Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:49 AM EDT

PDB ID	:	2FFD
Title	:	Fibrinogen Fragment D with "A" knob peptide mimic GPRVVE
Authors	:	Betts, L.
Deposited on	:	2005-12-19
Resolution	:	2.89 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:

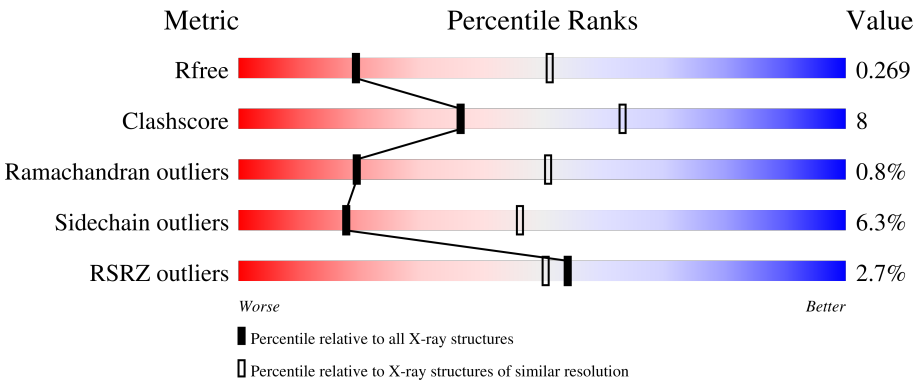
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	3%, 76%, 21%, • •
1	D	66	11%, 71%, 14%, •, 14%
2	B	313	2%, 78%, 17%, • •
2	E	313	2%, 72%, 19%, •, 6%
3	C	311	%, 77%, 17%, • •

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Mol	Chain	Length	Quality of chain
3	F	311	3% 73% 16% • 8%
4	G	6	33% 33% 33%
4	H	6	50% 17% 33%
4	I	6	33% 17% 17% 33%
4	J	6	50% 17% 33%
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	2	-	-	-	X
5	FUC	L	3	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10894 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	65	530	327	100	100	3	0	0	0
1	D	57	466	286	88	89	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	303	2428	1515	429	462	22	0	0	0
2	E	295	2369	1480	418	449	22	0	0	0

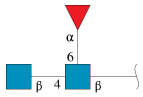
- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	298	2391	1517	402	461	11	0	0	0
3	F	285	2283	1450	384	438	11	0	0	0

- Molecule 4 is a protein called GLY-PRO-ARG-VAL-VAL-GLU peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	4	29	18	7	4	0	0	0
4	H	4	29	18	7	4	0	0	0
4	I	4	29	18	7	4	0	0	0
4	J	4	29	18	7	4	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	10	10	10	0	0
7	B	57	57	57	0	0
7	C	26	26	26	0	0
7	D	6	6	6	0	0
7	E	76	76	76	0	0
7	F	52	52	52	0	0
7	H	1	1	1	0	0
7	I	2	2	2	0	0

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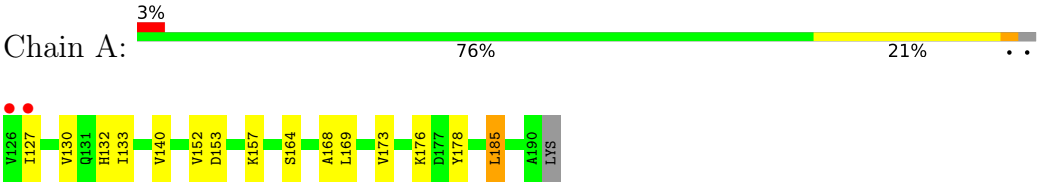
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	J	1	1	1	0	0

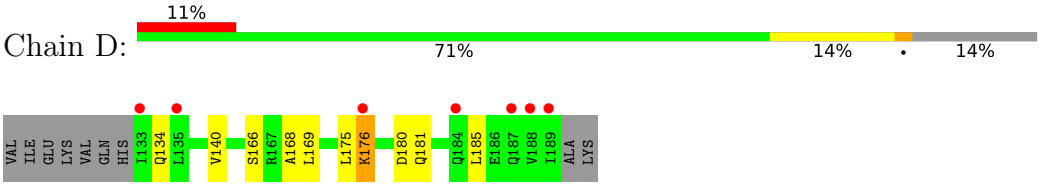
3 Residue-property plots (i)

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.

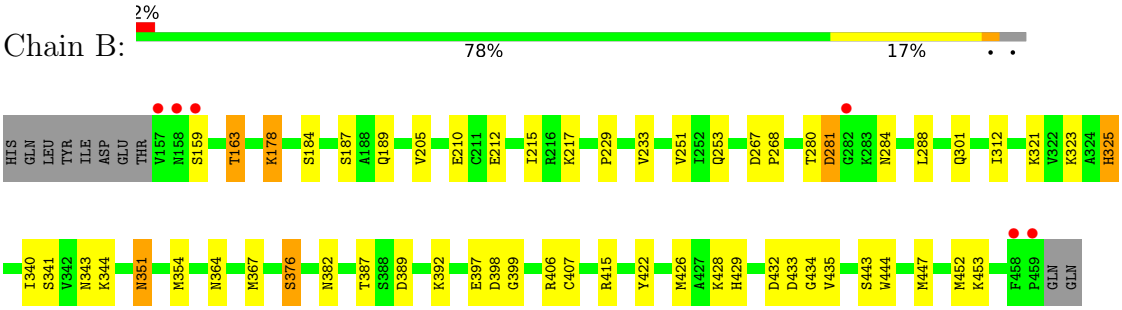
• Molecule 1: Fibrinogen alpha/alpha-E Chain



