Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:39 PM EDT

PDB ID	:	2OYI
Title	:	Crystal Structure of Fragment D of gammaD298,301A Fibrinogen with the Peptide Ligand Gly-Pro-Arg-Pro-Amide
Authors	:	Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on	:	2007-02-22
Resolution	:	2.70 Å(reported)

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

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

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

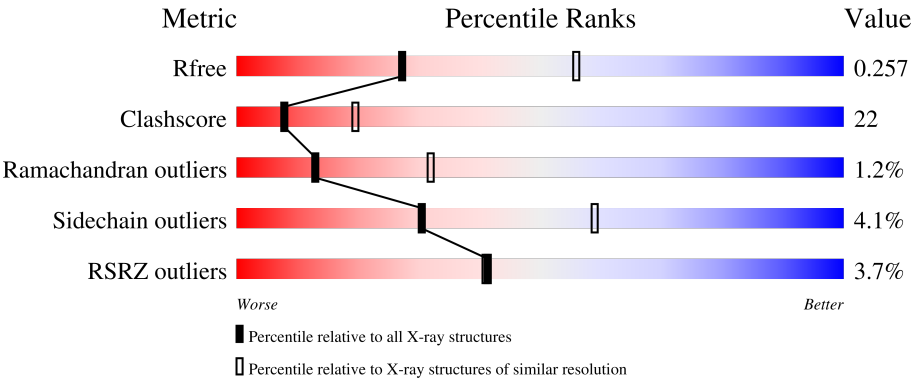
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	8% 45% 48% 5%
1	D	66	15% 35% 45% 5% 15%
2	B	313	2% 61% 33%
2	E	313	2% 64% 27% 6%
3	C	311	3% 66% 27%

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Mol	Chain	Length	Quality of chain
3	F	311	4% 60% 29% 8%
4	G	4	25% 50% 25%
4	H	4	25% 75%
4	I	4	25% 50% 25%
4	J	4	75% 25%
5	K	3	33% 33% 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
5	FUC	L	3	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10784 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	65	Total	C	N	O	S	0	0	0
			530	327	100	100	3			
1	D	56	Total	C	N	O	S	0	0	0
			458	280	87	88	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	0	0
			2414	1505	427	460	22			
2	E	294	Total	C	N	O	S	0	0	0
			2362	1475	417	448	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	299	Total	C	N	O	S	0	0	0
			2393	1521	403	458	11			
3	F	285	Total	C	N	O	S	0	0	0
			2277	1448	384	434	11			

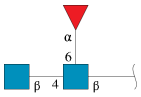
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	298	ALA	ASP	engineered mutation	UNP P02679
C	301	ALA	ASP	engineered mutation	UNP P02679
F	298	ALA	ASP	engineered mutation	UNP P02679
F	301	ALA	ASP	engineered mutation	UNP P02679

- Molecule 4 is a protein called GPRP Peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	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	I	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	3	Total O 3 3	0	0
7	B	27	Total O 27 27	0	0
7	C	18	Total O 18 18	0	0

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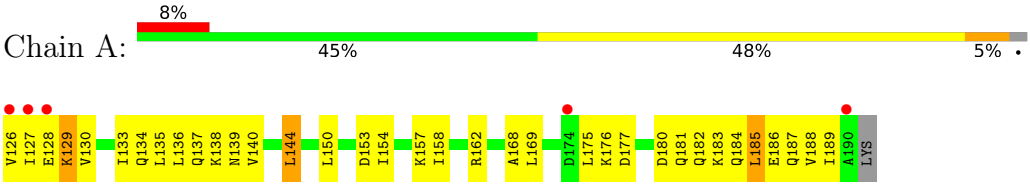
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	5	Total O 5 5	0	0
7	E	63	Total O 63 63	0	0
7	F	33	Total O 33 33	0	0
7	I	1	Total O 1 1	0	0

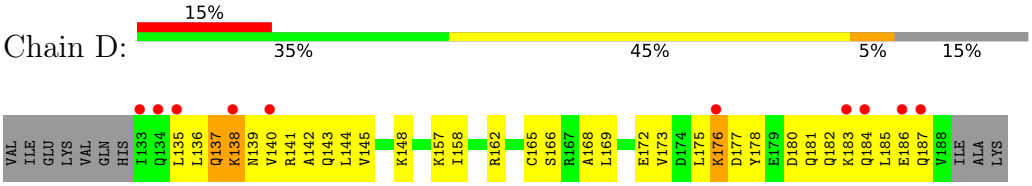
3 Residue-property plots (i)

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.

