Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 06:32 AM EDT

PDB ID	:	3BVH
Title	:	Crystal Structure of Recombinant gammaD364A Fibrinogen Fragment D with the Peptide Ligand Gly-Pro-Arg-Pro-Amide
Authors	:	Bowley, S.R.; Merenbloom, B.K.; Betts, L.; Okumura, N.; Heroux, A.; Gorkun, O.V.; Lord, S.T.
Deposited on	:	2008-01-07
Resolution	:	2.60 Å(reported)

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

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

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

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

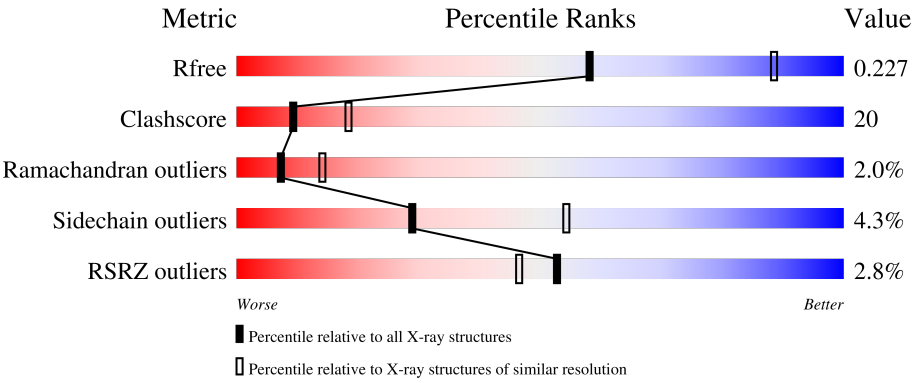
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	62	6% 39% 56% 5%
1	D	62	6% 39% 56% 5%
2	B	298	2% 73% 23% .
2	E	298	% 64% 33% .
3	C	293	2% 66% 31% .

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Mol	Chain	Length	Quality of chain
3	F	293	5% 56% 38% 6%
4	G	4	50% 25% 25%
4	H	4	25% 50% 25%
4	I	4	100%
4	J	4	75% 25%
5	K	3	33% 33% 33%
5	L	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	L	1	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			507	311	97	96	3			
1	D	62	Total	C	N	O	S	0	0	0
			507	311	97	96	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2393	1494	422	455	22			
2	E	298	Total	C	N	O	S	0	0	0
			2393	1494	422	455	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	293	Total	C	N	O	S	0	0	0
			2349	1490	397	451	11			
3	F	293	Total	C	N	O	S	0	0	0
			2349	1490	397	451	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	ASP	engineered mutation	UNP P02679
F	364	ALA	ASP	engineered mutation	UNP P02679

- Molecule 4 is a protein called 4-mer peptide GPRP.

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

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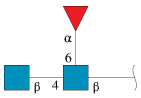
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	4	Total C N O 30 18 7 5	0	0	0
4	H	4	Total C N O 30 18 7 5	0	0	0
4	J	4	Total C N O 30 18 7 5	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	3	Total C N O 38 22 2 14	0	0	0
5	L	3	Total C N O 38 22 2 14	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	24	Total O 24 24	0	0
7	B	169	Total O 169 169	0	0
7	C	105	Total O 105 105	0	0

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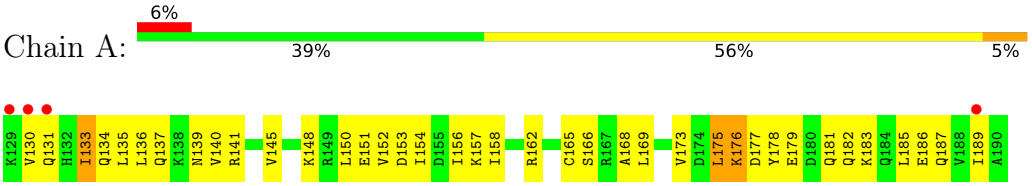
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	16	Total O 16 16	0	0
7	E	92	Total O 92 92	0	0
7	F	39	Total O 39 39	0	0
7	I	1	Total O 1 1	0	0

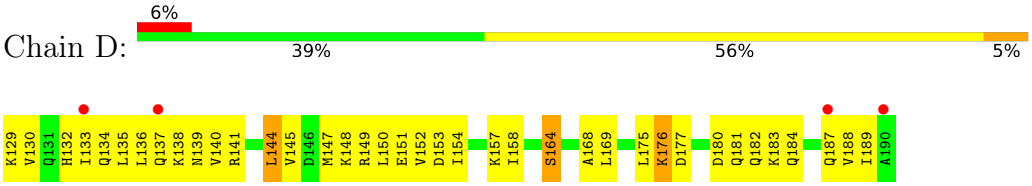
3 Residue-property plots (i)

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.