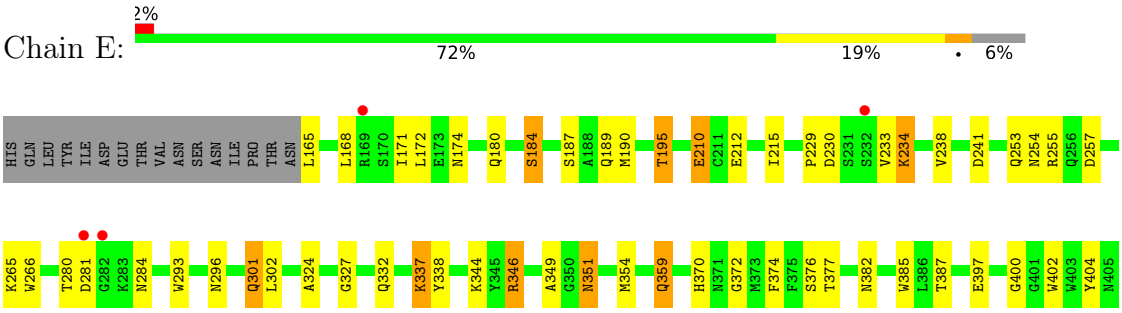
• Molecule 1: Fibrinogen alpha/alpha-E Chain



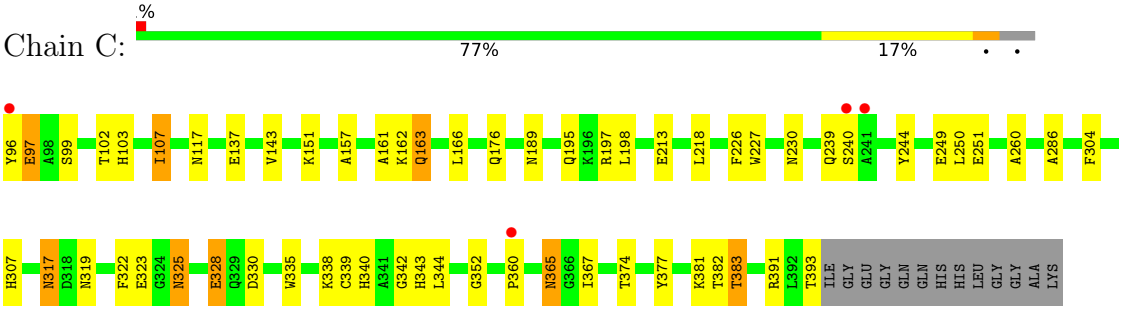
• Molecule 2: Fibrinogen beta chain



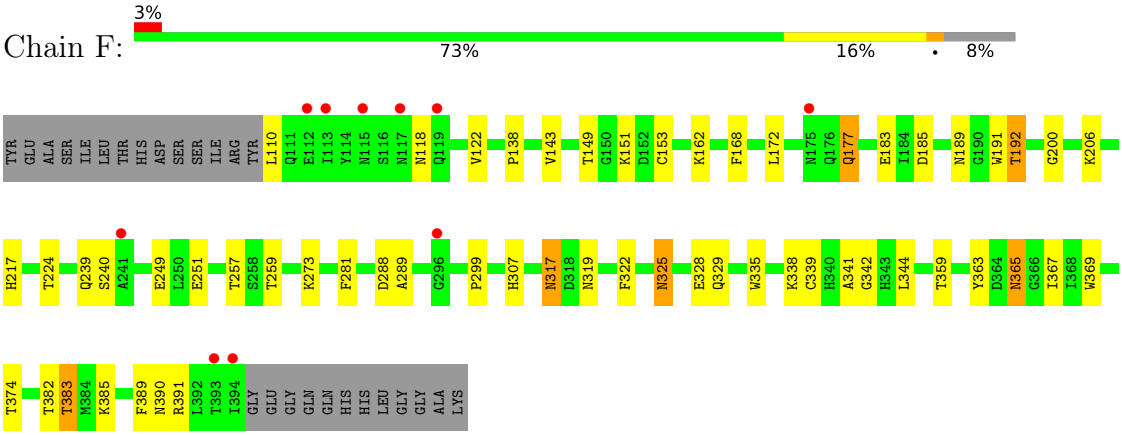
• Molecule 2: Fibrinogen beta chain



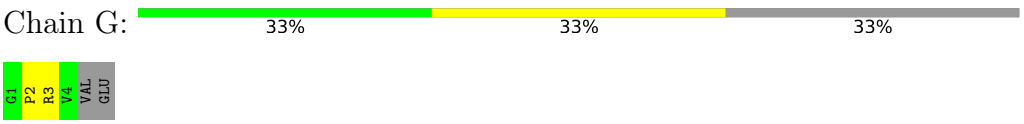
• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain

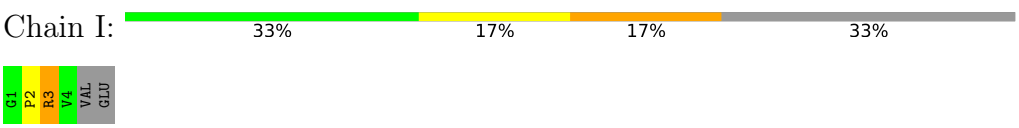


• Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



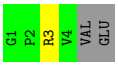
• Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide

• Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



• Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU 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	89.52Å 94.65Å 227.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.89 17.86 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.89) 98.2 (17.86-2.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.87Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.268 0.215 , 0.269	Depositor DCC
R_{free} test set	2160 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10894	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.26% 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: 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	0.39	0/531	0.54	0/709
1	D	0.38	0/466	0.59	0/621
2	B	0.42	0/2490	0.56	0/3364
2	E	0.44	0/2430	0.60	0/3280
3	C	0.40	0/2457	0.51	0/3324
3	F	0.44	0/2346	0.55	0/3173
4	G	0.65	0/29	0.53	0/38
4	H	0.66	0/29	0.61	0/38
4	I	0.73	0/29	0.69	0/38
4	J	0.52	0/29	0.46	0/38
All	All	0.42	0/10836	0.56	0/14623

There are no bond length outliers.