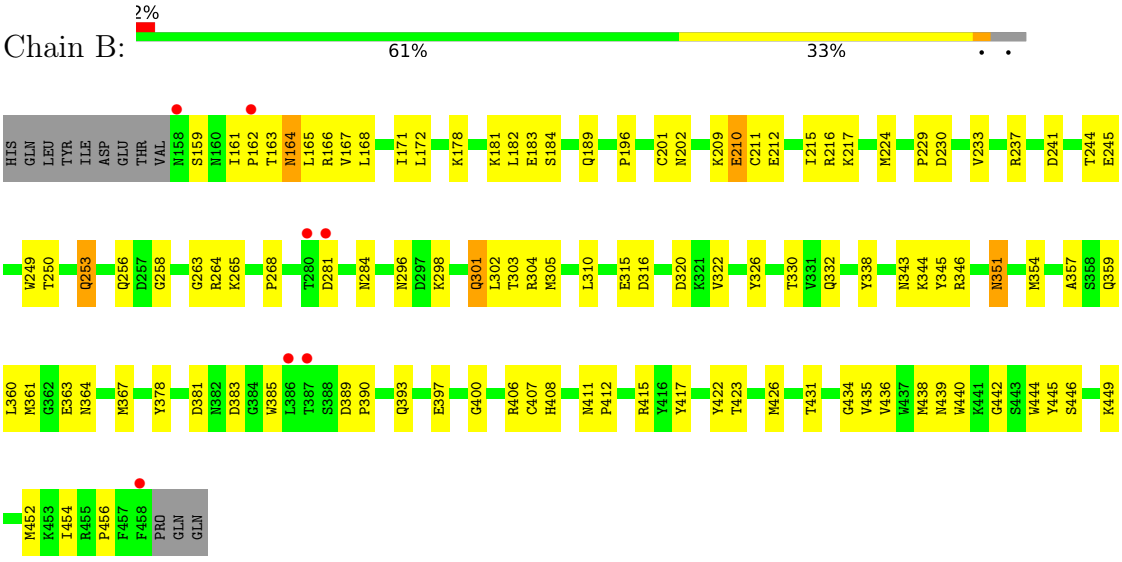
• Molecule 1: Fibrinogen alpha chain



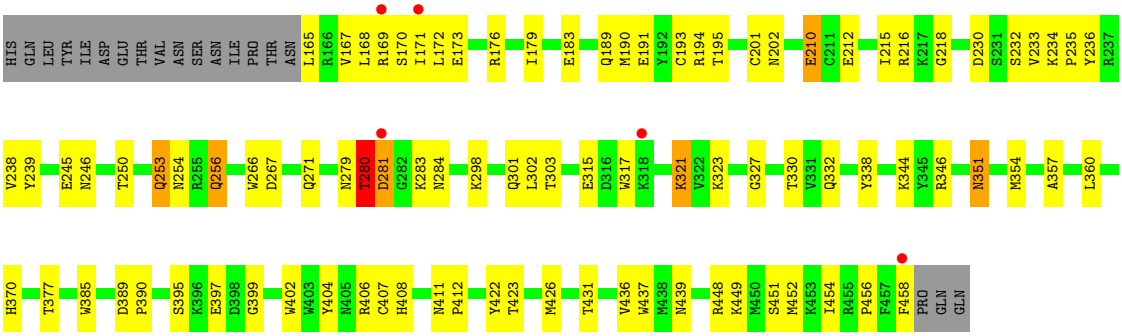
• Molecule 1: Fibrinogen alpha chain



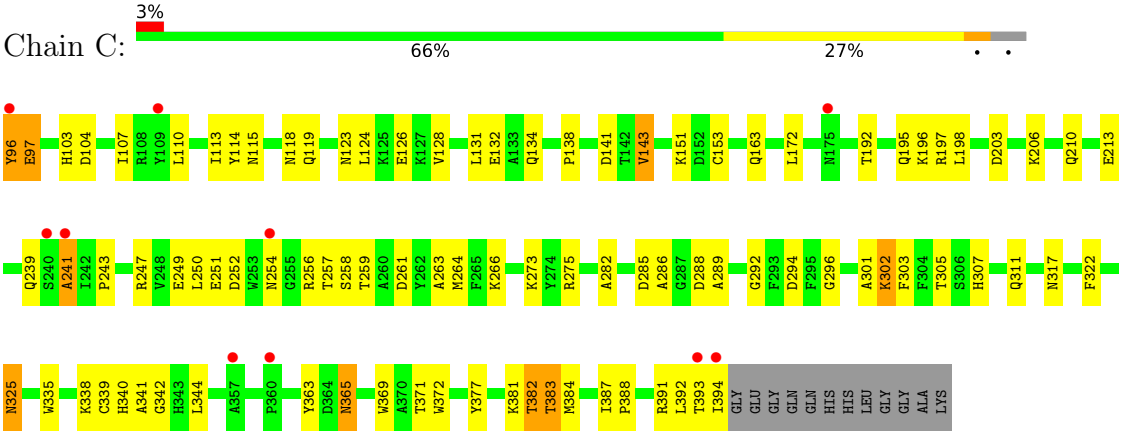
• Molecule 2: Fibrinogen beta chain



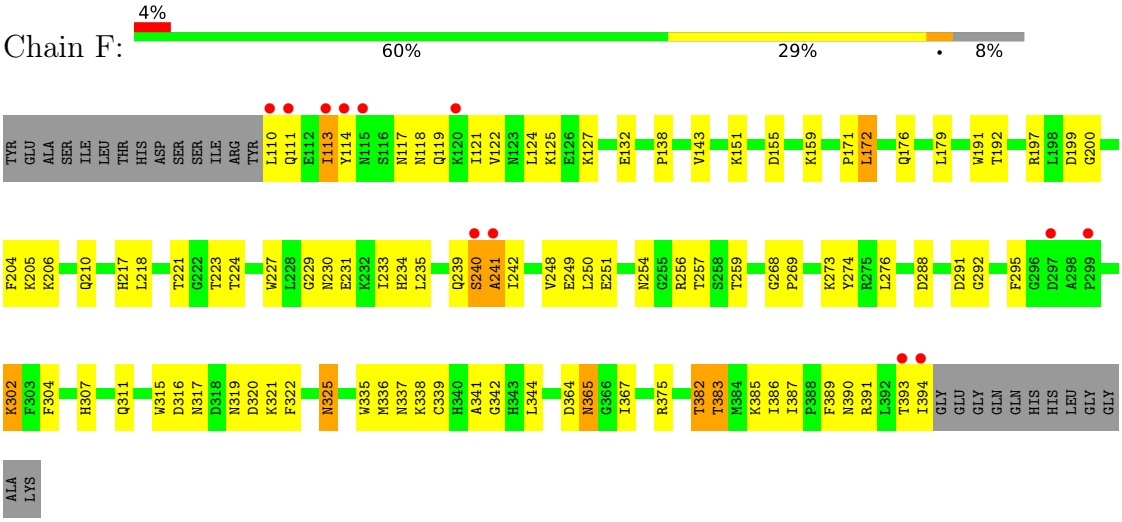
• Molecule 2: Fibrinogen beta chain



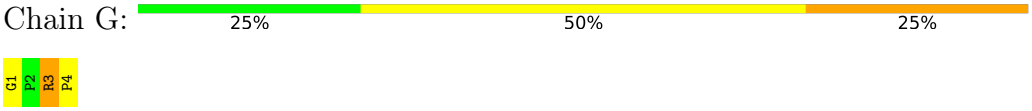
• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain

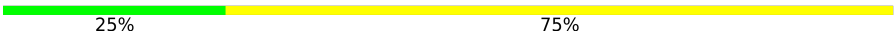


• Molecule 4: GPRP Peptide



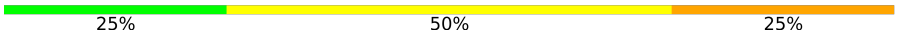
• Molecule 4: GPRP Peptide

Chain H:



• Molecule 4: GPRP Peptide

Chain I:

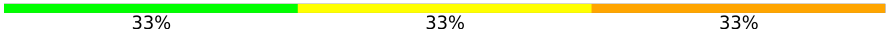


• Molecule 4: GPRP Peptide

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	88.99Å 94.04Å 226.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.70 17.97 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (17.97-2.70) 98.0 (17.97-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.256 0.218 , 0.257	Depositor DCC
R_{free} test set	2634 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10784	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% 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: CA, NAG, FUC

