLU	4.5
2	D	1072	ALA	4.5
2	D	1077	VAL	4.5
3	F	483	HIS	4.4
1	C	44	LYS	4.3
3	H	460	ARG	4.3
1	A	374	THR	4.3
2	D	1107	MET	4.2
2	D	1078	LEU	4.2
2	D	1049	LYS	4.2
2	D	1504	LYS	4.2
2	D	1096	PHE	4.1
2	D	1122	THR	4.0
2	D	1081	ALA	4.0
1	C	22	LEU	3.9
1	C	40	PHE	3.9
3	H	479	PRO	3.9
2	D	1131	GLU	3.9
2	B	1419	ARG	3.9
2	D	1071	ILE	3.9
1	C	323	GLY	3.8
2	D	1150	ALA	3.8
1	C	107	TYR	3.7
2	D	1099	ASP	3.7
1	A	497	LEU	3.7
3	H	484	GLU	3.7
1	C	314	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	1103	ILE	3.6
1	C	75	LYS	3.6
2	D	1155	GLU	3.6
2	D	1162	GLN	3.6
3	H	483	HIS	3.6
1	C	374	THR	3.6
1	C	70	ALA	3.5
2	D	1098	GLU	3.5
2	D	1120	ALA	3.5
1	C	194	GLN	3.5
2	D	1158	TYR	3.5
2	D	1018	GLU	3.5
1	C	19	THR	3.5
2	D	1059	TYR	3.5
2	D	1070	LEU	3.5
1	C	21	VAL	3.5
2	D	1177	MET	3.4
1	C	37	VAL	3.4
2	D	1161	LEU	3.4
2	D	1119	MET	3.4
1	C	36	THR	3.4
2	D	1424	ILE	3.4
1	A	102	SER	3.4
1	C	350	LEU	3.4
1	C	166	VAL	3.3
2	D	1056	LEU	3.3
2	D	1444	TYR	3.3
3	H	703	GLN	3.3
1	C	52	THR	3.2
1	C	378	LEU	3.2
1	A	376	GLN	3.2
1	A	514	THR	3.2
1	C	610	GLY	3.2
1	C	634	GLN	3.2
1	C	81	ASN	3.2
1	A	481	ALA	3.2
1	C	24	ALA	3.2
1	A	90	PHE	3.1
1	A	20	MET	3.1
1	C	382	ASP	3.1
1	C	104	GLN	3.1
2	D	1076	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	343	TRP	3.1
1	C	230	GLU	3.1
1	C	365	VAL	3.1
2	B	1119	MET	3.1
1	A	405	LYS	3.1
1	C	190	ASN	3.0
3	H	477	ILE	3.0
1	A	21	VAL	3.0
1	C	228	GLY	3.0
1	C	440	ARG	3.0
2	D	1036	ALA	3.0
1	A	468	TYR	3.0
3	H	611	GLU	3.0
2	B	1444	TYR	3.0
2	D	1023	ALA	3.0
2	D	1048	VAL	3.0
2	D	1085	LEU	2.9
1	C	609	SER	2.9
3	H	70	LYS	2.9
1	C	530	TRP	2.9
2	B	1078	LEU	2.9
2	D	1418	ASP	2.9
2	D	1419	ARG	2.9
1	C	72	ARG	2.9
1	A	105	SER	2.9
2	D	1102	VAL	2.8
2	D	1331	LYS	2.8
2	B	1418	ASP	2.8
1	A	68	ILE	2.8
1	C	101	VAL	2.8
2	B	985	PRO	2.8
1	C	87	GLN	2.8
3	F	481	LYS	2.8
1	A	515	LEU	2.8
3	H	482	GLY	2.8
2	D	1152	ASP	2.8
1	A	636	ALA	2.7
1	A	349	ASP	2.7
2	B	1411	GLU	2.7
2	D	1143	LEU	2.7
1	C	30	ASP	2.7
1	C	336	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	22	LEU	2.7
2	D	1147	ILE	2.7
2	D	1186	ASN	2.7
2	D	1178	GLY	2.7
1	C	156	ASP	2.6
1	C	405	LYS	2.6