There are no bond angle outliers.

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	530	0	556	12	0
1	D	466	0	488	7	0
2	B	2428	0	2295	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2369	0	2238	46	0
3	C	2391	0	2235	35	0
3	F	2283	0	2138	41	0
4	G	29	0	34	0	0
4	H	29	0	34	5	0
4	I	29	0	34	2	0
4	J	29	0	34	2	0
5	K	38	0	34	2	0
5	L	38	0	34	4	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	10	0	0	0	0
7	B	57	0	0	0	0
7	C	26	0	0	0	0
7	D	6	0	0	0	0
7	E	76	0	0	2	0
7	F	52	0	0	4	0
7	H	1	0	0	0	0
7	I	2	0	0	0	0
7	J	1	0	0	1	0
All	All	10894	0	10154	164	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 8.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ASN:OD1	2:B:344:LYS:HE3	1.70	0.92
3:F:153:CYS:SG	3:F:192:THR:HB	2.16	0.85
2:E:359:GLN:HE21	2:E:359:GLN:H	1.22	0.83
1:A:169:LEU:H	2:B:189:GLN:HE22	1.31	0.78
1:A:164:SER:HB3	3:C:137:GLU:O	1.85	0.76
2:B:351:ASN:HD21	2:B:354:MET:HG3	1.53	0.72
3:C:307:HIS:HD2	3:C:335:TRP:O	1.73	0.70
2:E:359:GLN:H	2:E:359:GLN:NE2	1.89	0.70
2:B:397:GLU:OE1	4:J:3:ARG:NH1	2.26	0.68
3:C:304:PHE:HB3	3:C:338:LYS:HB3	1.77	0.67
1:A:169:LEU:H	2:B:189:GLN:NE2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:307:HIS:HE1	3:F:341:ALA:H	1.44	0.65
2:E:415:ARG:O	2:E:434:GLY:HA2	1.98	0.64
3:F:189:ASN:HD22	3:F:391:ARG:HG3	1.63	0.64
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.33	0.64
3:F:325:ASN:HD22	3:F:325:ASN:C	2.01	0.63
3:F:307:HIS:HD2	3:F:335:TRP:O	1.82	0.63
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.80	0.62
3:C:197:ARG:HB2	3:C:382:THR:HB	1.83	0.61
3:C:322:PHE:HB2	3:C:338:LYS:HG3	1.81	0.61
1:A:153:ASP:O	1:A:157:LYS:HG2	2.00	0.60
5:L:1:NAG:H61	5:L:3:FUC:H3	1.81	0.60
3:F:149:THR:HG22	3:F:168:PHE:O	2.02	0.60
2:B:376:SER:HB3	2:B:382:ASN:H	1.67	0.59
2:B:415:ARG:O	2:B:434:GLY:HA2	2.00	0.59
3:C:189:ASN:ND2	3:C:391:ARG:HE	1.99	0.59
3:F:249:GLU:HG3	3:F:259:THR:HG22	1.83	0.59
1:D:169:LEU:H	2:E:189:GLN:HE22	1.49	0.59
3:F:359:THR:HG21	3:F:363:TYR:O	2.02	0.59
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.85	0.58
2:E:431:THR:HG21	4:H:3:ARG:NH1	2.18	0.58
2:B:280:THR:O	2:B:281:ASP:HB3	2.02	0.58
3:F:365:ASN:HD22	3:F:365:ASN:H	1.51	0.58
2:E:439:ASN:HD22	2:E:439:ASN:H	1.53	0.57
2:E:397:GLU:OE1	4:H:3:ARG:NH1	2.37	0.56
3:F:307:HIS:CE1	3:F:341:ALA:H	2.22	0.56
1:D:176:LYS:HD2	1:D:180:ASP:OD2	2.05	0.56
2:E:241:ASP:OD2	2:E:453:LYS:HE2	2.05	0.56
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.87	0.56
2:E:337:LYS:HG2	2:E:382:ASN:ND2	2.21	0.56
4:J:3:ARG:NH2	7:J:19:HOH:O	2.39	0.56
2:B:312:ILE:HG12	2:B:452:MET:HG2	1.87	0.55
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.89	0.55
3:F:239:GLN:HA	7:F:606:HOH:O	2.07	0.54
1:D:140:VAL:HG11	2:E:172:LEU:HD12	1.87	0.54
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.90	0.54
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.90	0.53
1:D:166:SER:HB3	2:E:195:THR:HB	1.91	0.53
3:F:338:LYS:N	3:F:339:CYS:HA	2.24	0.53
2:E:406:ARG:HG3	2:E:406:ARG:O	2.09	0.53
2:B:217:LYS:HG2	3:C:213:GLU:HG3	1.90	0.53
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.74	0.52
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.42	0.52
2:E:212:GLU:O	2:E:215:ILE:HG22	2.09	0.52
2:E:400:GLY:O	2:E:404:TYR:HE2	1.91	0.52
3:C:307:HIS:HE1	3:C:342:GLY:H	1.58	0.52
3:C:317:ASN:ND2	3:C:319:ASN:OD1	2.42	0.52
3:C:325:ASN:HB3	3:C:328:GLU:HB3	1.93	0.51
2:E:351:ASN:HD21	2:E:354:MET:HG3	1.76	0.51
3:F:325:ASN:ND2	3:F:328:GLU:H	2.08	0.51
2:B:159:SER:O	2:B:163:THR:HB	2.11	0.51
2:B:435:VAL:O	2:B:447:MET:HG2	2.11	0.51
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.76	0.51
2:B:217:LYS:HE3	3:C:213:GLU:CD	2.31	0.51
2:E:265:LYS:HB3	7:E:606:HOH:O	2.11	0.51
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.76	0.50
1:D:169:LEU:H	2:E:189:GLN:NE2	2.09	0.50
2:E:406:ARG:N	2:E:407:CYS:HA	2.26	0.50
3:F:200:GLY:HA2	7:F:604:HOH:O	2.11	0.50
2:B:323:LYS:NZ	2:B:325:HIS:HD2	2.10	0.50
2:E:346:ARG:O	2:E:346:ARG:HG2	2.12	0.50
2:B:340:ILE:HG12	2:B:341:SER:N	2.27	0.50
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.30	0.49
2:E:423:THR:O	2:E:426:MET:HB2	2.12	0.49
3:F:389:PHE:C	3:F:391:ARG:H	2.15	0.49
2:B:351:ASN:C	2:B:351:ASN:HD22	2.16	0.49
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.94	0.49
2:B:432:ASP:OD2	2:B:443:SER:OG	2.31	0.49
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.78	0.49
2:E:180:GLN:O	2:E:184:SER:HB2	2.13	0.48
2:B:389:ASP:HB3	2:B:392:LYS:HD2	1.95	0.48
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.60	0.48
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.26	0.48
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.95	0.48
1:A:169:LEU:N	2:B:189:GLN:HE22	2.07	0.48
3:C:103:HIS:O	3:C:107:ILE:HB	2.14	0.47
2:E:332:GLN:O	2:E:338:TYR:HA	2.14	0.47
3:C:338:LYS:N	3:C:339:CYS:HA	2.29	0.47