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	0.30	0/531	0.51	0/709
1	D	0.30	0/458	0.53	0/610
2	B	0.35	0/2475	0.60	0/3342
2	E	0.38	0/2422	0.65	1/3268 (0.0%)
3	C	0.36	0/2459	0.57	0/3327
3	F	0.39	0/2340	0.63	0/3165
4	G	0.46	0/31	0.63	0/40
4	H	0.48	0/31	0.66	0/40
4	I	0.58	0/31	0.68	0/40
4	J	0.60	0/31	0.68	0/40
All	All	0.37	0/10809	0.60	1/14581 (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	6.25	128.73	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	530	0	556	50	0
1	D	458	0	477	43	0
2	B	2414	0	2279	115	0
2	E	2362	0	2231	92	0
3	C	2393	0	2248	84	0
3	F	2277	0	2140	105	0
4	G	30	0	32	5	0
4	H	30	0	32	6	0
4	I	30	0	32	4	0
4	J	30	0	32	4	0
5	K	38	0	34	5	0
5	L	38	0	34	11	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	3	0	0	0	0
7	B	27	0	0	4	0
7	C	18	0	0	2	0
7	D	5	0	0	0	0
7	E	63	0	0	1	0
7	F	33	0	0	2	0
7	I	1	0	0	0	0
All	All	10784	0	10127	448	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 22.