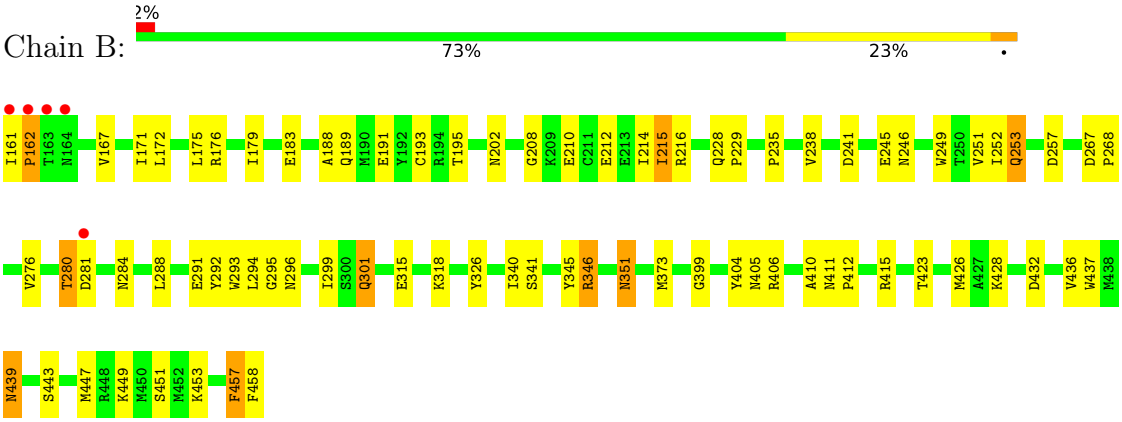
• Molecule 1: Fibrinogen alpha chain



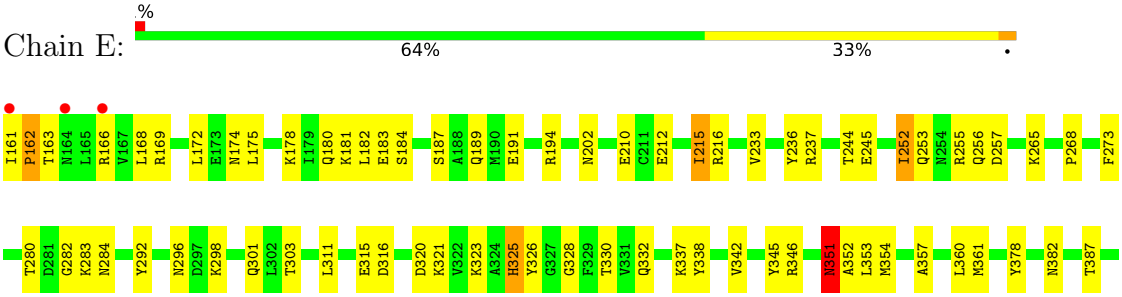
• Molecule 1: Fibrinogen alpha chain

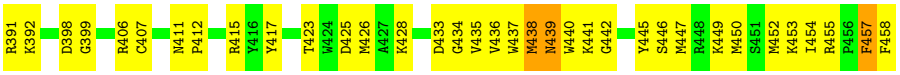


• Molecule 2: Fibrinogen beta chain



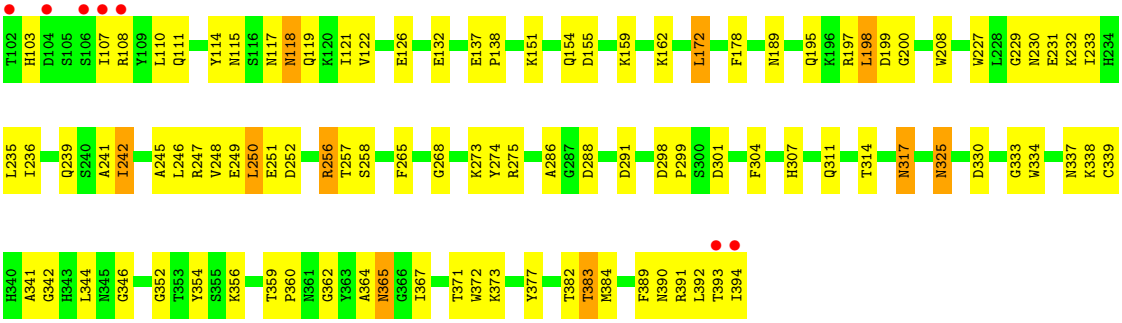
• Molecule 2: Fibrinogen beta chain





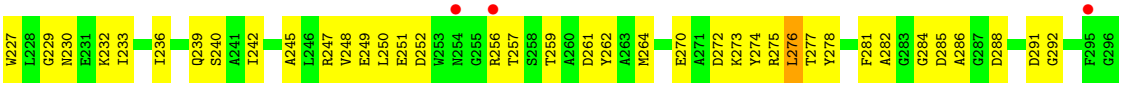
• Molecule 3: Fibrinogen gamma chain

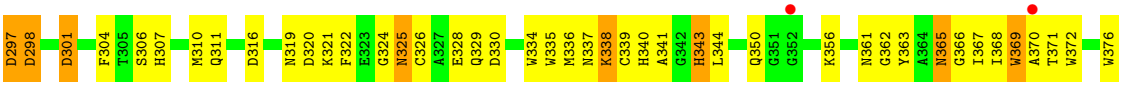
Chain C:

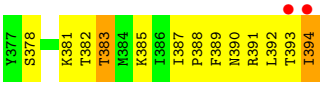


• Molecule 3: Fibrinogen gamma chain

Chain F:





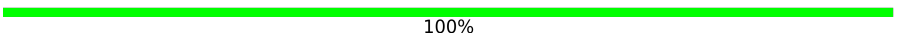


• Molecule 4: 4-mer peptide GPRP

Chain G:

• Molecule 4: 4-mer peptide GPRP

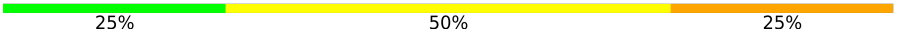
Chain I:



There are no outlier residues recorded for this chain.

• Molecule 4: 4-mer peptide GPRP

Chain H:

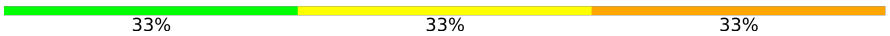


• Molecule 4: 4-mer peptide GPRP

Chain J:

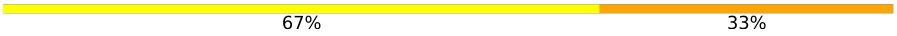
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.84Å 94.91Å 225.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.30 – 2.35	Depositor EDS
% Data completeness (in resolution range)	48.1 (50.00-2.60) 82.4 (49.30-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.260 0.222 , 0.227	Depositor DCC
R_{free} test set	3353 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.33% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/508	0.53	0/676
1	D	0.30	0/508	0.52	0/676
2	B	0.41	0/2454	0.67	1/3312 (0.0%)
2	E	0.34	0/2454	0.60	0/3312
3	C	0.39	0/2414	0.61	1/3264 (0.0%)
3	F	0.34	0/2414	0.54	0/3264
4	G	0.53	0/31	0.54	0/40
4	H	0.66	0/31	0.73	0/40
4	I	0.53	0/31	0.58	0/40
4	J	0.54	0/31	0.76	0/40
All	All	0.37	0/10876	0.60	2/14664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	399	GLY	N-CA-C	6.28	128.79	113.10
3	C	342	GLY	N-CA-C	-5.32	99.80	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	507	0	530	42	0
1	D	507	0	530	33	0
2	B	2393	0	2262	68	0
2	E	2393	0	2261	94	0
3	C	2349	0	2200	76	0
3	F	2349	0	2200	114	0
4	G	30	0	32	3	0
4	H	30	0	32	4	0
4	I	30	0	32	0	0
4	J	30	0	32	1	0
5	K	38	0	34	5	0
5	L	38	0	35	8	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	24	0	0	1	0
7	B	169	0	0	3	0
7	C	105	0	0	2	0
7	D	16	0	0	0	0
7	E	92	0	0	2	0
7	F	39	0	0	0	0
7	I	1	0	0	0	0
All	All	11144	0	10180	412	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 20.