1:D:181:GLN:HE22	2:E:174:ASN:ND2	2.13	0.47
5:L:1:NAG:H62	5:L:3:FUC:O2	2.14	0.47
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.97	0.47
2:E:372:GLY:HA2	7:E:661:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:415:ARG:N	2:E:434:GLY:HA2	2.30	0.47
3:F:307:HIS:HE1	3:F:342:GLY:H	1.62	0.47
3:F:149:THR:HG23	7:F:636:HOH:O	2.14	0.47
2:B:280:THR:HG22	2:B:288:LEU:HG	1.97	0.46
3:F:251:GLU:HB2	3:F:257:THR:HG22	1.95	0.46
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.98	0.46
1:A:132:HIS:HB3	3:C:107:ILE:HD12	1.96	0.46
3:F:217:HIS:O	3:F:224:THR:HG23	2.15	0.46
2:E:385:TRP:CH2	4:H:3:ARG:HD2	2.51	0.46
2:E:266:TRP:HA	2:E:377:THR:HG21	1.98	0.46
3:F:363:TYR:HB2	7:F:625:HOH:O	2.15	0.46
1:A:164:SER:CB	3:C:137:GLU:O	2.60	0.45
2:B:364:ASN:ND2	5:K:1:NAG:C7	2.79	0.45
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.16	0.45
3:C:249:GLU:CB	3:C:383:THR:HG23	2.46	0.45
1:A:152:VAL:HG21	2:B:426:MET:HG2	1.98	0.45
2:E:327:GLY:HA3	2:E:344:LYS:HB2	1.97	0.45
3:C:343:HIS:O	3:C:367:ILE:HA	2.17	0.45
2:E:234:LYS:H	2:E:234:LYS:HE2	1.82	0.45
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.14	0.45
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.99	0.45
2:B:212:GLU:HA	2:B:215:ILE:HG22	1.97	0.44
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.98	0.44
2:B:229:PRO:HB2	2:B:301:GLN:HE22	1.81	0.44
3:C:365:ASN:C	3:C:365:ASN:HD22	2.21	0.44
2:E:420:GLY:HA2	2:E:446:SER:O	2.18	0.44
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.52	0.44
5:L:1:NAG:C6	5:L:3:FUC:H3	2.48	0.44
3:C:96:TYR:O	3:C:97:GLU:CB	2.66	0.44
2:B:184:SER:O	2:B:187:SER:HB2	2.18	0.44
2:B:428:LYS:HG2	2:B:429:HIS:CD2	2.53	0.44
3:F:365:ASN:HD22	3:F:365:ASN:N	2.13	0.44
2:E:406:ARG:O	2:E:406:ARG:CG	2.66	0.43
2:B:422:TYR:O	2:B:444:TRP:HB3	2.17	0.43
3:C:99:SER:O	3:C:102:THR:HB	2.18	0.43
2:B:398:ASP:HA	2:B:433:ASP:HB3	2.01	0.43
3:C:96:TYR:O	3:C:97:GLU:HB3	2.18	0.43
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.54	0.43
3:F:338:LYS:O	4:I:2:PRO:HA	2.19	0.43
3:F:162:LYS:NZ	3:F:185:ASP:O	2.51	0.43
3:F:151:LYS:HB3	3:F:239:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:MET:HB2	2:B:406:ARG:HB3	2.01	0.42
3:C:166:LEU:HD22	3:C:218:LEU:HB3	2.01	0.42
3:C:330:ASP:OD2	3:C:340:HIS:NE2	2.52	0.42
3:F:325:ASN:C	3:F:325:ASN:ND2	2.71	0.42
3:F:344:LEU:HA	3:F:367:ILE:HG23	2.01	0.42
2:E:374:PHE:HB2	2:E:382:ASN:HB3	2.00	0.42
2:E:168:LEU:HD23	3:F:110:LEU:HD13	2.01	0.42
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.54	0.42
3:F:273:LYS:NZ	3:F:319:ASN:HD21	2.18	0.42
3:F:307:HIS:CE1	3:F:342:GLY:H	2.37	0.42
3:C:352:GLY:HA3	3:C:377:TYR:CE1	2.54	0.42
2:E:324:ALA:HB2	2:E:349:ALA:HB3	2.02	0.42
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.19	0.41
2:E:385:TRP:CZ3	4:H:3:ARG:HD2	2.55	0.41
2:B:364:ASN:HD22	5:K:1:NAG:C7	2.33	0.41
2:E:254:ASN:O	2:E:255:ARG:HD2	2.19	0.41
3:F:118:ASN:O	3:F:122:VAL:HG23	2.20	0.41
2:E:229:PRO:HB2	2:E:301:GLN:HE22	1.86	0.41
2:E:431:THR:HG21	4:H:3:ARG:HH12	1.84	0.41
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.56	0.41
2:B:406:ARG:N	2:B:407:CYS:HA	2.35	0.41
3:C:163:GLN:HE21	3:C:163:GLN:HB2	1.66	0.41
2:E:171:ILE:HG13	2:E:172:LEU:N	2.35	0.41
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.19	0.41
3:F:389:PHE:C	3:F:391:ARG:N	2.74	0.40
2:B:205:VAL:HG21	3:C:226:PHE:HB2	2.03	0.40
5:L:1:NAG:H61	5:L:3:FUC:H5	2.04	0.40
1:A:178:TYR:CZ	2:B:178:LYS:HD3	2.56	0.40
3:C:249:GLU:HB2	3:C:383:THR:HG23	2.03	0.40
3:F:177:GLN:HE21	3:F:177:GLN:HB2	1.64	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	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
1	D	55/66 (83%)	53 (96%)	2 (4%)	0	100	100
2	B	301/313 (96%)	280 (93%)	19 (6%)	2 (1%)	22	54
2	E	293/313 (94%)	271 (92%)	21 (7%)	1 (0%)	41	71
3	C	296/311 (95%)	271 (92%)	21 (7%)	4 (1%)	11	36
3	F	283/311 (91%)	264 (93%)	17 (6%)	2 (1%)	22	54
4	G	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
4	H	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
4	I	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
4	J	2/6 (33%)	0	2 (100%)	0	100	100
All	All	1299/1404 (92%)	1203 (93%)	86 (7%)	10 (1%)	19	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	198	LEU
3	C	240	SER
2	E	281	ASP
4	G	2	PRO
3	C	97	GLU
3	F	240	SER
2	B	281	ASP
2	B	399	GLY
3	C	360	PRO
3	F	299	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/61 (98%)	56 (93%)	4 (7%)	16	43
1	D	53/61 (87%)	49 (92%)	4 (8%)	13	37
2	B	261/271 (96%)	250 (96%)	11 (4%)	30	63
2	E	253/271 (93%)	233 (92%)	20 (8%)	12	34
3	C	251/259 (97%)	235 (94%)	16 (6%)	17	45
3	F	239/259 (92%)	226 (95%)	13 (5%)	22	54
4	G	3/5 (60%)	2 (67%)	1 (33%)	0	0
4	H	3/5 (60%)	2 (67%)	1 (33%)	0	0
4	I	3/5 (60%)	2 (67%)	1 (33%)	0	0
4	J	3/5 (60%)	3 (100%)	0	100	100
All	All	1129/1202 (94%)	1058 (94%)	71 (6%)	18	46

