Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 08:39 PM EDT

PDB ID	:	1RF1
Title	:	Crystal Structure of Fragment D of gammaE132A Fibrinogen with the Peptide Ligand Gly-His-Arg-Pro-amide
Authors	:	Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on	:	2003-11-07
Resolution	:	2.53 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:

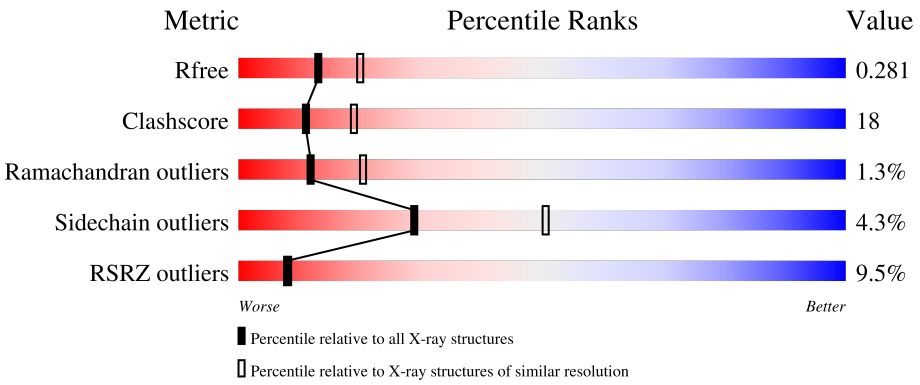
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	66	23% 53% 36% 8% •
1	D	66	29% 42% 39% • 15%
2	B	313	6% 68% 27% • •
2	E	313	3% 67% 24% • 6%
3	C	311	10% 65% 28% • •

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Mol	Chain	Length	Quality of chain
3	F	311	8% 64% 27% 6%
4	G	4	75% 75% 25%
4	H	4	25% 75% 25%
4	I	4	50% 25% 50% 25%
4	J	4	75% 25%
5	K	3	67% 33%
5	L	3	33% 67%

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	2	-	-	-	X
5	FUC	K	3	-	-	-	X
5	NAG	L	1	-	-	X	-
5	NAG	L	2	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10928 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/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	64	523	322	99	99	3	0	0	0
1	D	56	458	280	87	88	3	0	0	0

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	299	2399	1499	423	455	22	0	0	0
2	E	295	2369	1480	418	449	22	0	0	0

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	298	2387	1515	402	459	11	0	0	0
3	F	291	2332	1479	395	447	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	GLU	engineered mutation	UNP P02679
F	132	ALA	GLU	engineered mutation	UNP P02679

- Molecule 4 is a protein called GHRP peptide.

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

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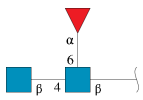
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	4	33	19	9	5	0	0	0
4	I	4	33	19	9	5	0	0	0
4	J	4	33	19	9	5	0	0	0

- 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
			Total	C	N	O			
5	K	3	38	22	2	14	0	0	0
5	L	3	38	22	2	14	0	0	0

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	6	6	6	0	0
7	B	51	51	51	0	0
7	C	30	30	30	0	0

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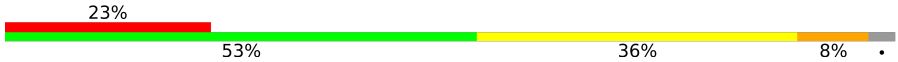
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	11	11	11	0	0
			Total	O		
7	E	89	89	89	0	0
			Total	O		
7	F	60	60	60	0	0
			Total	O		
7	J	1	1	1	0	0

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/alpha-E chain

Chain A:

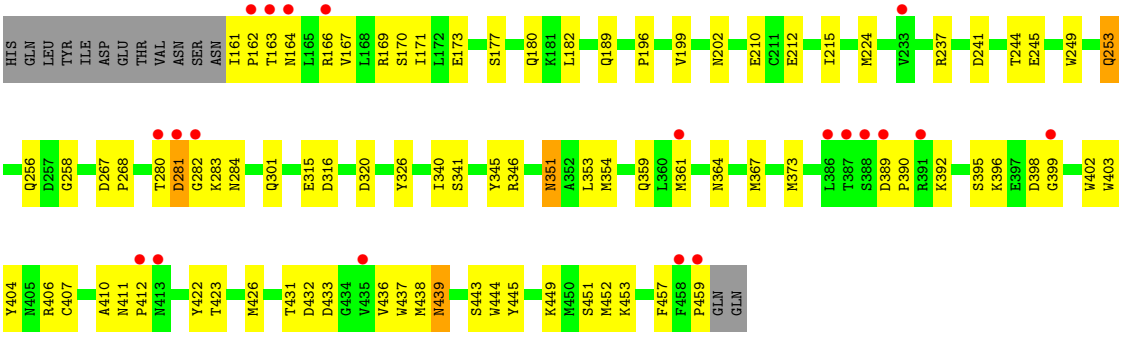


• Molecule 1: Fibrinogen alpha/alpha-E chain

Chain D:

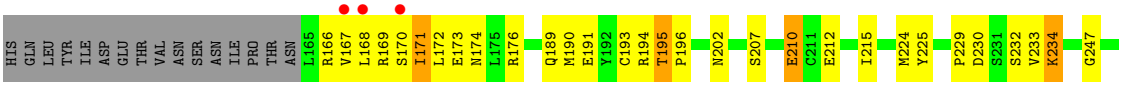
• Molecule 2: Fibrinogen beta chain

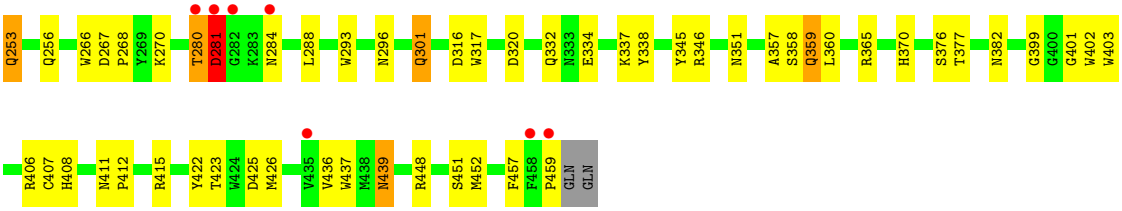
Chain B:



• Molecule 2: Fibrinogen beta chain

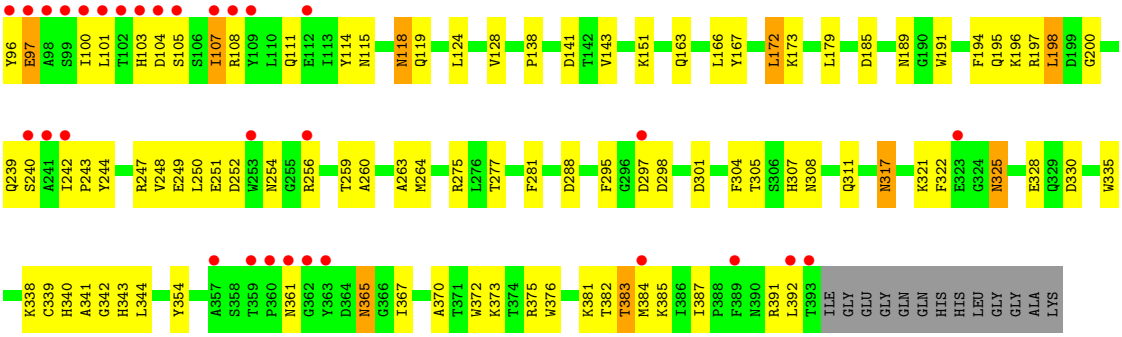
Chain E:





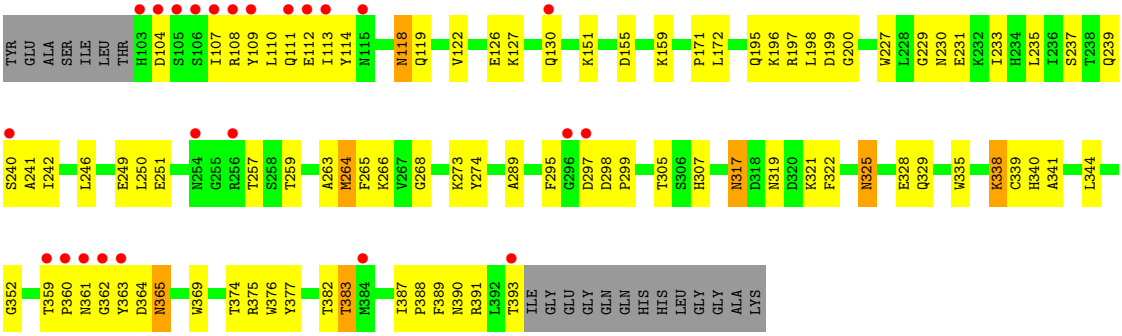
• Molecule 3: Fibrinogen gamma chain

Chain C:



• Molecule 3: Fibrinogen gamma chain

Chain F:



• Molecule 4: GHRP peptide

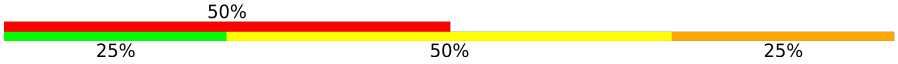
Chain G:

• Molecule 4: GHRP peptide

Chain H:

• Molecule 4: GHRP peptide

Chain I:

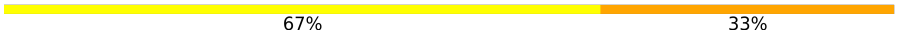


• Molecule 4: GHRP peptide

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	89.71Å 94.68Å 228.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.53 35.02 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.97-2.53) 99.7 (35.02-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.281 0.235 , 0.281	Depositor DCC
R_{free} test set	3316 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.33% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.29	0/524	0.52	0/699
1	D	0.29	0/458	0.50	0/610
2	B	0.36	0/2461	0.61	0/3324
2	E	0.39	0/2430	0.65	1/3280 (0.0%)
3	C	0.36	0/2453	0.56	0/3319
3	F	0.39	0/2397	0.60	0/3242
4	G	0.52	0/34	0.51	0/43
4	H	0.46	0/34	0.52	0/43
4	I	0.47	0/34	0.41	0/43
4	J	0.49	0/34	0.51	0/43
All	All	0.37	0/10859	0.60	1/14646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	399	GLY	N-CA-C	7.12	130.89	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	523	0	547	37	0
1	D	458	0	477	30	0
2	B	2399	0	2269	78	0
2	E	2369	0	2238	72	0
3	C	2387	0	2234	88	0
3	F	2332	0	2180	92	0
4	G	33	0	32	5	0
4	H	33	0	32	1	0
4	I	33	0	32	9	0
4	J	33	0	32	1	0
5	K	38	0	34	7	0
5	L	38	0	34	7	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	6	0	0	0	0
7	B	51	0	0	3	0
7	C	30	0	0	2	0
7	D	11	0	0	0	0
7	E	89	0	0	1	0
7	F	60	0	0	2	0
7	J	1	0	0	0	0
All	All	10928	0	10141	375	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 18.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:LEU:HD23	3:F:110:LEU:HD13	1.45	0.97
2:E:358:SER:HA	2:E:365:ARG:HH12	1.37	0.88
2:E:359:GLN:H	2:E:359:GLN:HE21	1.19	0.88
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.41	0.85
3:C:172:LEU:HD23	3:C:172:LEU:H	1.44	0.82
1:D:134:GLN:H	1:D:134:GLN:NE2	1.77	0.81
1:A:127:ILE:HG12	1:A:130:VAL:HG23	1.61	0.81
3:F:113:ILE:HD12	3:F:114:TYR:N	1.97	0.79
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.19	0.78
2:B:439:ASN:H	2:B:439:ASN:HD22	1.29	0.77
2:E:359:GLN:H	2:E:359:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1:NAG:H61	5:L:3:FUC:H5	1.66	0.76
1:A:143:GLN:HE21	3:C:118:ASN:ND2	1.83	0.76
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.66	0.76
2:B:389:ASP:HB3	2:B:392:LYS:HG3	1.67	0.76
3:C:197:ARG:HB2	3:C:382:THR:HB	1.67	0.75
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.69	0.75
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.69	0.74
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.35	0.74
2:B:423:THR:H	2:B:426:MET:HE3	1.53	0.74
2:E:439:ASN:HD22	2:E:439:ASN:H	1.35	0.74
3:C:325:ASN:C	3:C:325:ASN:HD22	1.90	0.73
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.70	0.73
2:B:359:GLN:HE22	2:B:438:MET:HB3	1.54	0.73
2:E:457:PHE:O	2:E:459:PRO:HD3	1.89	0.72
2:E:234:LYS:H	2:E:234:LYS:HD2	1.55	0.72
2:E:172:LEU:HD13	3:F:113:ILE:HD11	1.72	0.71
2:E:423:THR:N	2:E:426:MET:HE3	2.06	0.70
2:E:358:SER:HA	2:E:365:ARG:NH1	2.07	0.70
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.07	0.69
2:E:406:ARG:NH1	4:J:3:ARG:O	2.25	0.69
3:F:325:ASN:HD22	3:F:325:ASN:C	1.96	0.69
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.93	0.69
3:F:108:ARG:HA	3:F:111:GLN:HE21	1.55	0.69
3:F:365:ASN:HD22	3:F:365:ASN:H	1.41	0.69
2:B:316:ASP:OD2	2:B:320:ASP:HB2	1.92	0.69
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.92	0.69
3:C:307:HIS:CE1	3:C:341:ALA:H	2.11	0.68
1:D:179:GLU:O	1:D:183:LYS:HG3	1.93	0.68
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.75	0.68
5:K:1:NAG:H4	5:K:2:NAG:HN2	1.58	0.68
2:B:423:THR:N	2:B:426:MET:HE3	2.09	0.67
2:E:280:THR:HG23	2:E:288:LEU:HG	1.77	0.66
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.61	0.66
1:D:133:ILE:HD11	3:F:107:ILE:HD12	1.78	0.66
3:F:151:LYS:HD3	3:F:172:LEU:HD21	1.75	0.66
3:F:338:LYS:N	3:F:339:CYS:HA	2.09	0.66
1:A:169:LEU:H	2:B:189:GLN:NE2	1.93	0.66
1:A:169:LEU:H	2:B:189:GLN:HE22	1.43	0.66
2:B:361:MET:HB2	5:K:1:NAG:H81	1.77	0.65
3:C:101:LEU:HD12	3:C:101:LEU:H	1.61	0.65
3:F:307:HIS:HE1	3:F:341:ALA:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:172:LEU:H	3:F:239:GLN:HE21	1.45	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.45	0.65
3:C:101:LEU:HD12	3:C:101:LEU:N	2.14	0.63
2:E:234:LYS:H	2:E:234:LYS:CD	2.10	0.63
3:C:195:GLN:OE1	3:C:382:THR:HG22	1.99	0.63
3:F:118:ASN:O	3:F:122:VAL:HG23	1.99	0.63
3:C:295:PHE:HE2	3:C:305:THR:HG21	1.62	0.63
2:B:163:THR:HA	2:B:166:ARG:HD2	1.80	0.62
2:B:345:TYR:HB2	2:B:354:MET:CE	2.30	0.62
3:F:325:ASN:ND2	3:F:328:GLU:H	1.97	0.62
3:C:295:PHE:HB2	3:C:301:ASP:OD2	1.99	0.62
2:E:345:TYR:O	2:E:346:ARG:HG3	1.99	0.62
2:E:406:ARG:N	2:E:407:CYS:HA	2.13	0.62
2:B:351:ASN:HD22	2:B:351:ASN:C	2.00	0.62
3:C:105:SER:HA	3:C:108:ARG:HH21	1.63	0.62
2:E:439:ASN:HD22	2:E:439:ASN:N	1.97	0.62
5:L:1:NAG:H61	5:L:3:FUC:H3	1.80	0.62
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.65	0.62
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.65	0.61
2:E:270:LYS:HE2	2:E:334:GLU:OE1	2.00	0.61
3:F:240:SER:O	3:F:242:ILE:HG13	2.00	0.61
3:F:307:HIS:HD2	3:F:335:TRP:O	1.82	0.61
2:B:439:ASN:HD22	2:B:439:ASN:N	1.98	0.61
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.83	0.61
2:B:253:GLN:NE2	2:B:451:SER:HA	2.16	0.60
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.81	0.60
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.83	0.60
3:C:104:ASP:O	3:C:107:ILE:HG22	2.01	0.60
5:L:1:NAG:H61	5:L:3:FUC:C5	2.32	0.60
2:B:359:GLN:NE2	2:B:438:MET:HB3	2.17	0.59
1:A:132:HIS:HB3	3:C:107:ILE:HD11	1.84	0.59
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.17	0.59
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.82	0.59
2:B:351:ASN:ND2	2:B:354:MET:H	2.01	0.59
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.03	0.59
3:F:321:LYS:O	3:F:338:LYS:HD3	2.02	0.59
1:A:178:TYR:O	1:A:182:GLN:HG3	2.03	0.58
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.84	0.58
3:C:325:ASN:ND2	3:C:328:GLU:H	2.00	0.58
1:D:169:LEU:H	2:E:189:GLN:HE22	1.49	0.58
3:C:108:ARG:HA	3:C:111:GLN:HE21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HE3	3:C:100:ILE:HG23	1.85	0.58
2:E:229:PRO:HB2	2:E:301:GLN:HE22	1.67	0.58
3:C:307:HIS:HE1	3:C:342:GLY:H	1.52	0.58
2:E:212:GLU:O	2:E:215:ILE:HG22	2.04	0.58
3:C:103:HIS:O	3:C:107:ILE:HB	2.04	0.57
3:F:389:PHE:C	3:F:391:ARG:H	2.07	0.57
2:B:457:PHE:O	2:B:459:PRO:HD3	2.04	0.57
3:C:340:HIS:O	4:G:1:GLY:HA2	2.04	0.57
3:F:197:ARG:HB2	3:F:382:THR:HB	1.85	0.57
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.19	0.57
3:C:295:PHE:CE2	3:C:305:THR:HG21	2.39	0.57
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.03	0.57
3:C:307:HIS:CE1	3:C:342:GLY:H	2.23	0.57