All (412) 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)
3:C:172:LEU:H	3:C:239:GLN:HE21	1.11	0.97
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.25	0.96
2:B:439:ASN:H	2:B:439:ASN:HD22	1.16	0.91
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.53	0.88
2:B:280:THR:HG23	2:B:288:LEU:HG	1.55	0.86
1:A:130:VAL:HG12	1:A:134:GLN:HE21	1.44	0.83
3:C:365:ASN:HD22	3:C:365:ASN:H	1.25	0.82
3:C:189:ASN:ND2	3:C:391:ARG:HE	1.78	0.82
2:E:423:THR:N	2:E:426:MET:HE3	1.96	0.81
1:A:157:LYS:HE3	3:C:132:GLU:OE2	1.81	0.80
2:B:439:ASN:HD22	2:B:439:ASN:N	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:THR:N	2:B:426:MET:HE3	1.97	0.79
2:B:228:GLN:HG3	2:B:235:PRO:HG3	1.65	0.79
2:E:315:GLU:OE1	2:E:321:LYS:HE2	1.83	0.79
3:F:189:ASN:ND2	3:F:391:ARG:HE	1.79	0.79
3:C:241:ALA:O	3:C:242:ILE:HG13	1.83	0.78
2:E:202:ASN:ND2	2:E:284:ASN:HB2	1.98	0.78
1:A:178:TYR:O	1:A:182:GLN:HG3	1.85	0.77
3:F:197:ARG:HB2	3:F:382:THR:HB	1.68	0.75
2:E:252:ILE:HD12	2:E:454:ILE:HG23	1.67	0.75
2:E:346:ARG:O	2:E:346:ARG:HG3	1.86	0.74
2:E:361:MET:HB2	5:L:1:NAG:O7	1.87	0.74
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.23	0.73
2:E:323:LYS:NZ	2:E:325:HIS:HD2	1.86	0.73
2:B:295:GLY:O	2:B:299:ILE:HG12	1.88	0.73
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.69	0.72
3:F:107:ILE:HD13	3:F:107:ILE:O	1.89	0.72
2:B:161:ILE:N	2:B:162:PRO:HD2	2.05	0.72
3:F:240:SER:O	3:F:242:ILE:HG13	1.90	0.72
3:F:252:ASP:OD2	3:F:256:ARG:HB2	1.89	0.72
3:F:288:ASP:OD2	3:F:291:ASP:HB2	1.89	0.72
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.35	0.72
2:B:373:MET:HE1	2:B:405:ASN:HA	1.71	0.72
3:C:172:LEU:H	3:C:239:GLN:NE2	1.87	0.71
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.90	0.71
1:D:150:LEU:O	1:D:154:ILE:HG12	1.91	0.70
3:F:249:GLU:HB2	3:F:383:THR:CG2	2.22	0.69
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.58	0.68
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.76	0.68
2:B:423:THR:H	2:B:426:MET:HE3	1.59	0.68
2:E:423:THR:H	2:E:426:MET:HE3	1.56	0.68
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.08	0.67
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.09	0.67
3:C:338:LYS:N	3:C:339:CYS:HA	2.10	0.66
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.77	0.66
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.44	0.65
3:C:365:ASN:HD22	3:C:365:ASN:N	1.94	0.65
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.62	0.65
2:B:439:ASN:H	2:B:439:ASN:ND2	1.94	0.65
1:D:133:ILE:O	1:D:137:GLN:HG3	1.97	0.64
1:A:137:GLN:NE2	1:A:189:ILE:HA	2.12	0.64
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HG	1:D:139:ASN:HD21	1.64	0.63
5:L:1:NAG:C6	5:L:3:FUC:C1	2.76	0.63
1:A:166:SER:HB3	2:B:195:THR:OG1	1.99	0.63
2:E:351:ASN:ND2	2:E:354:MET:H	1.97	0.63
2:E:323:LYS:HZ1	2:E:325:HIS:HD2	1.46	0.63
1:D:177:ASP:O	1:D:181:GLN:HG3	1.99	0.62
3:F:124:LEU:O	3:F:128:VAL:HG23	2.00	0.62
2:B:252:ILE:HB	2:B:299:ILE:CD1	2.28	0.62
2:B:439:ASN:N	2:B:439:ASN:ND2	2.48	0.62
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.00	0.62
2:E:434:GLY:O	2:E:436:VAL:N	2.33	0.62
1:A:141:ARG:O	1:A:145:VAL:HG23	1.99	0.61
2:B:176:ARG:HG3	3:C:117:ASN:HD21	1.65	0.61
2:B:373:MET:CE	2:B:405:ASN:HA	2.30	0.61
3:F:276:LEU:HD12	3:F:277:THR:N	2.14	0.61
3:F:393:THR:O	3:F:394:ILE:HG22	2.00	0.61
3:F:203:ASP:O	3:F:206:LYS:HE2	2.00	0.61
2:E:168:LEU:HB3	3:F:110:LEU:HD13	1.81	0.61
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.65	0.61
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.83	0.61
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.15	0.61
1:A:150:LEU:O	1:A:154:ILE:HD13	2.00	0.61
7:B:502:HOH:O	5:K:2:NAG:H2	2.00	0.61
3:F:151:LYS:NZ	3:F:172:LEU:HD21	2.16	0.61
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.01	0.60
3:C:189:ASN:ND2	3:C:391:ARG:HG3	2.15	0.60
3:F:175:ASN:HB3	3:F:176:GLN:HE21	1.65	0.60
1:A:169:LEU:H	2:B:189:GLN:NE2	1.98	0.60
3:C:365:ASN:H	3:C:365:ASN:ND2	1.99	0.60
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.35	0.60
4:H:3:ARG:HB3	4:H:4:PRO:HD2	1.83	0.60
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.02	0.60
2:E:166:ARG:HG3	7:E:483:HOH:O	2.01	0.60
2:E:172:LEU:HD13	3:F:113:ILE:HG13	1.84	0.60
2:E:441:LYS:HG3	2:E:447:MET:HE1	1.84	0.60
3:F:232:LYS:O	3:F:236:ILE:HG13	2.01	0.60
5:L:1:NAG:HO6	5:L:3:FUC:C1	2.08	0.60
2:E:212:GLU:O	2:E:216:ARG:HG3	2.01	0.60
1:A:185:LEU:HD13	1:A:185:LEU:O	2.01	0.59
2:B:346:ARG:O	2:B:346:ARG:HG3	2.02	0.59
3:F:123:ASN:N	3:F:123:ASN:HD22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.37	0.59
2:B:188:ALA:O	2:B:191:GLU:HB3	2.02	0.59
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.38	0.59
2:E:168:LEU:CB	3:F:110:LEU:HD13	2.33	0.59
1:A:133:ILE:HD13	1:A:133:ILE:O	2.02	0.59
2:B:457:PHE:O	2:B:458:PHE:HB2	2.03	0.59
2:E:244:THR:HG22	2:E:245:GLU:HG2	1.82	0.59
2:E:316:ASP:OD2	2:E:320:ASP:HB2	2.03	0.59
3:F:338:LYS:N	3:F:339:CYS:HA	2.16	0.59
2:E:351:ASN:C	2:E:351:ASN:HD22	2.04	0.58
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.39	0.58
2:B:176:ARG:HG3	3:C:117:ASN:ND2	2.19	0.58
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.67	0.58
2:E:326:TYR:CE2	2:E:353:LEU:HD12	2.38	0.58
2:E:351:ASN:HD21	2:E:354:MET:H	1.52	0.58
5:L:1:NAG:H4	5:L:2:NAG:HN2	1.69	0.58
2:E:360:LEU:HD11	4:H:2:PRO:HD3	1.84	0.58
2:E:162:PRO:HG2	2:E:163:THR:H	1.69	0.58
3:F:297:ASP:O	3:F:298:ASP:HB2	2.03	0.58
3:C:393:THR:O	3:C:393:THR:HG22	2.04	0.57
2:B:167:VAL:O	2:B:171:ILE:HG12	2.04	0.57
2:B:252:ILE:HB	2:B:299:ILE:HD11	1.87	0.57
1:D:164:SER:HB3	3:F:137:GLU:O	2.04	0.57
5:K:1:NAG:H4	5:K:2:NAG:HN2	1.69	0.57
4:J:4:PRO:HG3	5:K:1:NAG:H62	1.86	0.57
3:C:248:VAL:HG12	3:C:250:LEU:HD13	1.86	0.57
2:E:202:ASN:HD22	2:E:284:ASN:HB2	1.66	0.57
1:D:144:LEU:HD13	1:D:182:GLN:HG2	1.86	0.56
4:H:3:ARG:O	4:H:4:PRO:C	2.43	0.56
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.71	0.56
1:D:130:VAL:O	1:D:133:ILE:HG22	2.05	0.56
1:D:141:ARG:O	1:D:145:VAL:HG23	2.05	0.56
2:E:406:ARG:O	2:E:406:ARG:HG2	2.05	0.56
1:A:133:ILE:HD13	1:A:133:ILE:C	2.26	0.55
1:A:186:GLU:OE1	1:A:189:ILE:HD12	2.05	0.55
3:F:247:ARG:HH22	3:F:392:LEU:HD11	1.72	0.55
3:C:304:PHE:O	3:C:337:ASN:HB3	2.07	0.55
3:C:307:HIS:CE1	3:C:341:ALA:H	2.24	0.55
2:E:387:THR:HG21	2:E:392:LYS:O	2.06	0.55
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.22	0.55
2:E:417:TYR:HB2	2:E:446:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LEU:H	2:E:189:GLN:NE2	2.05	0.54
2:E:161:ILE:N	2:E:162:PRO:HD2	2.23	0.54
1:A:148:LYS:HE3	1:A:175:LEU:CD1	2.37	0.54
1:A:177:ASP:O	1:A:181:GLN:HG3	2.08	0.54
2:E:252:ILE:HD13	2:E:452:MET:O	2.07	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.06	0.54