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ILE
1	A	173	VAL
1	A	176	LYS
1	A	185	LEU
2	B	163	THR
2	B	178	LYS
2	B	210	GLU
2	B	233	VAL
2	B	253	GLN
2	B	284	ASN
2	B	321	LYS
2	B	325	HIS
2	B	351	ASN
2	B	376	SER
2	B	387	THR
3	C	107	ILE
3	C	117	ASN
3	C	143	VAL
3	C	162	LYS
3	C	163	GLN
3	C	176	GLN
3	C	244	TYR
3	C	250	LEU
3	C	317	ASN

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Mol	Chain	Res	Type
3	C	323	GLU
3	C	325	ASN
3	C	328	GLU
3	C	365	ASN
3	C	374	THR
3	C	383	THR
3	C	393	THR
1	D	134	GLN
1	D	175	LEU
1	D	176	LYS
1	D	185	LEU
2	E	165	LEU
2	E	184	SER
2	E	187	SER
2	E	190	MET
2	E	195	THR
2	E	210	GLU
2	E	234	LYS
2	E	238	VAL
2	E	253	GLN
2	E	257	ASP
2	E	280	THR
2	E	284	ASN
2	E	301	GLN
2	E	337	LYS
2	E	346	ARG
2	E	351	ASN
2	E	359	GLN
2	E	376	SER
2	E	387	THR
2	E	406	ARG
3	F	138	PRO
3	F	143	VAL
3	F	172	LEU
3	F	177	GLN
3	F	192	THR
3	F	206	LYS
3	F	317	ASN
3	F	325	ASN
3	F	329	GLN
3	F	365	ASN
3	F	374	THR

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Mol	Chain	Res	Type
3	F	383	THR
3	F	390	ASN
4	G	3	ARG
4	H	3	ARG
4	I	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	284	ASN
2	B	301	GLN
2	B	325	HIS
2	B	351	ASN
2	B	359	GLN
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	136	GLN
3	C	163	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	311	GLN
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	365	ASN
1	D	143	GLN
1	D	181	GLN
2	E	189	GLN