1:D:177:ASP:O	1:D:181:GLN:HG3	2.04	0.56
1:A:188:VAL:CG2	2:B:167:VAL:HG21	2.35	0.56
3:C:200:GLY:HA2	7:C:408:HOH:O	2.05	0.56
3:F:200:GLY:HA2	7:F:408:HOH:O	2.05	0.56
2:B:282:GLY:O	2:B:283:LYS:HG2	2.05	0.56
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.05	0.56
3:C:361:ASN:N	3:C:361:ASN:HD22	2.03	0.56
1:D:169:LEU:H	2:E:189:GLN:NE2	2.04	0.56
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.06	0.56
3:F:322:PHE:HB2	3:F:338:LYS:HG3	1.88	0.56
3:C:101:LEU:H	3:C:101:LEU:CD1	2.19	0.56
3:C:172:LEU:H	3:C:172:LEU:CD2	2.10	0.56
2:B:345:TYR:CG	2:B:346:ARG:N	2.74	0.55
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.71	0.55
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.42	0.55
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.72	0.55
1:A:176:LYS:HB2	1:A:176:LYS:NZ	2.22	0.55
1:A:144:LEU:HD13	1:A:182:GLN:HG2	1.89	0.55
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.53	0.55
1:D:133:ILE:HD11	3:F:107:ILE:HG23	1.88	0.54
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.89	0.54
3:F:196:LYS:NZ	3:F:383:THR:HB	2.22	0.54
3:C:307:HIS:HD2	3:C:335:TRP:O	1.90	0.54
1:A:176:LYS:HB2	1:A:176:LYS:HZ3	1.73	0.54
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.88	0.54
3:C:96:TYR:CG	3:C:97:GLU:N	2.76	0.54
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.89	0.54
2:E:195:THR:HG22	2:E:196:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:365:ASN:HD22	3:F:365:ASN:N	2.03	0.53
3:C:305:THR:HB	3:C:341:ALA:HB2	1.91	0.53
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.08	0.53
1:A:136:LEU:HD21	3:C:111:GLN:HG2	1.91	0.53
1:D:140:VAL:HG23	1:D:141:ARG:N	2.24	0.53
1:D:140:VAL:HG23	1:D:141:ARG:H	1.74	0.53
2:E:337:LYS:HG2	2:E:382:ASN:ND2	2.24	0.53
2:E:171:ILE:HG13	2:E:172:LEU:N	2.24	0.53
5:K:1:NAG:C4	5:K:2:NAG:HN2	2.22	0.53
3:C:338:LYS:N	3:C:339:CYS:HA	2.23	0.52
3:F:172:LEU:H	3:F:172:LEU:HD22	1.75	0.52
3:F:307:HIS:CE1	3:F:341:ALA:H	2.26	0.52
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.23	0.52
2:B:253:GLN:HE22	2:B:451:SER:HA	1.75	0.52
2:B:432:ASP:OD2	2:B:443:SER:HB2	2.08	0.52
3:C:107:ILE:HD13	3:C:107:ILE:O	2.10	0.52
2:E:357:ALA:O	2:E:365:ARG:HG3	2.09	0.52
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.25	0.52
3:F:340:HIS:O	4:I:1:GLY:HA3	2.10	0.52
1:D:151:GLU:HG2	1:D:173:VAL:HG13	1.92	0.52
3:F:229:GLY:O	3:F:233:ILE:HG13	2.10	0.52
2:B:373:MET:HE2	2:B:404:TYR:O	2.10	0.51
1:A:175:LEU:HD22	1:A:175:LEU:H	1.76	0.51
5:L:1:NAG:H61	5:L:3:FUC:C3	2.40	0.51
2:B:432:ASP:N	2:B:432:ASP:OD1	2.43	0.51
2:B:410:ALA:C	2:B:412:PRO:HD3	2.31	0.51
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.92	0.51
5:L:1:NAG:C6	5:L:3:FUC:H5	2.36	0.51
1:D:144:LEU:HD13	1:D:182:GLN:HG2	1.93	0.51
3:F:352:GLY:O	3:F:377:TYR:HA	2.10	0.51
3:C:259:THR:HG22	3:C:260:ALA:N	2.26	0.51
2:E:436:VAL:HG12	2:E:437:TRP:N	2.25	0.51
1:D:178:TYR:O	1:D:182:GLN:HG3	2.11	0.51
2:E:415:ARG:HD3	7:E:484:HOH:O	2.11	0.51
1:A:181:GLN:NE2	2:B:171:ILE:HG23	2.27	0.50
3:C:243:PRO:HG2	7:C:435:HOH:O	2.11	0.50
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.93	0.50
2:B:361:MET:HB2	5:K:1:NAG:C8	2.41	0.50
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.93	0.50
2:B:163:THR:HG22	2:B:166:ARG:NH1	2.26	0.50
2:B:436:VAL:HG12	2:B:437:TRP:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:PHE:CE2	2:B:459:PRO:HG3	2.46	0.50
2:E:172:LEU:HB3	3:F:113:ILE:CD1	2.41	0.50
2:E:423:THR:H	2:E:426:MET:HE3	1.75	0.50
2:B:258:GLY:HA2	7:B:463:HOH:O	2.10	0.50
3:C:108:ARG:HA	3:C:111:GLN:NE2	2.27	0.50
3:F:108:ARG:O	3:F:111:GLN:HG2	2.12	0.50
3:F:389:PHE:O	3:F:391:ARG:N	2.45	0.50
2:E:253:GLN:NE2	2:E:451:SER:HA	2.27	0.50
3:F:249:GLU:O	3:F:250:LEU:HD13	2.12	0.50
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.94	0.49
3:C:365:ASN:HD22	3:C:365:ASN:H	1.60	0.49
2:E:436:VAL:CG1	2:E:437:TRP:N	2.74	0.49
3:F:389:PHE:C	3:F:391:ARG:N	2.66	0.49
2:B:167:VAL:O	2:B:170:SER:HB3	2.12	0.49
1:D:185:LEU:HD13	1:D:185:LEU:O	2.12	0.49
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.77	0.49
2:E:316:ASP:OD2	2:E:320:ASP:HB2	2.12	0.49
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.94	0.49
1:D:133:ILE:HD11	3:F:107:ILE:CG2	2.43	0.49
2:E:172:LEU:HD22	3:F:113:ILE:CD1	2.43	0.49
4:G:2:HIS:CD2	4:G:4:PRO:HD3	2.47	0.49
3:C:249:GLU:CB	3:C:383:THR:HG23	2.40	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.95	0.49
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.78	0.49
2:B:224:MET:CE	2:B:237:ARG:HD3	2.43	0.49
3:F:339:CYS:HB2	4:I:1:GLY:O	2.13	0.49
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.48	0.49
3:C:240:SER:O	3:C:242:ILE:HG13	2.12	0.49
1:A:175:LEU:HD22	1:A:175:LEU:N	2.29	0.48
3:C:107:ILE:O	3:C:111:GLN:HG3	2.14	0.48
3:C:361:ASN:N	3:C:361:ASN:ND2	2.60	0.48
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.28	0.48
3:C:263:ALA:HB1	3:C:264:MET:CE	2.44	0.48
5:L:1:NAG:C6	5:L:2:NAG:H2	2.43	0.48
2:B:280:THR:O	2:B:281:ASP:C	2.52	0.48
2:B:364:ASN:HD22	5:K:1:NAG:H82	1.79	0.48
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.48	0.48
2:B:326:TYR:HE1	2:B:354:MET:HE2	1.79	0.48
2:B:406:ARG:N	2:B:407:CYS:HA	2.26	0.48
3:C:297:ASP:HB3	4:G:2:HIS:NE2	2.28	0.48
3:C:325:ASN:C	3:C:325:ASN:ND2	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:HD22	1:D:175:LEU:N	2.29	0.48
3:F:151:LYS:HD3	3:F:172:LEU:CD2	2.44	0.48
5:K:1:NAG:H4	5:K:3:FUC:H5	1.95	0.48
3:F:375:ARG:HH22	4:I:2:HIS:CD2	2.31	0.48
3:C:321:LYS:O	3:C:338:LYS:HD3	2.14	0.48
3:F:127:LYS:HA	3:F:130:GLN:NE2	2.28	0.48
1:D:135:LEU:HD13	1:D:139:ASN:ND2	2.29	0.47
2:E:171:ILE:HG13	2:E:172:LEU:H	1.79	0.47
1:A:129:LYS:NZ	1:A:129:LYS:HB3	2.29	0.47
2:B:439:ASN:N	2:B:439:ASN:ND2	2.61	0.47
2:E:234:LYS:HD2	2:E:234:LYS:N	2.26	0.47
3:F:237:SER:HB2	3:F:266:LYS:HA	1.96	0.47
1:A:182:GLN:O	1:A:186:GLU:HG2	2.14	0.47
3:F:365:ASN:H	3:F:365:ASN:ND2	2.11	0.47
3:F:359:THR:HG21	3:F:363:TYR:O	2.14	0.47
3:C:317:ASN:HD22	3:C:317:ASN:C	2.18	0.47
3:F:196:LYS:HD2	3:F:383:THR:HB	1.96	0.47
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.30	0.47
3:C:322:PHE:CZ	4:G:3:ARG:HG2	2.50	0.47
3:F:155:ASP:O	3:F:159:LYS:HG3	2.15	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.97	0.47
2:E:411:ASN:N	2:E:412:PRO:HD3	2.29	0.47
2:E:439:ASN:N	2:E:439:ASN:ND2	2.61	0.47
2:B:351:ASN:HD21	2:B:354:MET:HB2	1.80	0.46
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.96	0.46
1:A:133:ILE:O	1:A:137:GLN:HG3	2.14	0.46
1:A:136:LEU:O	1:A:140:VAL:HG22	2.14	0.46
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.80	0.46
2:B:406:ARG:O	2:B:406:ARG:HG2	2.16	0.46
5:K:2:NAG:O3	5:K:2:NAG:C7	2.63	0.46