3:F:297:ASP:HB2	3:F:301:ASP:OD2	2.06	0.54
1:A:136:LEU:HD11	3:C:111:GLN:HG2	1.88	0.54
2:E:330:THR:HG22	7:E:477:HOH:O	2.08	0.54
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.89	0.54
2:B:228:GLN:HG3	2:B:235:PRO:CG	2.36	0.54
1:A:175:LEU:O	1:A:179:GLU:HG3	2.07	0.54
1:D:132:HIS:O	1:D:136:LEU:HG	2.07	0.54
2:E:411:ASN:N	2:E:412:PRO:HD3	2.23	0.54
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.73	0.54
3:F:350:GLN:HA	3:F:350:GLN:NE2	2.22	0.54
3:C:151:LYS:HE2	3:C:172:LEU:HD13	1.89	0.54
3:F:248:VAL:O	3:F:259:THR:HA	2.07	0.54
2:E:282:GLY:C	2:E:283:LYS:HD2	2.28	0.54
1:D:129:LYS:HA	1:D:132:HIS:HD2	1.72	0.53
2:E:212:GLU:OE1	2:E:455:ARG:HD2	2.07	0.53
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.72	0.53
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.09	0.53
3:C:390:ASN:O	3:C:394:ILE:HA	2.07	0.53
2:E:169:ARG:HA	3:F:110:LEU:HD22	1.91	0.53
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.43	0.53
3:C:338:LYS:O	3:C:338:LYS:HG2	2.08	0.53
3:F:247:ARG:HH21	3:F:392:LEU:HD21	1.72	0.53
2:E:215:ILE:HD13	2:E:215:ILE:O	2.09	0.53
2:E:328:GLY:O	2:E:342:VAL:HA	2.09	0.53
3:F:229:GLY:O	3:F:233:ILE:HG13	2.08	0.53
3:C:354:TYR:OH	3:C:364:ALA:HB1	2.09	0.53
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.74	0.53
3:F:321:LYS:O	3:F:338:LYS:HB2	2.08	0.53
1:A:185:LEU:O	1:A:189:ILE:HG13	2.09	0.53
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.73	0.53
2:B:228:GLN:CG	2:B:235:PRO:HG3	2.37	0.52
3:F:325:ASN:HD22	3:F:325:ASN:C	2.13	0.52
3:C:273:LYS:HB2	3:C:311:GLN:HB3	1.92	0.52
1:A:169:LEU:H	2:B:189:GLN:HE22	1.56	0.52
2:B:253:GLN:NE2	2:B:451:SER:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:361:ASN:N	3:F:361:ASN:HD22	2.08	0.52
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.58	0.52
3:F:350:GLN:HA	3:F:350:GLN:HE21	1.75	0.52
2:B:280:THR:CG2	2:B:288:LEU:HG	2.34	0.52
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.45	0.52
2:E:252:ILE:HD13	2:E:252:ILE:H	1.75	0.51
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.45	0.51
3:C:197:ARG:HB2	3:C:382:THR:HB	1.92	0.51
3:C:229:GLY:O	3:C:233:ILE:HG13	2.10	0.51
3:F:322:PHE:CZ	3:F:324:GLY:HA3	2.46	0.51
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.91	0.51
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.25	0.51
2:B:373:MET:HE2	2:B:404:TYR:O	2.10	0.51
3:C:189:ASN:HD22	3:C:391:ARG:HG3	1.76	0.51
3:C:352:GLY:O	3:C:377:TYR:HA	2.09	0.51
2:E:180:GLN:HA	2:E:183:GLU:OE1	2.10	0.51
1:D:175:LEU:H	1:D:175:LEU:HD22	1.76	0.51
3:F:189:ASN:HD21	3:F:391:ARG:HE	1.55	0.51
3:C:122:VAL:O	3:C:126:GLU:HG3	2.10	0.51
1:A:136:LEU:O	1:A:140:VAL:HG13	2.10	0.51
2:E:311:LEU:HD23	2:E:453:LYS:HD2	1.91	0.51
2:E:332:GLN:O	2:E:338:TYR:HA	2.10	0.51
3:F:365:ASN:HD22	3:F:366:GLY:N	2.08	0.51
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.11	0.50
3:C:307:HIS:HE1	3:C:341:ALA:H	1.59	0.50
1:D:154:ILE:O	1:D:158:ILE:HG12	2.11	0.50
4:G:3:ARG:HA	4:G:3:ARG:HE	1.76	0.50
1:D:134:GLN:O	1:D:138:LYS:HG3	2.12	0.50
3:F:247:ARG:NH2	3:F:392:LEU:HD21	2.27	0.50
3:C:298:ASP:HB3	3:C:301:ASP:OD1	2.12	0.50
3:F:108:ARG:O	3:F:112:GLU:HG3	2.11	0.50
3:F:325:ASN:CG	3:F:328:GLU:HB2	2.32	0.50
1:A:136:LEU:HD11	3:C:111:GLN:CG	2.41	0.50
3:C:286:ALA:O	3:C:372:TRP:HB2	2.12	0.49
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.94	0.49
2:B:175:LEU:O	2:B:179:ILE:HG13	2.12	0.49
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.74	0.49
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.93	0.49
2:E:361:MET:CB	5:L:1:NAG:H81	2.42	0.49
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.93	0.49
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:LEU:HB3	2:E:453:LYS:HG3	1.93	0.49
3:F:310:MET:HB2	3:F:335:TRP:HB3	1.94	0.49
2:E:280:THR:HB	2:E:283:LYS:HG2	1.93	0.49
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.78	0.49
1:D:135:LEU:HG	1:D:139:ASN:ND2	2.26	0.49
2:B:257:ASP:O	2:B:291:GLU:OE2	2.30	0.49
2:B:294:LEU:HB3	2:B:299:ILE:HD11	1.93	0.49
3:C:208:TRP:HA	3:C:314:THR:HG21	1.95	0.49
2:B:179:ILE:O	2:B:183:GLU:HG3	2.12	0.49
3:C:117:ASN:O	3:C:121:ILE:HG13	2.13	0.49
3:F:389:PHE:C	3:F:391:ARG:H	2.16	0.49
3:C:200:GLY:HA2	7:C:409:HOH:O	2.12	0.48
3:C:317:ASN:HD22	3:C:317:ASN:C	2.16	0.48
3:F:273:LYS:CB	3:F:311:GLN:HB3	2.43	0.48
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.27	0.48
1:A:162:ARG:CZ	7:A:196:HOH:O	2.61	0.48
3:C:268:GLY:O	3:C:274:TYR:HA	2.12	0.48
2:B:212:GLU:O	2:B:215:ILE:HG22	2.13	0.48
1:D:180:ASP:O	1:D:184:GLN:HB2	2.14	0.48
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.94	0.48
1:D:169:LEU:H	2:E:189:GLN:HE22	1.60	0.48
3:C:298:ASP:OD1	3:C:299:PRO:HD2	2.13	0.48
5:K:1:NAG:H4	5:K:2:NAG:N2	2.28	0.48
3:C:155:ASP:O	3:C:159:LYS:HG3	2.14	0.47
2:E:187:SER:O	2:E:191:GLU:HG3	2.14	0.47
2:E:265:LYS:HE3	2:E:378:TYR:OH	2.13	0.47
5:K:1:NAG:O3	5:K:2:NAG:H82	2.14	0.47
1:A:183:LYS:O	1:A:187:GLN:HG3	2.14	0.47
3:F:307:HIS:CE1	3:F:341:ALA:H	2.31	0.47
5:L:1:NAG:O3	5:L:2:NAG:H82	2.14	0.47
1:A:130:VAL:HA	1:A:133:ILE:HG22	1.96	0.47
3:F:141:ASP:OD1	3:F:143:VAL:HG13	2.15	0.47
3:C:231:GLU:O	3:C:235:LEU:HG	2.15	0.47
3:F:338:LYS:O	3:F:338:LYS:HG2	2.14	0.47
1:D:153:ASP:O	1:D:157:LYS:HG2	2.15	0.47
3:F:307:HIS:HD2	3:F:335:TRP:O	1.97	0.47
2:E:351:ASN:ND2	2:E:351:ASN:C	2.68	0.47
3:F:356:LYS:HG3	3:F:362:GLY:O	2.15	0.47
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.27	0.47
2:E:361:MET:HB3	5:L:1:NAG:H81	1.96	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:439:ASN:HD22	2:E:439:ASN:H	1.64	0.46
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.50	0.46
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.30	0.46
2:E:346:ARG:O	2:E:346:ARG:CG	2.58	0.46
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.36	0.46
2:B:406:ARG:O	2:B:406:ARG:HG2	2.15	0.46
2:E:174:ASN:O	2:E:178:LYS:HG3	2.16	0.46
2:E:345:TYR:CE2	2:E:351:ASN:HB2	2.50	0.46
1:A:151:GLU:HG2	1:A:173:VAL:HG13	1.97	0.46
3:C:103:HIS:O	3:C:107:ILE:HG22	2.16	0.46
2:B:161:ILE:N	2:B:162:PRO:CD	2.76	0.46
1:A:176:LYS:HA	1:A:179:GLU:OE1	2.16	0.45
2:B:212:GLU:OE2	2:B:216:ARG:HD2	2.16	0.45
3:C:154:GLN:OE1	3:C:391:ARG:HG2	2.15	0.45
3:C:249:GLU:CB	3:C:383:THR:HG23	2.42	0.45
2:E:417:TYR:HB2	2:E:446:SER:CB	2.45	0.45
1:D:136:LEU:O	1:D:140:VAL:HG22	2.17	0.45
2:E:191:GLU:HG2	2:E:194:ARG:HH21	1.82	0.45
3:F:239:GLN:HB3	3:F:242:ILE:HD12	1.98	0.45
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.98	0.45
3:C:344:LEU:HD12	3:C:384:MET:SD	2.57	0.45
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.14	0.45
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.99	0.45