3	H	461	LYS	2.6
1	C	379	THR	2.6
2	D	1127	ILE	2.6
1	C	386	LYS	2.6
1	C	465	ILE	2.6
1	A	351	MET	2.6
1	A	440	ARG	2.6
1	C	481	ALA	2.6
2	D	1114	ASN	2.6
1	A	449	LEU	2.6
2	D	1251	PHE	2.5
2	D	1125	VAL	2.5
1	A	480	LYS	2.5
3	H	476	VAL	2.5
2	D	1498	ILE	2.5
3	H	641	TYR	2.5
2	D	1359	LYS	2.5
1	C	38	HIS	2.5
2	D	1250	THR	2.5
2	D	1132	ALA	2.5
1	A	386	LYS	2.4
2	B	1151	GLY	2.4
1	A	3	MET	2.4
1	A	43	LYS	2.4
2	D	1062	LYS	2.4
1	A	517	GLY	2.4
1	C	82	LYS	2.4
3	H	17	VAL	2.4
2	D	999	THR	2.4
2	D	1104	HIS	2.4
2	D	1017	LEU	2.4
2	D	1054	THR	2.4
1	A	516	ILE	2.4
2	B	1154	LEU	2.4
2	D	1160	ASN	2.4
1	C	98	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	480	LYS	2.4
2	D	1170	ALA	2.4
1	A	630	GLN	2.4
2	B	1188	PHE	2.4
3	H	610	GLU	2.4
1	C	54	LEU	2.3
2	D	1052	PRO	2.3
2	D	1236	GLU	2.3
1	C	348	PHE	2.3
1	A	25	HIS	2.3
3	H	525	ILE	2.3
1	C	304	VAL	2.3
2	D	1063	VAL	2.3
2	D	1183	PRO	2.3
3	H	635	ALA	2.3
1	A	45	LEU	2.3
1	A	387	LEU	2.3
1	C	324	ILE	2.3
2	D	1037	PHE	2.3
1	C	12	LEU	2.2
1	C	7	ILE	2.2
1	C	339	PRO	2.2
2	D	1146	SER	2.2
1	C	71	ASN	2.2
3	H	465	TYR	2.2
1	C	49	SER	2.2
2	D	1446	ASN	2.2
1	A	377	SER	2.2
1	A	624	PHE	2.2
1	A	496	PRO	2.2
1	C	129	THR	2.2
2	B	1420	ASN	2.2
2	D	1094	GLY	2.2
1	A	350	LEU	2.2
2	D	1124	PHE	2.2
2	D	1163	ARG	2.2
1	A	385	ALA	2.2
1	C	479	LEU	2.2
3	H	478	ARG	2.2
2	D	1047	PHE	2.2
3	H	481	LYS	2.2
1	A	218	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	544	ILE	2.2
1	A	5	SER	2.1
1	C	86	VAL	2.1
1	C	297	LEU	2.1
4	J	43	LEU	2.1
2	D	1138	GLU	2.1
3	F	460	ARG	2.1
1	C	23	GLU	2.1
2	D	1129	LEU	2.1
3	F	641	TYR	2.1
1	A	453	PHE	2.1
1	A	443	LEU	2.1
2	B	1391	PRO	2.1
2	D	1416	PHE	2.1
1	C	184	ILE	2.1
1	C	325	PRO	2.1
3	H	713	ALA	2.1
2	B	1503	ASP	2.1
1	C	376	GLN	2.1
1	A	485	VAL	2.1
1	C	79	GLY	2.1
3	H	503	PHE	2.1
2	B	1422	LEU	2.1
1	C	464	LYS	2.0
1	A	257	GLU	2.0
1	A	471	LEU	2.0
3	H	14	LEU	2.0
1	A	406	LYS	2.0
1	C	193	GLN	2.0
1	C	335	PHE	2.0
1	C	8	THR	2.0
1	A	7	ILE	2.0
1	A	459	ARG	2.0
1	C	347	PRO	2.0
2	D	1497	PHE	2.0
1	C	218	GLU	2.0
2	B	1128	SER	2.0
1	C	227	LYS	2.0
3	H	614	LYS	2.0
2	B	1504	LYS	2.0
1	C	85	THR	2.0
2	D	1381	LEU	2.0