All (448) 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)
5:L:1:NAG:H62	5:L:2:NAG:H2	1.30	1.11
2:B:397:GLU:HB3	2:B:431:THR:HG21	1.40	1.04
1:A:188:VAL:HG11	2:B:167:VAL:HG21	1.35	1.03
2:E:165:LEU:HD11	2:E:168:LEU:HD22	1.49	0.94
4:G:3:ARG:HG3	4:G:4:PRO:HD2	1.51	0.91
3:F:172:LEU:H	3:F:239:GLN:HE21	1.15	0.88
2:B:423:THR:H	2:B:426:MET:HE3	1.38	0.87
3:C:322:PHE:CZ	4:G:3:ARG:HG2	2.10	0.86
5:L:1:NAG:H61	5:L:3:FUC:H5	1.54	0.85
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.26	0.82
2:E:168:LEU:HD21	3:F:110:LEU:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.62	0.82
1:A:176:LYS:HE2	1:A:180:ASP:OD1	1.79	0.82
3:F:119:GLN:HE21	3:F:119:GLN:HA	1.45	0.81
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.44	0.81
3:C:393:THR:O	3:C:394:ILE:HG22	1.80	0.80
2:E:168:LEU:O	2:E:172:LEU:HB2	1.82	0.79
3:F:307:HIS:HE1	3:F:341:ALA:H	1.32	0.78
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.49	0.77
2:B:415:ARG:O	2:B:434:GLY:HA2	1.84	0.77
1:A:130:VAL:O	1:A:134:GLN:HG3	1.85	0.76
1:D:185:LEU:HD13	1:D:185:LEU:O	1.86	0.76
2:E:423:THR:N	2:E:426:MET:HE3	2.01	0.75
2:B:345:TYR:HB2	2:B:354:MET:HE3	1.68	0.73
5:L:1:NAG:C6	5:L:2:NAG:H2	2.15	0.73
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.53	0.73
2:E:172:LEU:HB3	3:F:113:ILE:HG21	1.69	0.72
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.05	0.72
2:B:423:THR:N	2:B:426:MET:HE3	2.04	0.72
1:A:188:VAL:HG11	2:B:167:VAL:CG2	2.17	0.71
1:A:128:GLU:HG2	1:A:129:LYS:N	2.05	0.71
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.71	0.71
3:C:365:ASN:HD22	3:C:365:ASN:H	1.37	0.70
3:F:254:ASN:HB2	3:F:256:ARG:HH21	1.56	0.70
1:D:178:TYR:O	1:D:182:GLN:HG3	1.91	0.70
2:B:351:ASN:ND2	2:B:354:MET:H	1.90	0.70
2:B:163:THR:HA	2:B:166:ARG:HD2	1.74	0.70
5:L:1:NAG:H61	5:L:3:FUC:H3	1.74	0.70
1:D:140:VAL:HG11	2:E:172:LEU:HD11	1.74	0.69
3:F:241:ALA:O	3:F:242:ILE:HG12	1.91	0.69
1:A:188:VAL:CG1	2:B:167:VAL:HG21	2.17	0.69
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.75	0.69
2:E:321:LYS:NZ	2:E:321:LYS:HB3	2.09	0.68
4:H:4:PRO:HG3	5:K:1:NAG:H62	1.76	0.68
2:E:321:LYS:HB3	2:E:321:LYS:HZ3	1.59	0.68
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.40	0.68
2:B:212:GLU:HG3	2:B:216:ARG:HH11	1.59	0.68
2:B:351:ASN:HD21	2:B:354:MET:H	1.41	0.68
5:L:1:NAG:H61	5:L:3:FUC:C5	2.23	0.68
1:A:127:ILE:HG12	1:A:128:GLU:H	1.59	0.67
1:D:157:LYS:HE2	3:F:132:GLU:OE2	1.94	0.67
2:B:230:ASP:O	2:B:233:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.08	0.67
3:C:254:ASN:HD22	3:C:256:ARG:HH12	1.41	0.66
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.78	0.66
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.78	0.66
2:B:316:ASP:HB2	2:B:445:TYR:OH	1.95	0.66
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.76	0.66
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.78	0.66
2:B:359:GLN:O	2:B:360:LEU:HD23	1.96	0.65
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.97	0.65
3:C:261:ASP:OD2	3:C:392:LEU:HD21	1.96	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.43	0.65
3:C:241:ALA:O	3:C:243:PRO:HD3	1.97	0.65
3:C:307:HIS:CE1	3:C:341:ALA:H	2.15	0.65
1:D:138:LYS:H	1:D:138:LYS:HD3	1.63	0.64
2:E:212:GLU:O	2:E:215:ILE:HG22	1.96	0.64
2:B:351:ASN:HD22	2:B:351:ASN:C	2.00	0.64
3:F:307:HIS:CE1	3:F:341:ALA:H	2.14	0.64
2:E:172:LEU:HD13	3:F:113:ILE:HD12	1.79	0.64
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.12	0.63
3:F:365:ASN:HD22	3:F:365:ASN:H	1.45	0.63
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.98	0.63