2:B:410:ALA:C	2:B:412:PRO:HD3	2.38	0.45
3:C:393:THR:O	3:C:394:ILE:OXT	2.35	0.45
3:F:167:TYR:O	3:F:179:LEU:HD12	2.17	0.45
1:A:185:LEU:CD1	1:A:189:ILE:HD11	2.47	0.44
2:B:340:ILE:HG12	2:B:341:SER:N	2.31	0.44
3:F:326:CYS:HB3	3:F:336:MET:HE3	1.99	0.44
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.99	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.79	0.44
3:F:262:TYR:CE2	3:F:288:ASP:OD1	2.71	0.44
3:C:118:ASN:HB3	7:C:480:HOH:O	2.16	0.44
3:F:247:ARG:NH2	3:F:392:LEU:HD11	2.32	0.44
2:B:428:LYS:HE3	2:B:428:LYS:HB2	1.81	0.44
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.52	0.44
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.16	0.44
2:E:433:ASP:OD1	2:E:433:ASP:O	2.36	0.44
3:F:325:ASN:O	3:F:328:GLU:HB3	2.17	0.44
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.18	0.44
2:E:406:ARG:N	2:E:407:CYS:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD13	1:A:185:LEU:C	2.38	0.44
2:B:432:ASP:CB	2:B:443:SER:HB3	2.48	0.44
3:C:189:ASN:HD22	3:C:391:ARG:NE	2.11	0.44
3:F:276:LEU:HD12	3:F:276:LEU:C	2.38	0.44
1:A:148:LYS:HE3	1:A:175:LEU:HD12	1.98	0.44
1:D:148:LYS:O	1:D:152:VAL:HG23	2.17	0.43
1:D:175:LEU:HD22	1:D:175:LEU:N	2.33	0.43
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.17	0.43
1:A:137:GLN:CG	1:A:189:ILE:HG12	2.48	0.43
1:D:147:MET:HG3	2:E:175:LEU:HD22	2.00	0.43
3:F:172:LEU:H	3:F:239:GLN:HE21	1.64	0.43
3:F:276:LEU:HD23	3:F:335:TRP:CD2	2.54	0.43
2:E:273:PHE:O	2:E:292:TYR:HB2	2.18	0.43
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.84	0.43
5:L:1:NAG:H4	5:L:2:NAG:N2	2.28	0.43
3:C:391:ARG:HD2	3:C:391:ARG:HA	1.83	0.43
2:E:391:ARG:HG3	2:E:391:ARG:HH11	1.84	0.43
3:F:239:GLN:CB	3:F:242:ILE:HD12	2.49	0.43
3:F:350:GLN:HE21	3:F:350:GLN:CA	2.30	0.43
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.54	0.43
3:C:333:GLY:O	3:C:334:TRP:HB2	2.19	0.43
2:B:436:VAL:CG1	2:B:437:TRP:N	2.82	0.43
3:C:356:LYS:HG3	3:C:362:GLY:O	2.19	0.43
2:E:169:ARG:HB2	3:F:110:LEU:HD21	2.00	0.43
2:E:178:LYS:O	2:E:182:LEU:HG	2.19	0.43
3:C:245:ALA:HB2	3:C:389:PHE:HD1	1.84	0.42
3:F:151:LYS:HZ3	3:F:172:LEU:HD21	1.84	0.42
3:F:251:GLU:CG	3:F:257:THR:HG22	2.49	0.42
1:D:183:LYS:O	1:D:187:GLN:HG3	2.19	0.42
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.55	0.42
2:E:161:ILE:N	2:E:162:PRO:CD	2.82	0.42
3:F:387:ILE:HG13	3:F:388:PRO:HD2	2.01	0.42
2:B:208:GLY:N	2:B:214:ILE:HD11	2.35	0.42
2:B:436:VAL:HG12	2:B:437:TRP:N	2.34	0.42
3:C:197:ARG:CZ	3:C:367:ILE:HD11	2.50	0.42
1:D:150:LEU:HD21	3:F:124:LEU:HD23	2.02	0.42
2:E:440:TRP:CE3	2:E:441:LYS:HG2	2.53	0.42
3:F:363:TYR:HE1	4:G:4:PRO:HD2	1.84	0.42
1:A:137:GLN:HE22	1:A:189:ILE:HA	1.81	0.42
1:A:153:ASP:O	1:A:157:LYS:HG2	2.19	0.42
2:B:423:THR:O	2:B:426:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:ASP:HB3	2:B:443:SER:HB3	2.01	0.42
3:C:346:GLY:O	3:C:367:ILE:HD11	2.20	0.42
3:C:359:THR:HA	3:C:360:PRO:HD3	1.92	0.42
3:F:250:LEU:HD21	3:F:369:TRP:CG	2.54	0.42
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.54	0.42
1:A:152:VAL:O	1:A:156:ILE:HG12	2.20	0.42
3:F:320:ASP:OD1	3:F:322:PHE:HB3	2.19	0.42
3:F:367:ILE:O	3:F:378:SER:HA	2.20	0.42
3:C:107:ILE:HG23	3:C:108:ARG:N	2.34	0.42
2:E:265:LYS:O	2:E:268:PRO:HD2	2.19	0.42
3:F:261:ASP:HB2	3:F:282:ALA:HB3	2.01	0.42
3:F:370:ALA:C	3:F:372:TRP:H	2.22	0.42
2:E:202:ASN:HD21	2:E:284:ASN:HB2	1.82	0.42
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.55	0.42
3:F:389:PHE:O	3:F:391:ARG:N	2.49	0.42
2:B:423:THR:HG23	2:B:426:MET:HE3	2.01	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.88	0.42
3:C:137:GLU:HA	3:C:138:PRO:HD3	1.84	0.42
3:F:272:ASP:OD2	3:F:275:ARG:NE	2.52	0.42
3:F:304:PHE:O	3:F:337:ASN:HB3	2.20	0.42
3:F:304:PHE:HB3	3:F:338:LYS:HB3	2.02	0.42
2:B:411:ASN:N	2:B:412:PRO:HD3	2.35	0.41
3:F:276:LEU:HD23	3:F:335:TRP:CG	2.55	0.41
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.50	0.41
3:F:393:THR:O	3:F:394:ILE:OXT	2.37	0.41
1:A:131:GLN:HA	1:A:131:GLN:NE2	2.34	0.41
1:D:157:LYS:HE3	3:F:132:GLU:OE2	2.19	0.41
2:E:296:ASN:HB3	2:E:338:TYR:CD1	2.55	0.41
2:E:303:THR:HB	2:E:330:THR:HA	2.02	0.41
2:E:337:LYS:HG2	2:E:382:ASN:ND2	2.35	0.41
3:F:151:LYS:HZ1	3:F:172:LEU:HD21	1.84	0.41
1:D:136:LEU:HD21	3:F:111:GLN:HG2	2.02	0.41
2:E:428:LYS:HB2	2:E:428:LYS:HE3	1.86	0.41
1:A:150:LEU:HG	1:A:154:ILE:HD13	2.02	0.41
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.69	0.41
3:C:232:LYS:O	3:C:236:ILE:HG13	2.19	0.41
3:C:246:LEU:HD22	3:C:265:PHE:CE1	2.56	0.41
2:E:181:LYS:O	2:E:184:SER:HB2	2.20	0.41
3:F:248:VAL:HG12	3:F:250:LEU:CD1	2.50	0.41
3:F:329:GLN:OE1	4:G:3:ARG:HD3	2.20	0.41
2:B:318:LYS:HD2	7:B:597:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG12	1:A:130:VAL:O	2.21	0.41
3:F:356:LYS:HA	3:F:376:TRP:CZ3	2.56	0.41
3:C:258:SER:OG	3:C:286:ALA:HB2	2.21	0.41
2:E:457:PHE:O	2:E:458:PHE:HB2	2.21	0.41
3:F:193:VAL:HG12	3:F:226:PHE:CZ	2.55	0.41
3:F:198:LEU:O	3:F:199:ASP:HB3	2.20	0.41
2:B:415:ARG:HD3	7:B:490:HOH:O	2.20	0.41
1:D:187:GLN:O	1:D:189:ILE:N	2.43	0.41
2:E:438:MET:HA	2:E:442:GLY:O	2.21	0.41
3:F:123:ASN:N	3:F:123:ASN:ND2	2.69	0.41
3:F:365:ASN:HD22	3:F:365:ASN:C	2.23	0.41
3:F:370:ALA:O	3:F:372:TRP:N	2.53	0.41
3:C:373:LYS:HD3	3:C:373:LYS:HA	1.90	0.41
3:F:361:ASN:N	3:F:361:ASN:ND2	2.68	0.41
2:B:326:TYR:OH	2:B:351:ASN:ND2	2.53	0.40
2:E:280:THR:HB	2:E:283:LYS:CG	2.51	0.40
2:B:245:GLU:O	2:B:246:ASN:HB2	2.21	0.40
3:C:325:ASN:C	3:C:325:ASN:HD22	2.24	0.40
2:E:323:LYS:HZ2	2:E:325:HIS:HD2	1.67	0.40
3:F:284:GLY:C	3:F:286:ALA:H	2.24	0.40
2:B:172:LEU:CD1	3:C:110:LEU:HB3	2.51	0.40
2:B:405:ASN:HB3	2:B:406:ARG:H	1.62	0.40
1:D:149:ARG:HG3	2:E:425:ASP:O	2.22	0.40
2:E:212:GLU:O	2:E:215:ILE:HG22	2.21	0.40
2:E:255:ARG:N	2:E:450:MET:O	2.51	0.40
3:F:202:VAL:HG21	3:F:225:GLU:O	2.20	0.40
4:H:3:ARG:HD3	4:H:3:ARG:HA	1.84	0.40
1:A:165:CYS:HB3	2:B:193:CYS:HA	2.04	0.40
2:B:276:VAL:HA	2:B:292:TYR:CD1	2.56	0.40
2:E:415:ARG:O	2:E:434:GLY:HA2	2.21	0.40
3:F:250:LEU:HD12	3:F:250:LEU:N	2.36	0.40
3:F:292:GLY:H	3:F:306:SER:HA	1.86	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	60/62 (97%)	56 (93%)	4 (7%)	0	100 100
1	D	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9 18
2	B	296/298 (99%)	275 (93%)	18 (6%)	3 (1%)	15 32
2	E	296/298 (99%)	267 (90%)	20 (7%)	9 (3%)	4 7
3	C	291/293 (99%)	267 (92%)	19 (6%)	5 (2%)	9 18
3	F	291/293 (99%)	253 (87%)	30 (10%)	8 (3%)	5 8
4	G	2/4 (50%)	2 (100%)	0	0	100 100
4	H	2/4 (50%)	2 (100%)	0	0	100 100
4	I	2/4 (50%)	2 (100%)	0	0	100 100
4	J	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
All	All	1302/1322 (98%)	1182 (91%)	94 (7%)	26 (2%)	7 14