3:C:254:ASN:HB2	3:C:256:ARG:NH1	2.29	0.46
1:D:140:VAL:HG12	2:E:172:LEU:HD21	1.96	0.46
3:F:339:CYS:N	4:I:1:GLY:O	2.45	0.46
2:B:402:TRP:CG	2:B:403:TRP:N	2.83	0.46
3:F:295:PHE:HE2	3:F:305:THR:HG21	1.80	0.46
1:D:136:LEU:O	1:D:140:VAL:HG22	2.16	0.46
2:B:390:PRO:O	2:B:396:LYS:HE3	2.16	0.46
3:C:304:PHE:CD1	3:C:338:LYS:HE3	2.51	0.46
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.81	0.46
3:C:124:LEU:O	3:C:128:VAL:HG23	2.15	0.46
3:C:259:THR:CG2	3:C:260:ALA:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.98	0.45
1:A:151:GLU:OE2	2:B:182:LEU:HD21	2.16	0.45
2:E:172:LEU:HB3	3:F:113:ILE:HD13	1.97	0.45
3:F:365:ASN:N	3:F:365:ASN:ND2	2.64	0.45
3:C:101:LEU:N	3:C:101:LEU:CD1	2.79	0.45
3:C:185:ASP:OD2	3:C:189:ASN:HB2	2.15	0.45
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.29	0.45
1:D:181:GLN:HE22	2:E:174:ASN:HD21	1.64	0.45
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.97	0.45
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.99	0.45
2:B:395:SER:HA	2:B:404:TYR:CE2	2.51	0.45
1:D:135:LEU:HD13	1:D:135:LEU:C	2.37	0.45
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.32	0.45
2:E:233:VAL:HG22	2:E:234:LYS:HD2	1.99	0.45
1:A:153:ASP:O	1:A:157:LYS:HG2	2.16	0.45
1:D:139:ASN:O	1:D:142:ALA:HB3	2.15	0.45
1:A:127:ILE:HG12	1:A:130:VAL:CG2	2.40	0.45
2:E:281:ASP:OD2	2:E:281:ASP:N	2.50	0.45
5:L:1:NAG:H62	5:L:2:NAG:H2	1.98	0.45
2:B:169:ARG:O	2:B:173:GLU:HG3	2.17	0.45
3:C:196:LYS:O	3:C:197:ARG:HD2	2.17	0.45
3:C:354:TYR:CE1	3:C:376:TRP:HA	2.51	0.45
3:F:268:GLY:O	3:F:274:TYR:HA	2.17	0.45
2:B:161:ILE:N	2:B:162:PRO:HD2	2.32	0.44
2:E:207:SER:HB3	7:F:461:HOH:O	2.16	0.44
3:C:340:HIS:N	4:G:1:GLY:O	2.45	0.44
1:A:127:ILE:HD11	1:A:129:LYS:HG2	1.99	0.44
2:B:411:ASN:N	2:B:412:PRO:HD3	2.33	0.44
1:D:141:ARG:O	1:D:145:VAL:HG23	2.17	0.44
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.52	0.44
2:B:177:SER:O	2:B:180:GLN:HB3	2.17	0.44
3:F:325:ASN:C	3:F:325:ASN:ND2	2.66	0.44
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.99	0.44
2:B:351:ASN:C	2:B:351:ASN:ND2	2.71	0.44
3:F:329:GLN:OE1	4:I:3:ARG:HD3	2.18	0.44
3:F:393:THR:HG22	3:F:393:THR:O	2.18	0.44
1:A:188:VAL:C	1:A:190:ALA:H	2.21	0.44
3:C:248:VAL:HG12	3:C:250:LEU:CD2	2.48	0.44
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.53	0.43
3:F:196:LYS:HZ2	3:F:383:THR:CG2	2.32	0.43
3:C:194:PHE:CD1	3:C:194:PHE:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:TYR:O	3:C:376:TRP:HB3	2.18	0.43
3:F:263:ALA:HB1	3:F:264:MET:CE	2.48	0.43
3:F:375:ARG:NH2	4:I:2:HIS:CD2	2.86	0.43
3:C:167:TYR:O	3:C:179:LEU:HD12	2.18	0.43
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.17	0.43
2:E:332:GLN:O	2:E:338:TYR:HA	2.19	0.43
2:E:169:ARG:HH12	3:F:109:TYR:HE2	1.61	0.43
2:E:173:GLU:HG2	2:E:176:ARG:NH2	2.33	0.43
3:F:172:LEU:CD2	3:F:239:GLN:NE2	2.81	0.43
3:F:231:GLU:O	3:F:235:LEU:HG	2.18	0.43
1:A:129:LYS:HE3	3:C:100:ILE:CG2	2.49	0.43
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.01	0.43
3:F:374:THR:HG22	3:F:376:TRP:H	1.83	0.43
2:B:351:ASN:ND2	2:B:351:ASN:O	2.51	0.43
7:B:506:HOH:O	3:C:138:PRO:HG3	2.18	0.43
2:E:253:GLN:HE21	2:E:253:GLN:C	2.23	0.42
3:F:297:ASP:HB3	4:I:2:HIS:CE1	2.54	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.87	0.42
2:B:315:GLU:HB3	2:B:449:LYS:HB2	2.00	0.42
3:F:109:TYR:C	3:F:111:GLN:H	2.22	0.42
3:F:298:ASP:HA	3:F:299:PRO:HD3	1.89	0.42
2:B:162:PRO:C	2:B:164:ASN:N	2.72	0.42
2:B:163:THR:HA	2:B:166:ARG:CD	2.47	0.42
2:B:212:GLU:O	2:B:215:ILE:HG22	2.19	0.42
3:C:173:LYS:HB2	3:C:173:LYS:HE3	1.80	0.42
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.54	0.42
3:C:250:LEU:HD22	3:C:250:LEU:N	2.35	0.42
3:C:365:ASN:H	3:C:365:ASN:ND2	2.17	0.42
1:A:140:VAL:HG23	1:A:141:ARG:N	2.34	0.42
2:B:315:GLU:HA	2:B:320:ASP:O	2.20	0.42
2:B:345:TYR:O	2:B:346:ARG:HB3	2.20	0.42
3:F:340:HIS:CE1	4:I:1:GLY:HA2	2.54	0.42
3:F:172:LEU:HD22	3:F:239:GLN:NE2	2.34	0.42
3:F:251:GLU:HG3	3:F:257:THR:HG22	2.00	0.42
2:E:422:TYR:HA	2:E:426:MET:CE	2.49	0.42
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.85	0.41
3:F:387:ILE:HG12	3:F:388:PRO:HD2	2.01	0.41
2:B:453:LYS:HG3	7:B:467:HOH:O	2.19	0.41
1:D:165:CYS:HB3	2:E:193:CYS:HA	2.03	0.41
2:E:166:ARG:O	2:E:168:LEU:N	2.53	0.41
2:E:224:MET:HG2	2:E:225:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.55	0.41
1:D:134:GLN:O	1:D:138:LYS:HE2	2.19	0.41
2:B:398:ASP:HA	2:B:433:ASP:HB3	2.02	0.41
3:C:172:LEU:CD2	3:C:239:GLN:HE21	2.33	0.41
1:D:149:ARG:HH21	2:E:425:ASP:HA	1.83	0.41
2:E:402:TRP:CG	2:E:403:TRP:N	2.89	0.41
3:F:364:ASP:OD1	3:F:375:ARG:HB2	2.20	0.41
2:B:431:THR:HG21	4:H:3:ARG:NH2	2.36	0.41
3:F:113:ILE:HD12	3:F:113:ILE:C	2.39	0.41
1:A:169:LEU:N	2:B:189:GLN:HE22	2.14	0.41
3:C:263:ALA:HB1	3:C:264:MET:HE1	2.03	0.41
3:C:372:TRP:C	3:C:373:LYS:HG2	2.41	0.41
2:E:376:SER:O	2:E:401:GLY:HA2	2.21	0.41
3:F:104:ASP:O	3:F:108:ARG:HG3	2.19	0.41
3:F:198:LEU:HD12	3:F:199:ASP:N	2.36	0.41
3:F:239:GLN:O	3:F:240:SER:C	2.58	0.41
1:A:136:LEU:O	1:A:140:VAL:HG13	2.21	0.41
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.53	0.41
3:F:359:THR:OG1	3:F:362:GLY:HA2	2.21	0.41
3:C:343:HIS:O	3:C:367:ILE:HA	2.20	0.41
2:E:172:LEU:HD22	3:F:113:ILE:HD11	2.03	0.41
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.84	0.41
3:F:122:VAL:O	3:F:126:GLU:HG3	2.21	0.41
3:F:295:PHE:CE2	3:F:305:THR:HG21	2.55	0.41
1:A:127:ILE:N	1:A:130:VAL:HB	2.36	0.40
3:C:295:PHE:CD1	3:C:375:ARG:HD2	2.56	0.40
2:B:340:ILE:HG12	2:B:341:SER:N	2.36	0.40
2:B:436:VAL:CG1	2:B:437:TRP:N	2.83	0.40
1:D:181:GLN:HE22	2:E:174:ASN:ND2	2.19	0.40
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.56	0.40
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.51	0.40
3:C:96:TYR:O	3:C:97:GLU:HB2	2.20	0.40
3:C:277:THR:HA	3:C:308:ASN:OD1	2.22	0.40
1:A:189:ILE:HG22	1:A:189:ILE:O	2.22	0.40
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.96	0.40
2:E:267:ASP:HB3	2:E:268:PRO:HD3	2.03	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	62/66 (94%)	54 (87%)	7 (11%)	1 (2%)	9	16
1	D	54/66 (82%)	51 (94%)	3 (6%)	0	100	100
2	B	297/313 (95%)	266 (90%)	28 (9%)	3 (1%)	15	27
2	E	293/313 (94%)	269 (92%)	18 (6%)	6 (2%)	7	11
3	C	296/311 (95%)	273 (92%)	20 (7%)	3 (1%)	15	27
3	F	289/311 (93%)	264 (91%)	21 (7%)	4 (1%)	11	19
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%)	2 (100%)	0	0	100	100
All	All	1299/1396 (93%)	1185 (91%)	97 (8%)	17 (1%)	12	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	97	GLU
2	E	170	SER
2	E	281	ASP
2	B	281	ASP
3	C	198	LEU
3	F	241	ALA
3	F	360	PRO
3	F	390	ASN
2	E	167	VAL
2	B	256	GLN
3	C	370	ALA
2	E	256	GLN
3	F	338	LYS
2	E	171	ILE