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Mol	Chain	Res	Type
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	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	115	ASN
3	F	117	ASN
3	F	144	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	365	ASN
3	F	390	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	0.71	0	17,19,21	0.68	0
5	NAG	K	2	5	14,14,15	0.75	0	17,19,21	0.69	0
5	FUC	K	3	5	10,10,11	0.64	0	14,14,16	0.36	0
5	NAG	L	1	2,5	14,14,15	0.64	0	17,19,21	1.31	2 (11%)
5	NAG	L	2	5	14,14,15	0.58	0	17,19,21	0.62	0
5	FUC	L	3	5	10,10,11	0.78	0	14,14,16	0.83	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	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	6/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1	NAG	C3-C4-C5	2.58	114.85	110.24
5	L	3	FUC	C1-C2-C3	2.52	112.77	109.67
5	L	1	NAG	C2-N2-C7	-2.12	119.89	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
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	1	NAG	C8-C7-N2-C2
5	K	2	NAG	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C3-C2-N2-C7

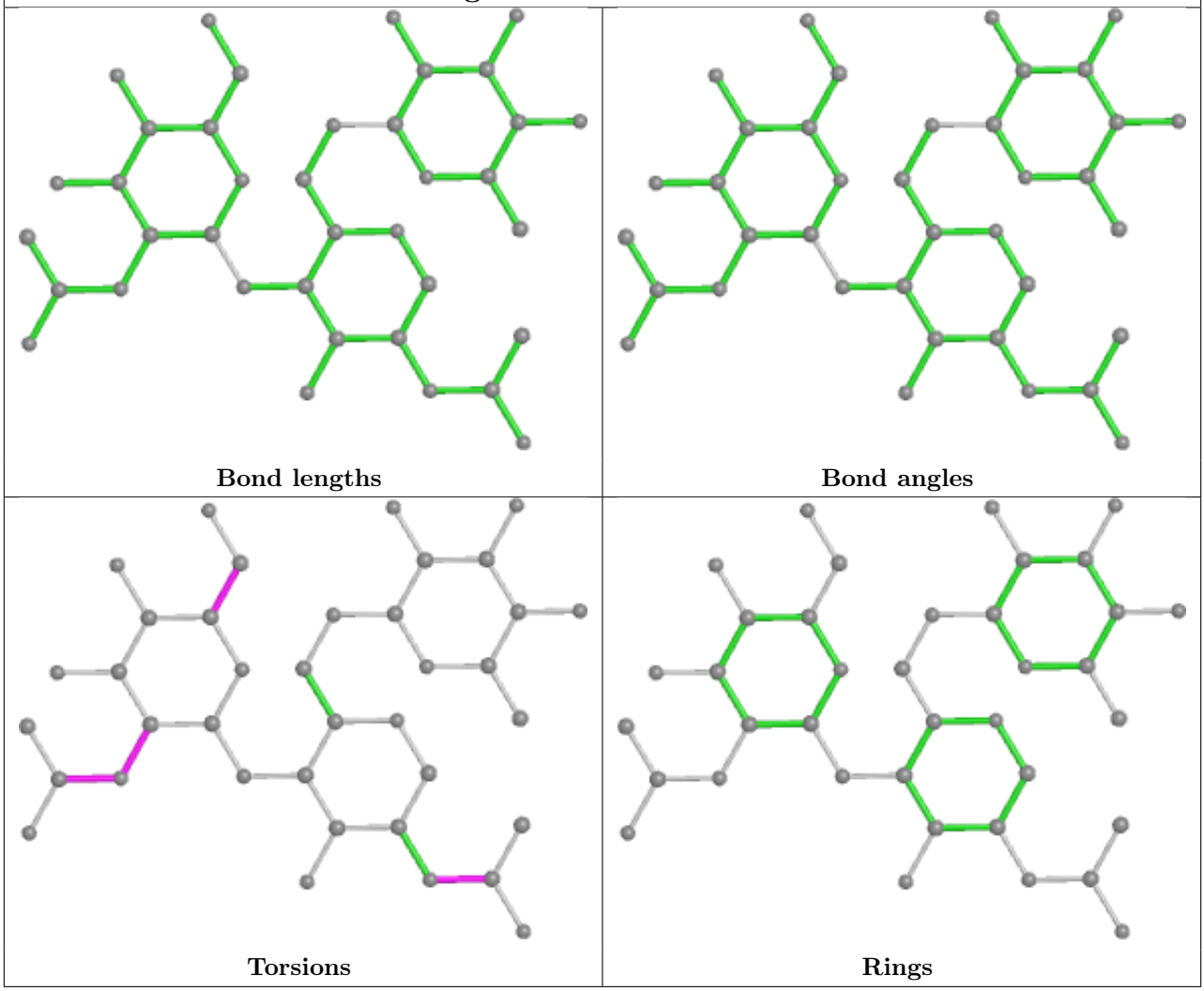
There are no ring outliers.