3:F:172:LEU:N	3:F:239:GLN:HE21	1.92	0.63
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.62	0.63
3:F:338:LYS:N	3:F:339:CYS:HA	2.13	0.63
2:B:439:ASN:H	2:B:439:ASN:HD22	1.47	0.62
1:D:169:LEU:H	2:E:189:GLN:NE2	1.96	0.62
1:A:128:GLU:HG2	1:A:129:LYS:H	1.63	0.62
1:A:157:LYS:HE3	3:C:132:GLU:OE2	1.99	0.62
2:B:343:ASN:OD1	2:B:344:LYS:HE2	1.99	0.62
3:F:321:LYS:O	3:F:338:LYS:HD3	1.98	0.62
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.81	0.62
3:C:338:LYS:N	3:C:339:CYS:HA	2.13	0.62
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.63	0.62
1:D:157:LYS:HD3	3:F:132:GLU:HG3	1.82	0.62
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.64	0.61
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.00	0.61
1:A:133:ILE:O	1:A:137:GLN:HG3	2.00	0.61
4:I:3:ARG:HG3	4:I:4:PRO:HD2	1.82	0.61
1:A:127:ILE:HG12	1:A:128:GLU:OE2	2.00	0.61
2:E:245:GLU:OE2	2:E:323:LYS:NZ	2.33	0.61
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:TYR:CG	2:B:346:ARG:N	2.69	0.60
3:F:118:ASN:O	3:F:122:VAL:HG23	2.01	0.60
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.01	0.60
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.65	0.60
2:B:397:GLU:OE1	4:H:3:ARG:NH1	2.34	0.60
1:D:176:LYS:HG3	1:D:180:ASP:OD2	2.01	0.60
2:E:423:THR:H	2:E:426:MET:HE3	1.67	0.60
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.37	0.59
1:A:144:LEU:HD13	1:A:182:GLN:HG2	1.84	0.59
7:E:476:HOH:O	3:F:138:PRO:HG3	2.02	0.59
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.38	0.59
1:D:185:LEU:HB2	2:E:171:ILE:CD1	2.32	0.59
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.68	0.58
2:E:253:GLN:NE2	2:E:451:SER:HA	2.18	0.58
1:A:126:VAL:HG13	1:A:126:VAL:O	2.03	0.58
3:C:197:ARG:HG2	3:C:382:THR:HG22	1.85	0.58
2:B:202:ASN:ND2	2:B:284:ASN:HD22	2.01	0.58
3:F:172:LEU:HD22	3:F:239:GLN:NE2	2.18	0.58
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.84	0.58
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.85	0.58
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.17	0.58
1:A:127:ILE:CG2	1:A:130:VAL:H	2.16	0.58
3:F:192:THR:HG23	3:F:386:ILE:HG13	1.86	0.58
2:E:168:LEU:CD2	3:F:110:LEU:HB2	2.33	0.57
1:A:169:LEU:H	2:B:189:GLN:HE22	1.51	0.57
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.70	0.57
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.86	0.57
5:L:1:NAG:H61	5:L:3:FUC:C3	2.34	0.57
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.52	0.57
3:C:365:ASN:H	3:C:365:ASN:ND2	2.03	0.57
1:D:136:LEU:O	1:D:139:ASN:N	2.38	0.57
1:D:143:GLN:HE22	3:F:117:ASN:HB2	1.69	0.57
3:F:389:PHE:C	3:F:391:ARG:H	2.08	0.57
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.35	0.56
5:L:1:NAG:H62	5:L:2:NAG:C2	2.20	0.56
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.41	0.56
3:F:205:LYS:NZ	3:F:205:LYS:HB3	2.21	0.56
2:E:165:LEU:CD1	2:E:168:LEU:HD22	2.31	0.56
2:E:283:LYS:HE2	2:E:283:LYS:HA	1.88	0.55
3:F:200:GLY:HA2	7:F:409:HOH:O	2.05	0.55
3:F:268:GLY:O	3:F:274:TYR:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:HD21	3:C:107:ILE:HD13	1.89	0.55
3:C:288:ASP:O	3:C:371:THR:HG21	2.07	0.55
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.71	0.55
3:F:224:THR:HG23	7:F:413:HOH:O	2.07	0.55
3:F:291:ASP:O	3:F:302:LYS:HD2	2.07	0.55
1:A:127:ILE:HG22	1:A:130:VAL:CG2	2.37	0.55
2:B:422:TYR:O	2:B:444:TRP:HB3	2.07	0.55
2:B:201:CYS:O	3:C:143:VAL:HG11	2.07	0.54
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.89	0.54
1:A:181:GLN:OE1	2:B:171:ILE:HG23	2.08	0.54