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Mol	Chain	Res	Type
2	B	399	GLY
1	A	130	VAL
2	E	247	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/61 (97%)	55 (93%)	4 (7%)	16	29
1	D	52/61 (85%)	48 (92%)	4 (8%)	13	23
2	B	257/271 (95%)	251 (98%)	6 (2%)	50	74
2	E	253/271 (93%)	242 (96%)	11 (4%)	29	50
3	C	250/258 (97%)	237 (95%)	13 (5%)	23	41
3	F	244/258 (95%)	236 (97%)	8 (3%)	38	62
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1127/1192 (94%)	1079 (96%)	48 (4%)	29	50

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

Mol	Chain	Res	Type
1	A	129	LYS
1	A	169	LEU
1	A	176	LYS
1	A	185	LEU
2	B	196	PRO
2	B	210	GLU
2	B	253	GLN
2	B	301	GLN
2	B	351	ASN
2	B	439	ASN

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Mol	Chain	Res	Type
3	C	107	ILE
3	C	118	ASN
3	C	143	VAL
3	C	163	GLN
3	C	172	LEU
3	C	198	LEU
3	C	244	TYR
3	C	298	ASP
3	C	317	ASN
3	C	325	ASN
3	C	330	ASP
3	C	365	ASN
3	C	383	THR
1	D	134	GLN
1	D	180	ASP
1	D	185	LEU
1	D	187	GLN
2	E	190	MET
2	E	195	THR
2	E	210	GLU
2	E	234	LYS
2	E	253	GLN
2	E	280	THR
2	E	281	ASP
2	E	301	GLN
2	E	351	ASN
2	E	359	GLN
2	E	439	ASN
3	F	112	GLU
3	F	118	ASN
3	F	264	MET
3	F	317	ASN
3	F	325	ASN
3	F	361	ASN
3	F	365	ASN
3	F	383	THR
4	G	3	ARG
4	I	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	139	ASN
1	A	187	GLN
2	B	164	ASN
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	339	GLN
2	B	351	ASN
2	B	359	GLN
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	118	ASN
3	C	119	GLN
3	C	134	GLN
3	C	163	GLN
3	C	177	GLN
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	361	ASN
3	C	365	ASN
1	D	134	GLN
1	D	139	ASN
1	D	181	GLN
1	D	184	GLN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	243	ASN
2	E	253	GLN
2	E	271	GLN

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Mol	Chain	Res	Type
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	103	HIS
3	F	111	GLN
3	F	117	ASN
3	F	119	GLN
3	F	123	ASN
3	F	130	GLN
3	F	176	GLN
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	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	0.67	0	17,19,21	0.92	1 (5%)
5	NAG	K	2	5	14,14,15	0.55	0	17,19,21	0.59	0
5	FUC	K	3	5	10,10,11	0.55	0	14,14,16	0.41	0
5	NAG	L	1	2,5	14,14,15	0.63	0	17,19,21	1.18	2 (11%)
5	NAG	L	2	5	14,14,15	0.48	0	17,19,21	0.65	0
5	FUC	L	3	5	10,10,11	0.58	0	14,14,16	0.76	1 (7%)

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	-	4/6/23/26	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	-	3/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	1	NAG	C2-N2-C7	-2.63	119.15	122.90
5	L	1	NAG	C4-C3-C2	2.34	114.44	111.02
5	L	1	NAG	C3-C4-C5	2.06	113.92	110.24
5	L	3	FUC	C1-C2-C3	2.04	112.17	109.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
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	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6

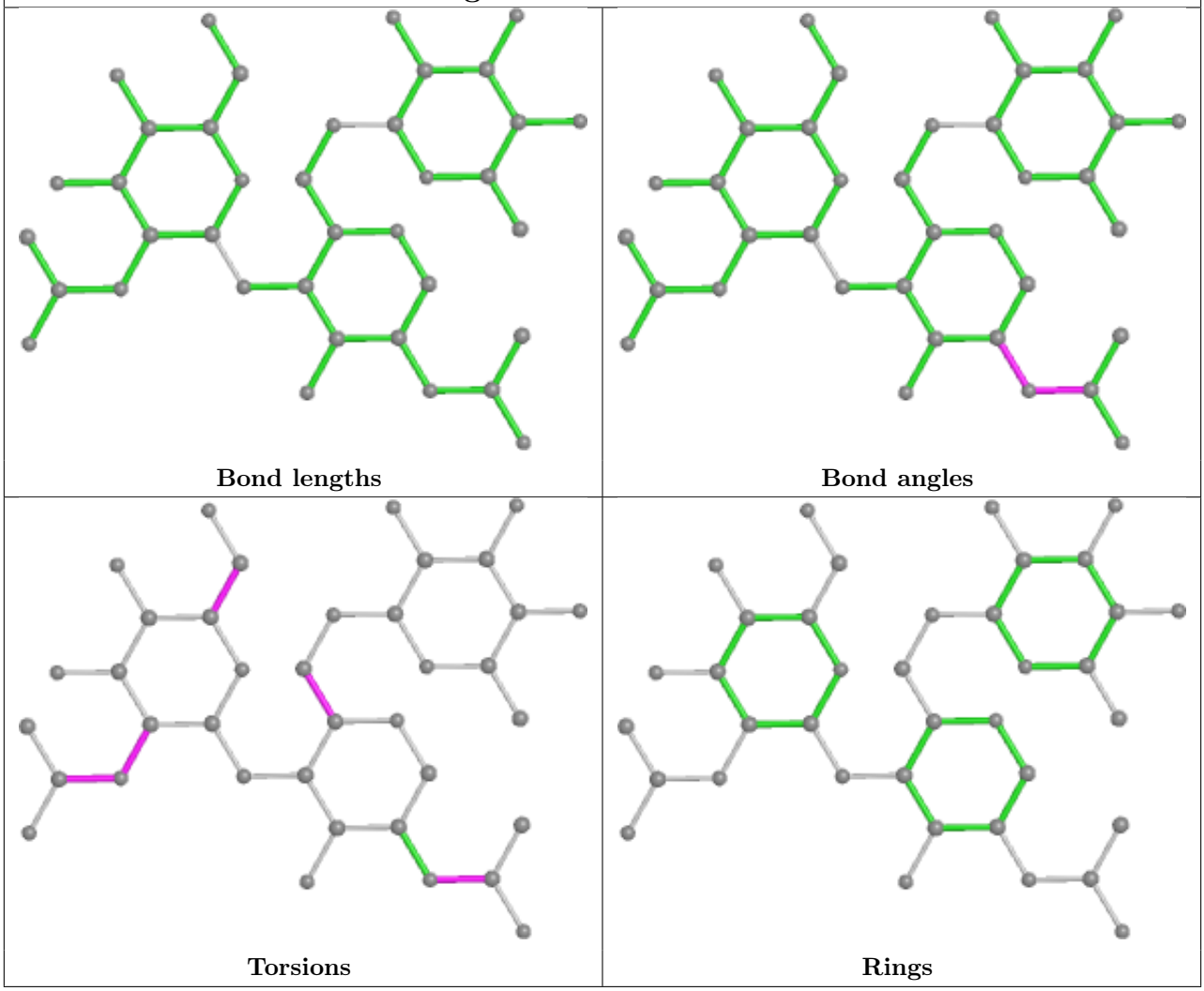
There are no ring outliers.