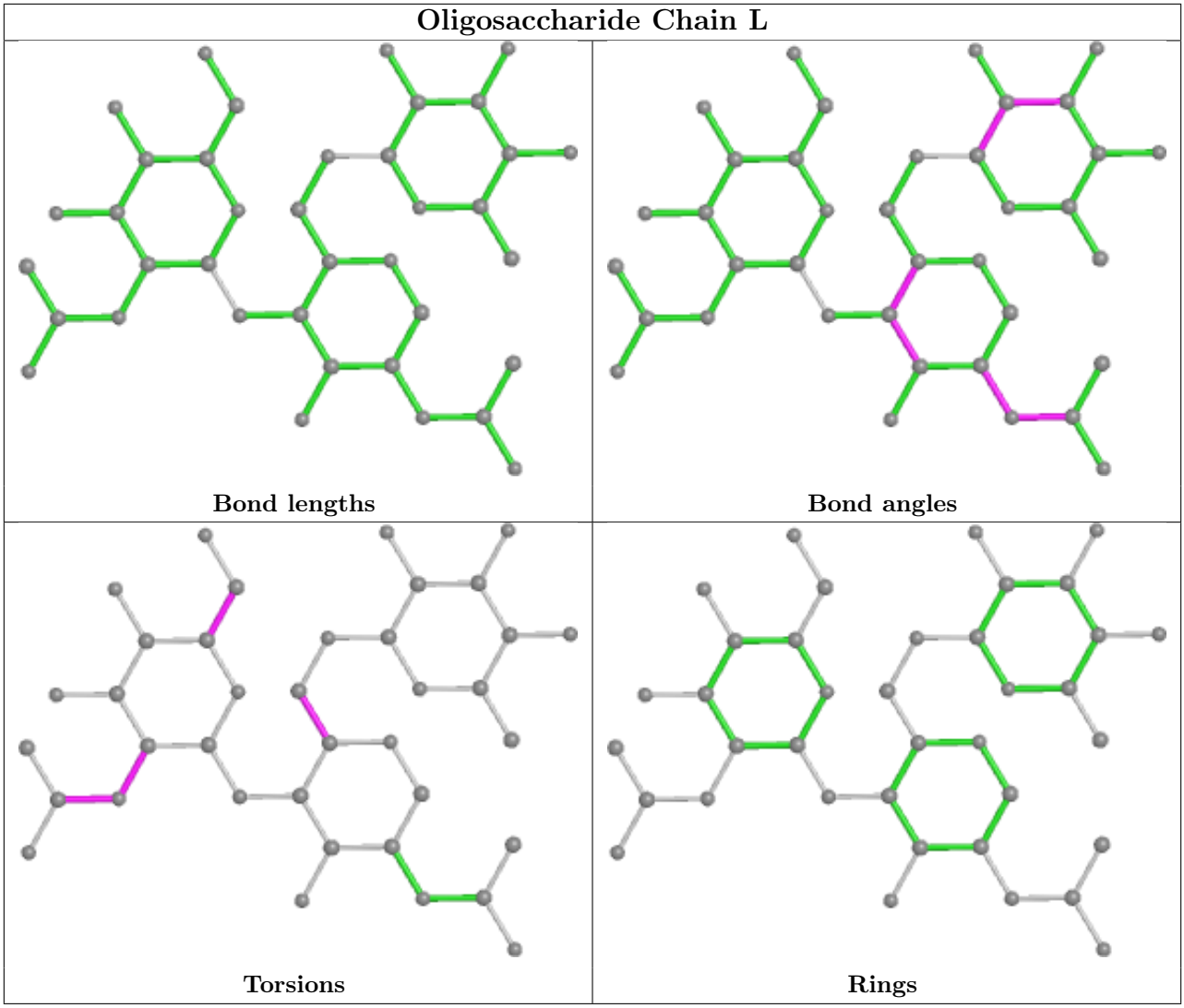
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1	NAG	4	0
5	L	3	FUC	4	0
5	K	1	NAG	2	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	65/66 (98%)	0.09	2 (3%) 49 44	26, 53, 78, 81	0
1	D	57/66 (86%)	0.39	7 (12%) 4 3	27, 56, 96, 99	0
2	B	303/313 (96%)	-0.24	6 (1%) 65 63	22, 35, 55, 82	0
2	E	295/313 (94%)	-0.41	6 (2%) 65 63	14, 23, 53, 88	0
3	C	298/311 (95%)	-0.14	4 (1%) 77 77	25, 41, 65, 82	0
3	F	285/311 (91%)	-0.24	10 (3%) 44 38	17, 29, 50, 84	0
4	G	4/6 (66%)	1.00	0 100 100	72, 72, 72, 73	0
4	H	4/6 (66%)	-0.40	0 100 100	31, 31, 32, 33	0
4	I	4/6 (66%)	0.03	0 100 100	33, 34, 34, 37	0
4	J	4/6 (66%)	0.25	0 100 100	53, 54, 54, 55	0
All	All	1319/1404 (93%)	-0.21	35 (2%) 54 50	14, 33, 72, 99	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	393	THR	4.9
3	F	394	ILE	4.1
1	D	187	GLN	4.1
1	A	126	VAL	4.1
3	F	112	GLU	3.9
2	B	459	PRO	3.6
2	B	157	VAL	3.5
2	E	459	PRO	3.4
2	E	282	GLY	3.3
3	C	241	ALA	3.3
3	F	115	ASN	3.2
2	B	282	GLY	3.0
1	D	184	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	96	TYR	2.8
3	F	113	ILE	2.7
2	E	281	ASP	2.6
1	D	188	VAL	2.6
1	D	176	LYS	2.6
3	F	241	ALA	2.5
3	C	360	PRO	2.5
1	D	135	LEU	2.5
3	F	296	GLY	2.3
2	B	458	PHE	2.3
2	E	232	SER	2.3
1	D	189	ILE	2.2
3	C	240	SER	2.2
3	F	175	ASN	2.2
2	B	159	SER	2.2
2	E	458	PHE	2.2
1	D	133	ILE	2.1
3	F	119	GLN	2.1
3	F	117	ASN	2.1
2	E	169	ARG	2.0
2	B	158	ASN	2.0
1	A	127	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)