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	162	PRO
2	E	457	PHE
3	F	199	ASP
3	C	198	LEU
1	D	188	VAL
2	E	162	PRO
2	E	399	GLY
2	E	435	VAL
3	F	371	THR
3	F	390	ASN
2	B	281	ASP
2	B	457	PHE
3	C	371	THR
2	E	256	GLN
2	E	438	MET
3	F	198	LEU
3	F	338	LYS
2	E	439	ASN
3	F	285	ASP
3	F	369	TRP

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Mol	Chain	Res	Type
3	C	199	ASP
3	C	172	LEU
3	C	242	ILE
2	E	257	ASP
2	E	351	ASN
3	F	298	ASP

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	57/57 (100%)	54 (95%)	3 (5%)	22 45
1	D	57/57 (100%)	54 (95%)	3 (5%)	22 45
2	B	256/256 (100%)	246 (96%)	10 (4%)	32 58
2	E	256/256 (100%)	248 (97%)	8 (3%)	40 66
3	C	246/246 (100%)	236 (96%)	10 (4%)	30 56
3	F	246/246 (100%)	233 (95%)	13 (5%)	22 45
4	G	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	H	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	I	3/3 (100%)	3 (100%)	0	100 100
4	J	3/3 (100%)	3 (100%)	0	100 100
All	All	1130/1130 (100%)	1081 (96%)	49 (4%)	29 54

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ILE
1	A	175	LEU
1	A	176	LYS
2	B	210	GLU
2	B	215	ILE
2	B	238	VAL
2	B	253	GLN

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Mol	Chain	Res	Type
2	B	280	THR
2	B	301	GLN
2	B	346	ARG
2	B	351	ASN
2	B	439	ASN
2	B	447	MET
3	C	118	ASN
3	C	162	LYS
3	C	198	LEU
3	C	250	LEU
3	C	256	ARG
3	C	317	ASN
3	C	325	ASN
3	C	330	ASP
3	C	365	ASN
3	C	383	THR
1	D	144	LEU
1	D	164	SER
1	D	176	LYS
2	E	210	GLU
2	E	215	ILE
2	E	233	VAL
2	E	252	ILE
2	E	253	GLN
2	E	301	GLN
2	E	325	HIS
2	E	351	ASN
3	F	107	ILE
3	F	123	ASN
3	F	143	VAL
3	F	163	GLN
3	F	176	GLN
3	F	276	LEU
3	F	297	ASP
3	F	301	ASP
3	F	325	ASN
3	F	343	HIS
3	F	365	ASN
3	F	383	THR
3	F	394	ILE
4	G	3	ARG
4	H	4	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	134	GLN
1	A	137	GLN
1	A	139	ASN
1	A	184	GLN
1	A	187	GLN
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	339	GLN
2	B	351	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	119	GLN
3	C	134	GLN
3	C	146	HIS
3	C	176	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	365	ASN
1	D	132	HIS
1	D	137	GLN
1	D	139	ASN
1	D	187	GLN
2	E	164	ASN
2	E	189	GLN

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Mol	Chain	Res	Type
2	E	202	ASN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	429	HIS
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	176	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	350	GLN
3	F	361	ASN
3	F	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	K	1	2,5	14,14,15	0.68	0	17,19,21	0.83	0
5	NAG	K	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.84	1 (5%)
5	FUC	K	3	5	10,10,11	0.45	0	14,14,16	0.42	0
5	NAG	L	1	2,5	14,14,15	0.69	0	17,19,21	0.84	0
5	NAG	L	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.84	1 (5%)
5	FUC	L	3	5	10,10,11	0.45	0	14,14,16	0.42	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
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	5/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	5/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	C1-C2	2.08	1.55	1.52
5	K	2	NAG	C1-C2	2.05	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	2	NAG	C2-N2-C7	-2.01	120.04	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	2	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6

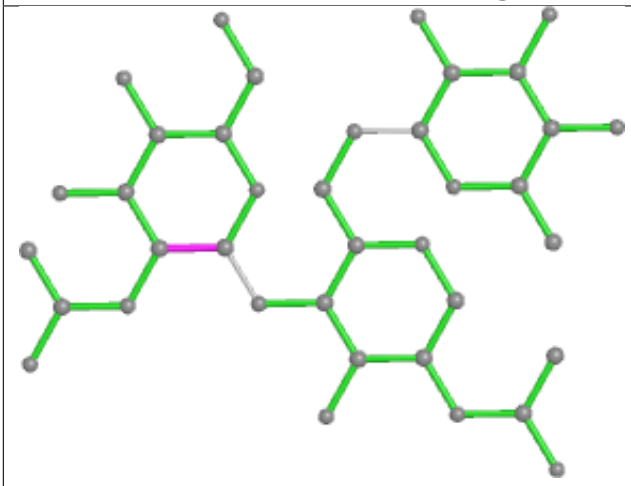
There are no ring outliers.