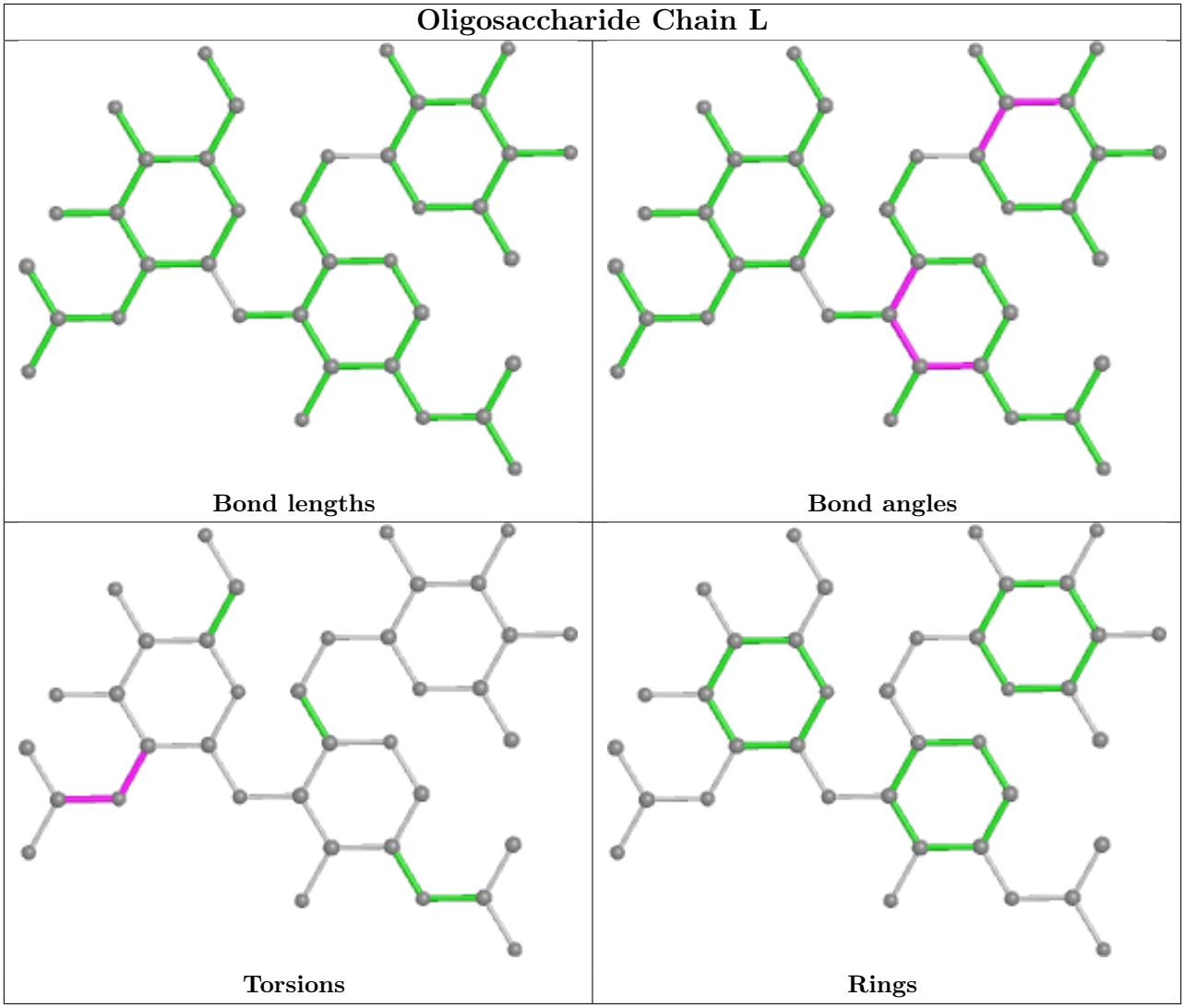
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	3	0
5	K	3	FUC	1	0
5	L	2	NAG	2	0
5	K	1	NAG	6	0
5	L	1	NAG	7	0
5	L	3	FUC	5	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





5.6 Ligand geometry (i)

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 (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	64/66 (96%)	0.95	15 (23%)	0	0	21, 55, 95, 100	0
1	D	56/66 (84%)	0.98	19 (33%)	0	0	20, 55, 109, 113	0
2	B	299/313 (95%)	0.35	20 (6%)	17	18	16, 33, 62, 94	0
2	E	295/313 (94%)	0.18	10 (3%)	45	49	10, 23, 57, 98	0
3	C	298/311 (95%)	0.62	31 (10%)	6	6	20, 39, 84, 101	0
3	F	291/311 (93%)	0.48	24 (8%)	11	12	10, 31, 70, 121	0
4	G	4/4 (100%)	2.76	3 (75%)	0	0	90, 93, 94, 95	0
4	H	4/4 (100%)	1.09	1 (25%)	0	0	50, 55, 55, 58	0
4	I	4/4 (100%)	2.95	2 (50%)	0	0	73, 75, 77, 82	0
4	J	4/4 (100%)	0.11	0	100	100	28, 29, 31, 40	0
All	All	1319/1396 (94%)	0.47	125 (9%)	8	8	10, 33, 87, 121	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	106	SER	7.8
4	I	4	PRO	6.3
3	F	107	ILE	6.2
3	F	393	THR	5.8
3	C	360	PRO	5.6
3	C	362	GLY	5.6
3	F	105	SER	5.4
2	B	281	ASP	5.3
3	F	104	ASP	5.2
3	C	100	ILE	5.2
1	D	187	GLN	5.1
2	B	459	PRO	5.0
1	A	130	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
3	C	96	TYR	4.8
2	E	459	PRO	4.8
2	E	458	PHE	4.5
3	F	108	ARG	4.5
4	G	4	PRO	4.5
3	C	392	LEU	4.4
3	F	109	TYR	4.3
3	C	241	ALA	4.2
3	F	103	HIS	4.1
3	F	362	GLY	4.1
3	C	101	LEU	4.1
3	F	361	ASN	4.0
2	B	162	PRO	4.0
1	D	185	LEU	3.9
3	C	361	ASN	4.0
2	B	458	PHE	3.7
3	C	105	SER	3.7
1	A	128	GLU	3.7
3	F	112	GLU	3.7
2	B	388	SER	3.7
3	C	107	ILE	3.7
3	C	297	ASP	3.7
1	D	140	VAL	3.6
1	A	131	GLN	3.5
3	C	108	ARG	3.5
2	B	164	ASN	3.5
1	D	135	LEU	3.5
1	A	129	LYS	3.4
3	F	363	TYR	3.4
4	G	1	GLY	3.4
2	E	167	VAL	3.3
3	F	296	GLY	3.3
2	B	282	GLY	3.3
1	D	184	GLN	3.2
1	A	127	ILE	3.2
2	E	168	LEU	3.2
1	A	189	ILE	3.2
1	D	133	ILE	3.1
1	A	133	ILE	3.1
3	C	242	ILE	3.1
3	C	359	THR	3.1
3	C	99	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	281	ASP	3.0
3	F	360	PRO	3.0
1	A	140	VAL	3.0
1	A	183	LYS	3.0
2	E	282	GLY	3.0
2	B	389	ASP	3.0
3	C	240	SER	3.0
3	F	254	ASN	2.9
3	F	297	ASP	2.9
4	I	2	HIS	2.9
1	D	138	LYS	2.9
2	E	170	SER	2.9
2	B	387	THR	2.8
1	A	190	ALA	2.8
3	C	389	PHE	2.8
1	D	175	LEU	2.8
2	B	361	MET	2.8
2	B	233	VAL	2.7
3	C	363	TYR	2.7
1	D	186	GLU	2.7
1	D	137	GLN	2.7
2	B	163	THR	2.7
3	C	98	ALA	2.6
1	A	134	GLN	2.6
2	B	166	ARG	2.6
2	E	280	THR	2.6
3	C	97	GLU	2.5
2	B	280	THR	2.5
1	D	136	LEU	2.5
3	F	256	ARG	2.5
1	D	188	VAL	2.5
1	D	180	ASP	2.5
3	C	109	TYR	2.4
3	C	104	ASP	2.4
2	E	284	ASN	2.4
1	D	179	GLU	2.4
2	B	391	ARG	2.4
4	G	2	HIS	2.4
3	C	357	ALA	2.4
1	D	176	LYS	2.4
1	A	132	HIS	2.3
3	C	103	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	134	GLN	2.3
2	B	435	VAL	2.3
3	F	384	MET	2.3
3	C	112	GLU	2.2
3	C	323	GLU	2.2
3	C	102	THR	2.2
2	B	399	GLY	2.2
3	C	393	THR	2.2
1	D	182	GLN	2.2
1	D	178	TYR	2.2
3	C	256	ARG	2.2
1	A	188	VAL	2.1
3	F	359	THR	2.1
3	C	384	MET	2.1
2	E	435	VAL	2.1
2	B	413	ASN	2.1
4	H	4	PRO	2.1
3	F	113	ILE	2.1
1	D	174	ASP	2.1
3	C	253	TRP	2.1
1	A	177	ASP	2.0
3	F	115	ASN	2.0
3	F	240	SER	2.0
1	A	187	GLN	2.0
2	B	386	LEU	2.0
2	B	412	PRO	2.0
3	F	111	GLN	2.0
3	F	130	GLN	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)