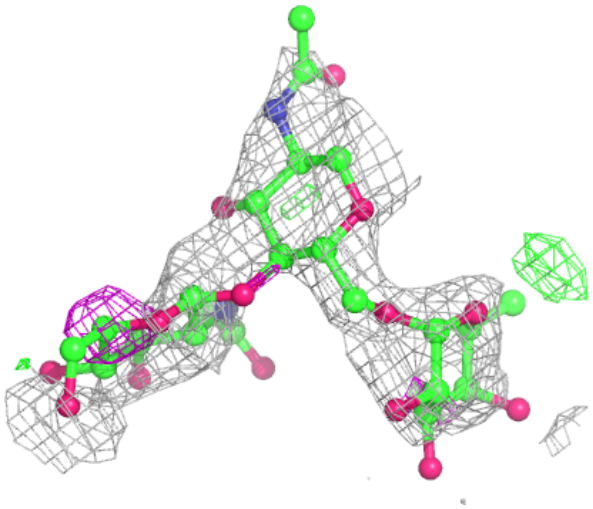
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

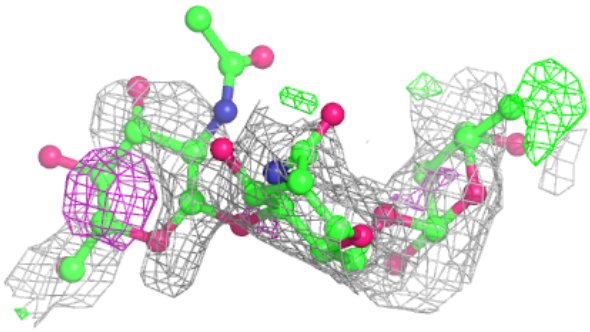
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	K	2	14/15	0.37	0.64	100,102,103,103	0
5	FUC	K	3	10/11	0.57	0.48	96,97,98,99	0
5	FUC	L	3	10/11	0.68	0.54	71,72,72,73	0
5	NAG	L	2	14/15	0.74	0.49	76,78,79,81	0
5	NAG	K	1	14/15	0.78	0.40	85,88,95,96	0
5	NAG	L	1	14/15	0.78	0.31	53,58,69,70	0

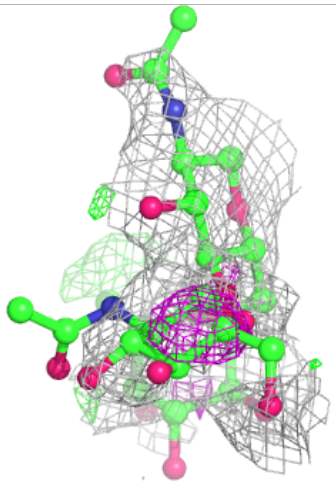
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

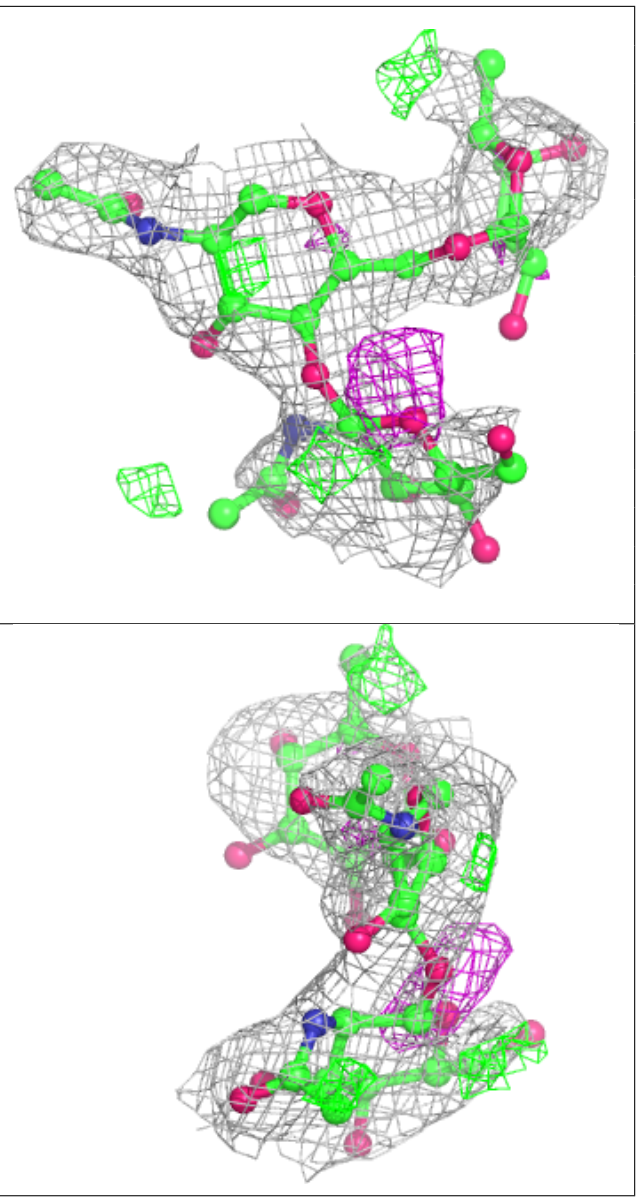






Electron density around Chain L:

$2mF_o$-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	F	603	1/1	0.94	0.07	24,24,24,24	0
6	CA	B	600	1/1	0.95	0.12	44,44,44,44	0
6	CA	E	602	1/1	0.97	0.12	28,28,28,28	0
6	CA	C	601	1/1	0.97	0.04	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.