5 monomers are involved in 13 short contacts:

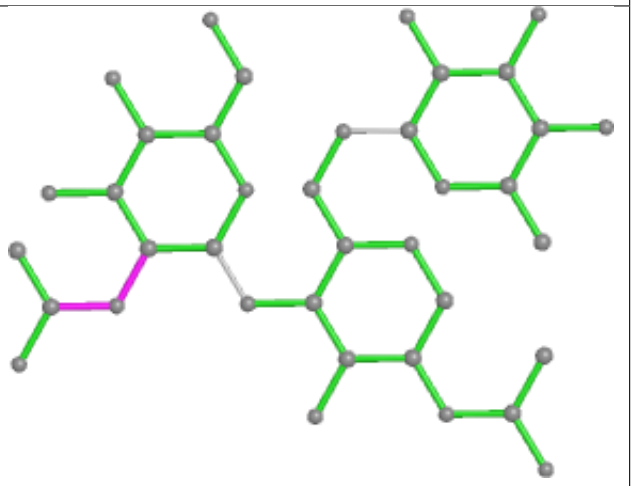
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	4	0
5	L	1	NAG	8	0
5	L	3	FUC	2	0
5	K	1	NAG	4	0
5	L	2	NAG	3	0

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

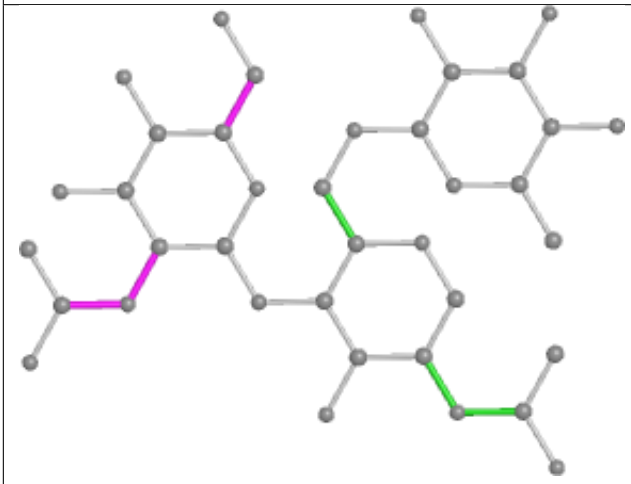
Oligosaccharide Chain K



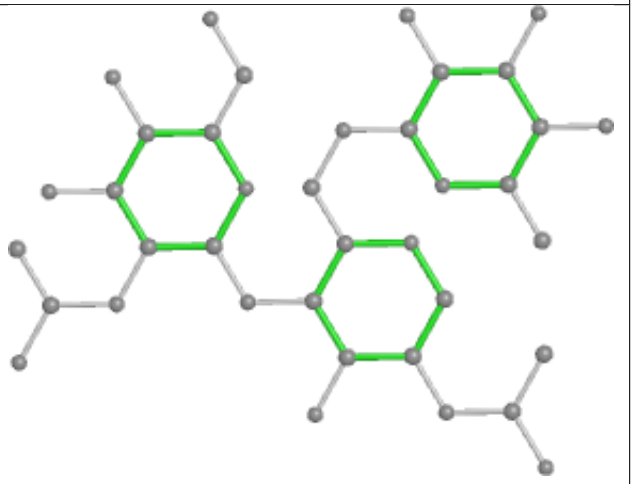
Bond lengths



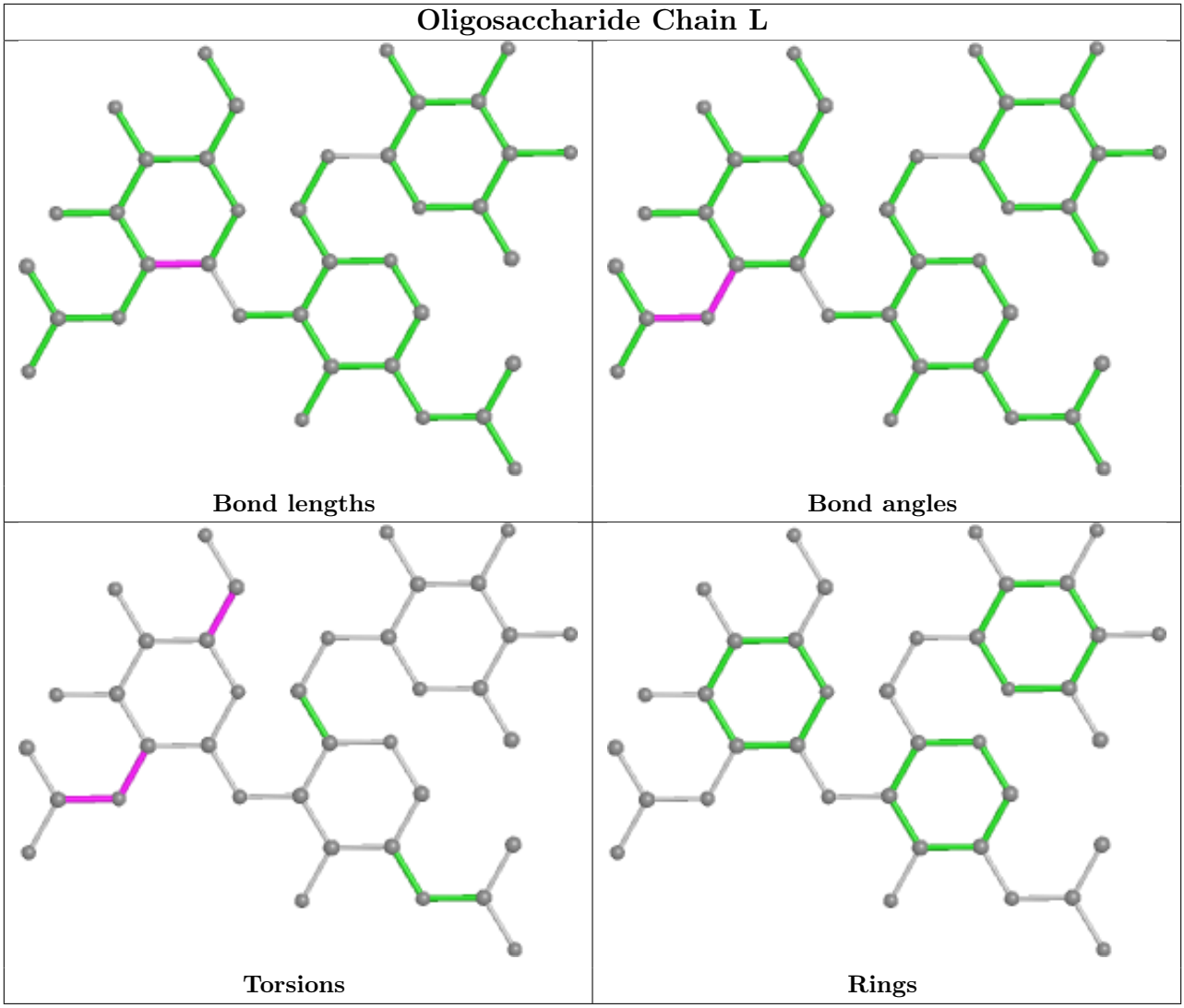
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	62/62 (100%)	0.08	4 (6%) 18 14	22, 49, 94, 108	0
1	D	62/62 (100%)	0.15	4 (6%) 18 14	24, 60, 99, 101	0
2	B	298/298 (100%)	-0.52	5 (1%) 70 66	10, 24, 61, 98	0
2	E	298/298 (100%)	-0.38	3 (1%) 82 80	19, 39, 68, 97	0
3	C	293/293 (100%)	-0.42	7 (2%) 59 53	16, 32, 67, 111	0
3	F	293/293 (100%)	0.02	14 (4%) 30 24	29, 52, 86, 116	0
4	G	4/4 (100%)	0.08	0 100 100	85, 87, 87, 92	0
4	H	4/4 (100%)	-0.53	0 100 100	52, 59, 59, 63	0
4	I	4/4 (100%)	-0.67	0 100 100	34, 34, 36, 46	0
4	J	4/4 (100%)	-0.64	0 100 100	25, 25, 28, 35	0
All	All	1322/1322 (100%)	-0.28	37 (2%) 53 46	10, 37, 86, 116	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	394	ILE	6.9
3	C	107	ILE	5.6
3	F	102	THR	4.5
3	F	104	ASP	4.2
3	C	102	THR	4.1
3	F	393	THR	3.9
3	F	107	ILE	3.8
1	A	129	LYS	3.7
2	E	164	ASN	3.6
3	C	394	ILE	3.5
2	B	161	ILE	3.3
1	D	190	ALA	3.3
2	B	164	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	254	ASN	3.2
3	F	352	GLY	3.2
2	B	163	THR	3.2
3	F	108	ARG	3.2
3	F	256	ARG	3.1
3	C	104	ASP	3.0
3	F	105	SER	2.9
2	B	281	ASP	2.8
3	C	106	SER	2.7
3	C	393	THR	2.7
1	A	130	VAL	2.7
2	E	161	ILE	2.6
3	F	103	HIS	2.6
2	B	162	PRO	2.5
1	A	189	ILE	2.5
3	C	108	ARG	2.5
3	F	295	PHE	2.3
3	F	370	ALA	2.3
1	A	131	GLN	2.2
1	D	137	GLN	2.1
1	D	187	GLN	2.1
3	F	112	GLU	2.1
2	E	166	ARG	2.1
1	D	133	ILE	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
5	NAG	L	2	14/15	0.61	0.34	68,71,75,77	0
5	NAG	K	2	14/15	0.66	0.29	68,71,75,77	0
5	FUC	L	3	10/11	0.82	0.31	57,59,60,61	0
5	NAG	L	1	14/15	0.83	0.29	42,51,56,63	0