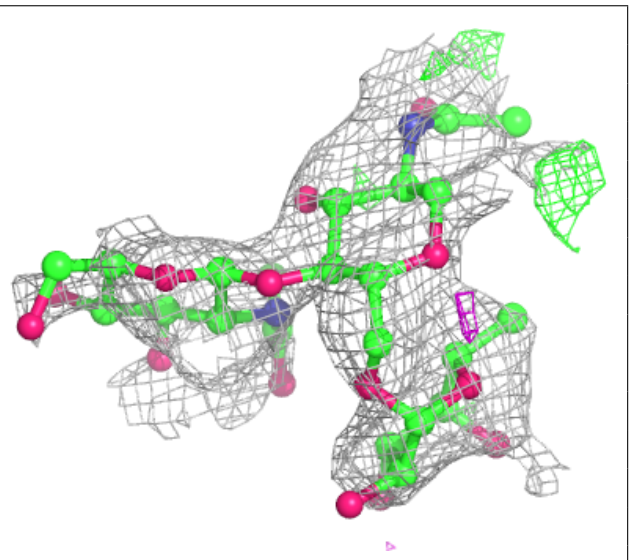
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

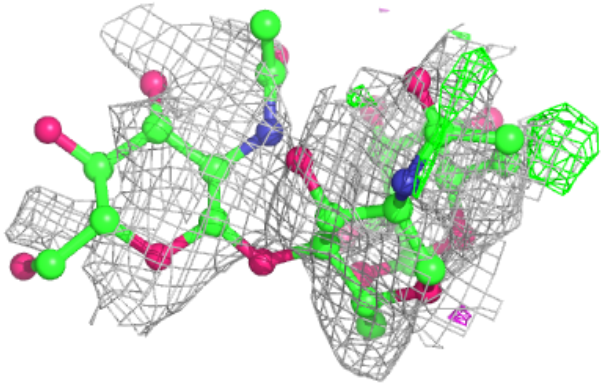
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	K	1	14/15	0.56	0.40	79,82,87,91	0
5	NAG	K	2	14/15	0.65	0.56	95,98,100,100	0
5	FUC	K	3	10/11	0.75	0.43	87,88,88,89	0
5	NAG	L	2	14/15	0.75	0.45	66,68,70,70	0
5	FUC	L	3	10/11	0.80	0.37	63,63,64,64	0
5	NAG	L	1	14/15	0.82	0.26	48,54,61,63	0

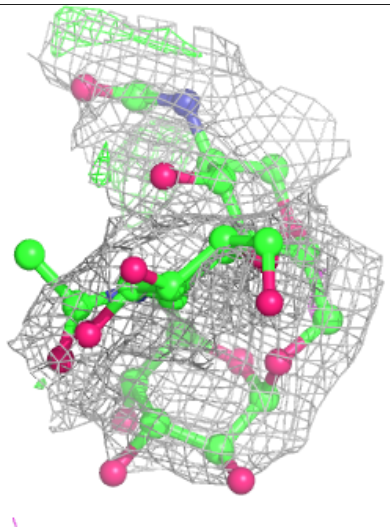
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

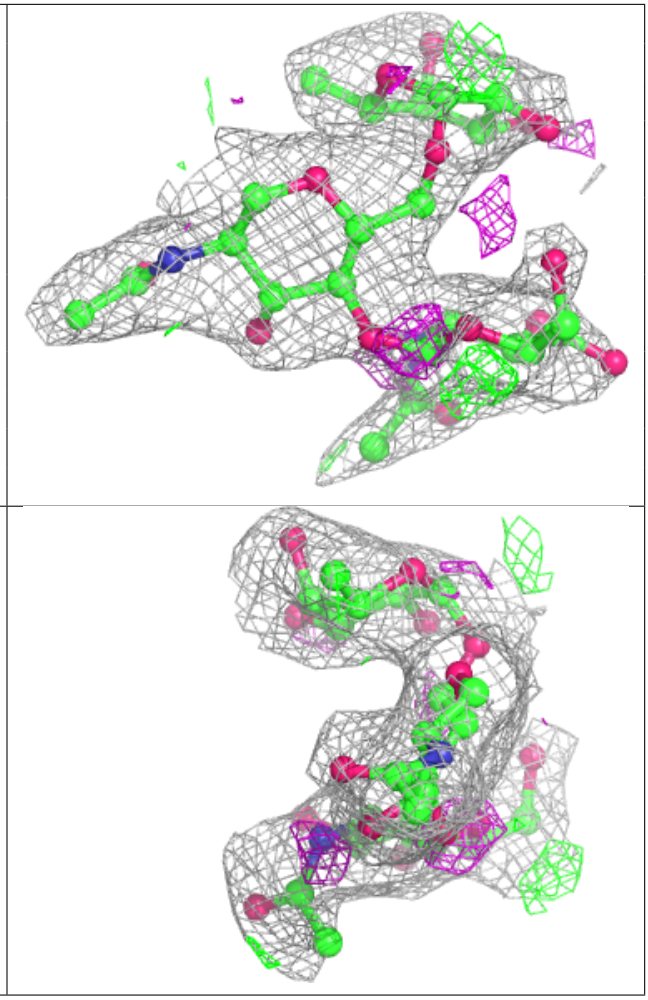






Electron density around Chain L:

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



6.4 Ligands (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
6	CA	C	407	1/1	0.94	0.12	37,37,37,37	0
6	CA	B	462	1/1	0.96	0.05	47,47,47,47	0
6	CA	F	407	1/1	0.96	0.05	29,29,29,29	0
6	CA	E	462	1/1	0.98	0.06	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.