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

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

6.3 Carbohydrates (i)

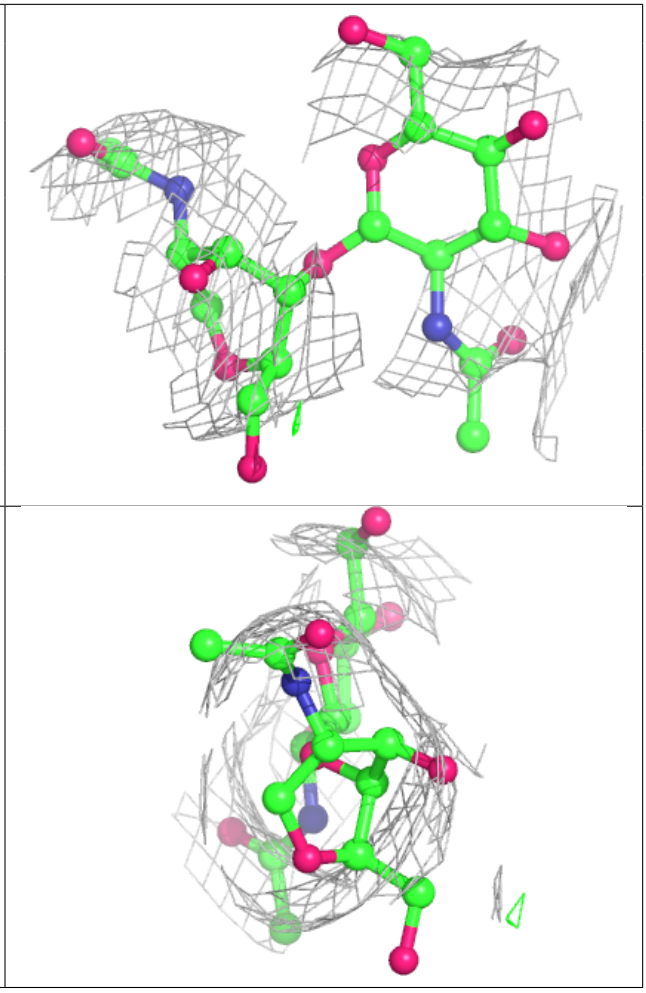
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	K	2	14/15	0.35	0.35	155,202,219,222	0
6	BMA	M	3	11/12	0.59	0.29	132,155,186,196	0
6	NAG	M	2	14/15	0.63	0.32	160,172,206,213	0
6	BMA	L	3	11/12	0.69	0.31	128,162,204,271	0
5	NAG	K	1	14/15	0.75	0.24	123,187,212,212	0
5	NAG	E	2	14/15	0.78	0.17	160,201,217,223	0
6	NAG	L	2	14/15	0.82	0.22	118,138,166,168	0
5	NAG	G	2	14/15	0.86	0.24	114,185,200,200	0
6	NAG	L	1	14/15	0.86	0.21	91,116,131,137	0
5	NAG	E	1	14/15	0.87	0.25	129,188,212,214	0
5	NAG	G	1	14/15	0.89	0.19	102,141,165,192	0
6	NAG	M	1	14/15	0.90	0.23	96,122,150,154	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.

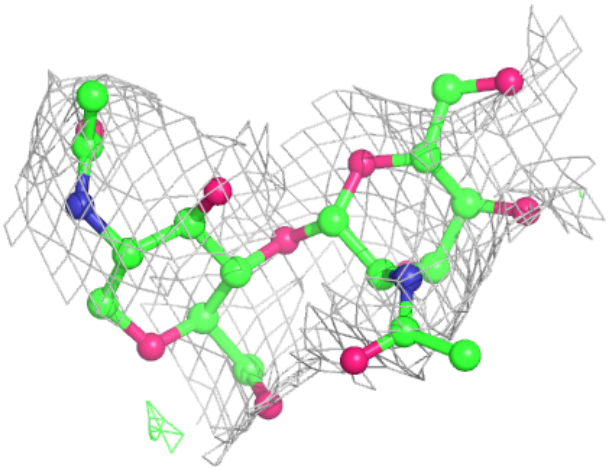
Electron density around Chain E:

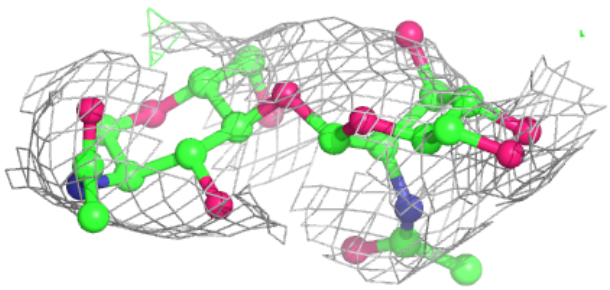
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

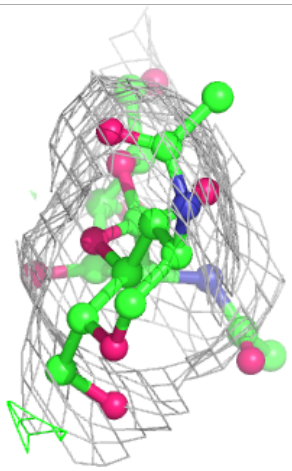


Electron density around Chain G:

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

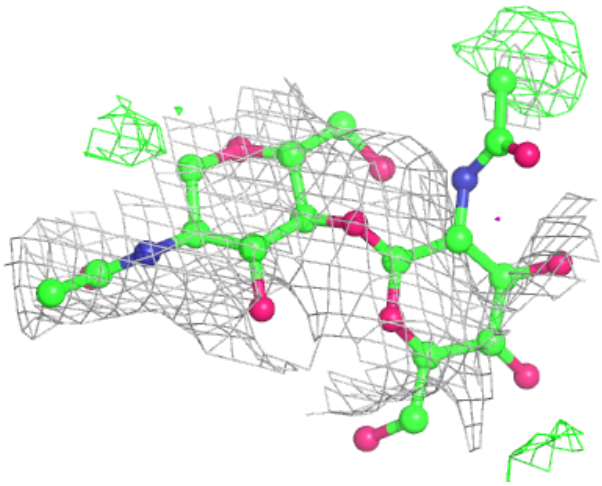


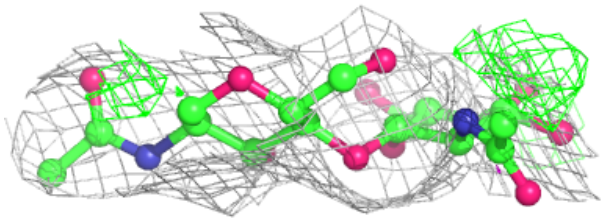


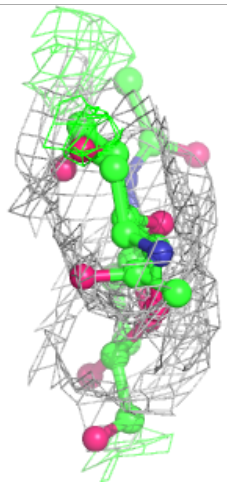


Electron density around Chain K:

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

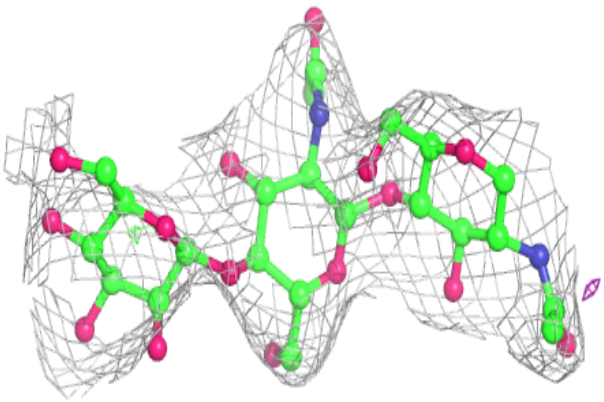


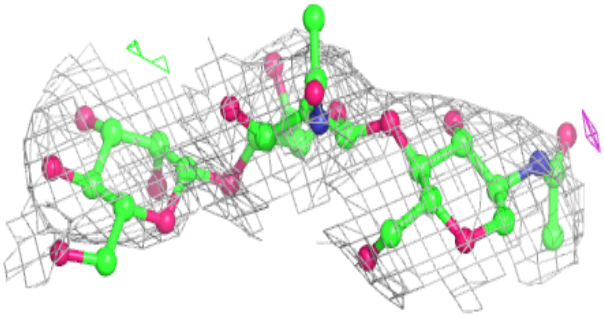


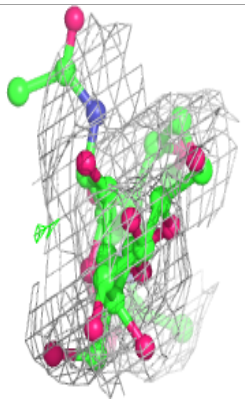


Electron density around Chain L:

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

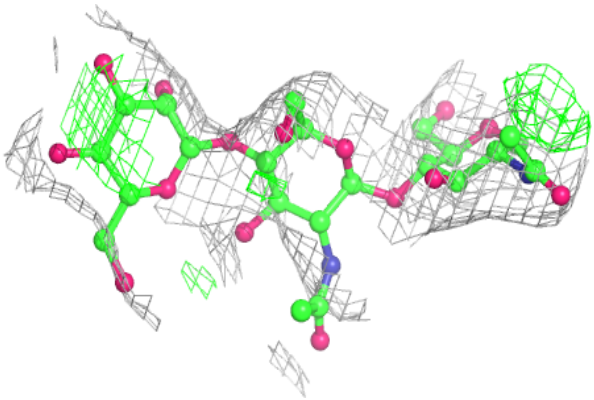


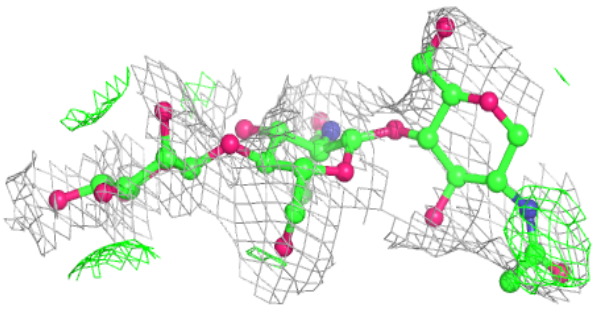


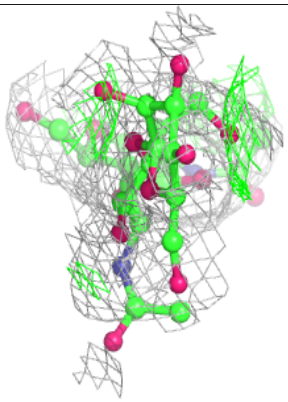


Electron density around Chain M:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	F	1743	14/15	0.73	0.37	97,143,202,215	0
8	NAG	D	2642	14/15	0.81	0.22	104,146,166,179	0
8	NAG	H	1747	14/15	0.81	0.28	118,163,182,198	0
8	NAG	F	1747	14/15	0.85	0.26	135,154,184,195	0
8	NAG	H	1743	14/15	0.85	0.27	117,167,189,193	0
7	MG	H	1742	1/1	0.85	0.30	140,140,140,140	0
7	MG	C	1645	1/1	0.89	0.04	127,127,127,127	0
7	MG	A	1645	1/1	0.92	0.12	108,108,108,108	0
9	GOL	J	1229	6/6	0.95	0.25	58,74,87,95	0
9	GOL	I	1229	6/6	0.96	0.37	73,107,124,127	0
7	MG	F	1742	1/1	0.99	0.20	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.