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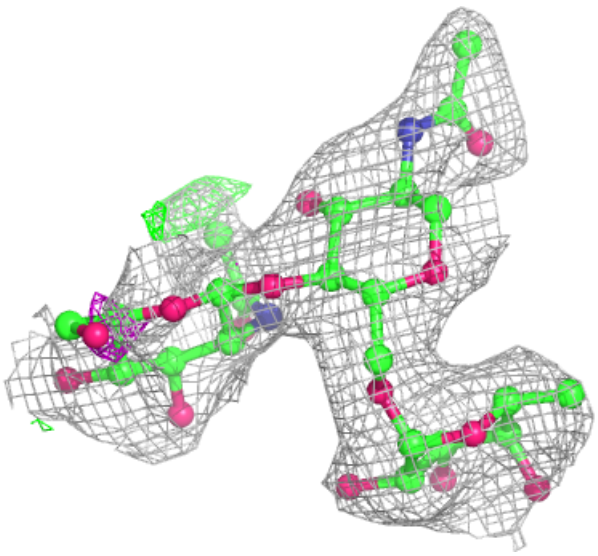
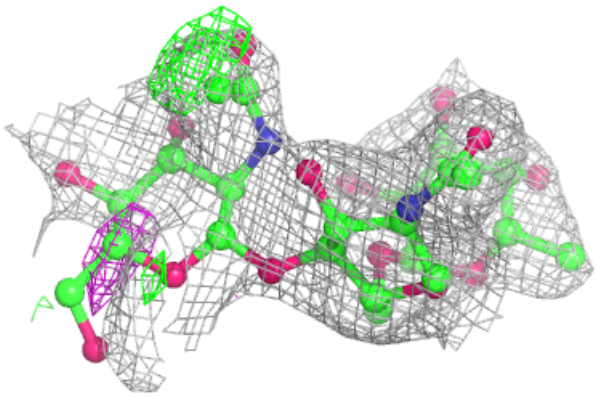
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FUC	K	3	10/11	0.88	0.18	57,59,60,61	0
5	NAG	K	1	14/15	0.91	0.13	42,51,56,63	0

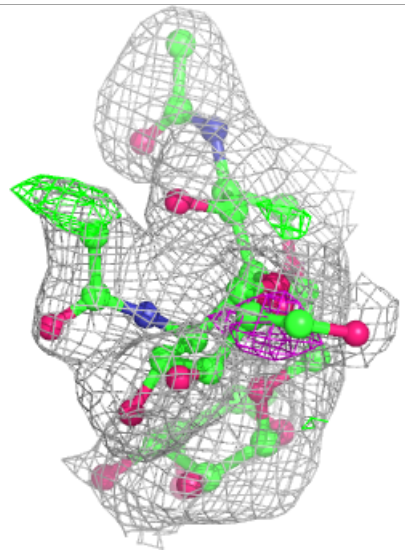
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

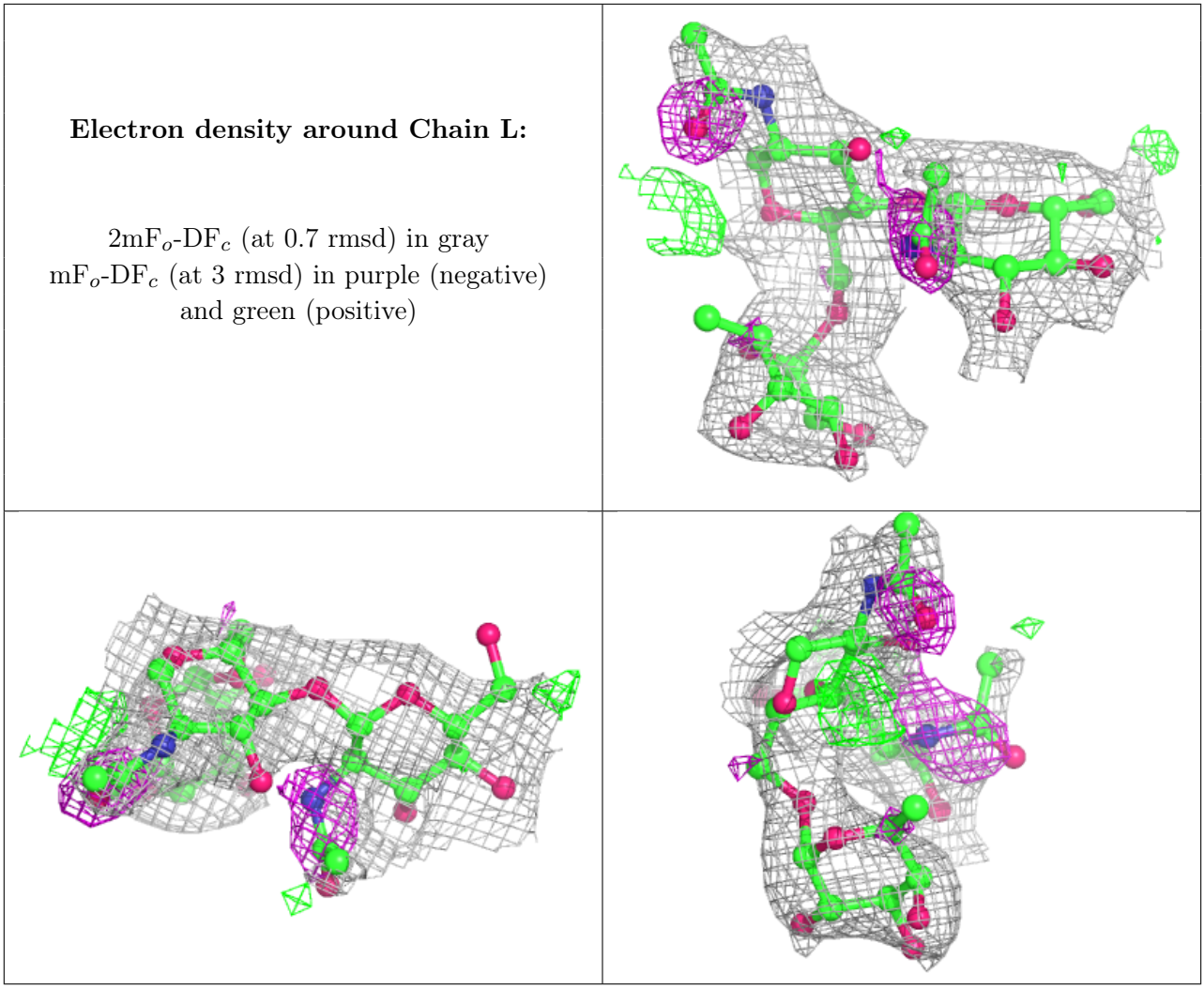






Electron density around Chain L:

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



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
6	CA	F	1	1/1	0.91	0.08	51,51,51,51	0
6	CA	E	1	1/1	0.97	0.16	49,49,49,49	0
6	CA	C	1	1/1	0.97	0.15	31,31,31,31	0
6	CA	B	1	1/1	0.98	0.14	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.