2:B:212:GLU:HG3	2:B:216:ARG:NH1	2.23	0.54
1:A:177:ASP:O	1:A:181:GLN:HG3	2.07	0.54
3:C:273:LYS:HB2	3:C:311:GLN:HB3	1.89	0.54
2:B:161:ILE:H	2:B:161:ILE:HD12	1.73	0.54
3:C:340:HIS:O	4:G:1:GLY:N	2.37	0.54
3:C:365:ASN:HD22	3:C:365:ASN:N	2.00	0.54
2:E:280:THR:HB	2:E:283:LYS:HG3	1.89	0.53
3:F:254:ASN:HD22	3:F:256:ARG:NH2	2.07	0.53
2:E:327:GLY:HA3	2:E:344:LYS:HE2	1.90	0.53
3:C:307:HIS:HE1	3:C:342:GLY:H	1.57	0.53
2:E:439:ASN:HD22	2:E:439:ASN:H	1.56	0.53
3:C:103:HIS:O	3:C:107:ILE:HG12	2.09	0.53
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.90	0.53
2:B:438:MET:HA	2:B:442:GLY:O	2.08	0.53
3:F:179:LEU:HD23	3:F:218:LEU:HD12	1.91	0.53
1:A:127:ILE:HG22	1:A:130:VAL:H	1.72	0.53
3:C:172:LEU:HD12	3:C:239:GLN:HB3	1.90	0.53
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.53
1:D:136:LEU:O	1:D:139:ASN:HB3	2.09	0.53
2:E:176:ARG:HB2	3:F:117:ASN:HD21	1.74	0.53
1:A:130:VAL:O	1:A:133:ILE:HG22	2.09	0.52
3:F:254:ASN:CB	3:F:256:ARG:HH21	2.20	0.52
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.08	0.52
2:B:439:ASN:HD22	2:B:439:ASN:N	2.07	0.52
3:F:192:THR:HG23	3:F:386:ILE:CG1	2.39	0.52
1:A:169:LEU:H	2:B:189:GLN:NE2	2.08	0.52
2:B:268:PRO:HG2	7:B:466:HOH:O	2.09	0.52
2:E:230:ASP:OD2	2:E:232:SER:HB2	2.09	0.52
3:F:276:LEU:HD23	3:F:276:LEU:C	2.30	0.52
2:B:172:LEU:HB3	3:C:113:ILE:CD1	2.39	0.52
1:D:169:LEU:H	2:E:189:GLN:HE22	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ASP:O	1:D:184:GLN:HG3	2.09	0.52
2:B:178:LYS:HA	2:B:178:LYS:HE2	1.91	0.52
3:C:172:LEU:H	3:C:239:GLN:HE21	1.58	0.52
1:D:141:ARG:O	1:D:145:VAL:HG23	2.10	0.52
3:F:254:ASN:HD22	3:F:256:ARG:HH21	1.57	0.52
2:B:364:ASN:OD1	4:H:4:PRO:HB3	2.10	0.52
1:D:183:LYS:O	1:D:186:GLU:HB2	2.09	0.52
2:E:408:HIS:CD2	2:E:408:HIS:C	2.83	0.52
2:E:167:VAL:HA	2:E:170:SER:HB3	1.91	0.52
3:F:365:ASN:H	3:F:365:ASN:ND2	2.09	0.52
3:C:292:GLY:HA2	3:C:305:THR:O	2.10	0.51
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.91	0.51
3:F:217:HIS:HB2	3:F:224:THR:HG21	1.92	0.51
2:B:351:ASN:ND2	2:B:351:ASN:C	2.63	0.51
2:E:216:ARG:HH12	2:E:458:PHE:HZ	1.58	0.51
2:E:238:VAL:HG21	2:E:250:THR:CG2	2.40	0.51
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.23	0.51
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.11	0.51
3:C:96:TYR:O	3:C:97:GLU:HB2	2.10	0.51
3:C:124:LEU:O	3:C:128:VAL:HG23	2.10	0.51
2:E:346:ARG:HG3	2:E:346:ARG:NH1	2.25	0.51
3:F:192:THR:CG2	3:F:386:ILE:HG13	2.41	0.51
1:A:136:LEU:HD13	3:C:110:LEU:HD12	1.93	0.51
2:E:238:VAL:HG21	2:E:250:THR:HG23	1.92	0.51
2:E:332:GLN:O	2:E:338:TYR:HA	2.11	0.51
2:E:395:SER:HA	2:E:404:TYR:CE2	2.45	0.51
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.93	0.51
2:B:201:CYS:C	3:C:143:VAL:HG11	2.31	0.51
2:B:202:ASN:HD22	2:B:284:ASN:ND2	2.09	0.51
2:B:229:PRO:HB3	2:B:301:GLN:HE22	1.76	0.51
2:B:357:ALA:HB3	2:B:360:LEU:HD12	1.93	0.51
1:D:166:SER:HB3	2:E:195:THR:HB	1.93	0.51
2:B:422:TYR:HA	2:B:426:MET:HE1	1.93	0.50
3:C:172:LEU:HG	3:C:239:GLN:HE21	1.77	0.50
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.93	0.50
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.92	0.50
3:C:307:HIS:CE1	3:C:342:GLY:H	2.29	0.50
1:D:186:GLU:O	1:D:187:GLN:HG3	2.11	0.50
1:A:182:GLN:O	1:A:186:GLU:HG2	2.12	0.50
2:B:303:THR:HB	2:B:330:THR:HA	1.93	0.50
2:E:172:LEU:HD13	3:F:113:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:CB	3:F:117:ASN:HD21	2.24	0.50
1:D:136:LEU:HD21	3:F:111:GLN:OE1	2.11	0.50
2:B:364:ASN:HD22	5:K:1:NAG:C7	2.24	0.50
1:D:185:LEU:HB2	2:E:171:ILE:HD13	1.93	0.50
2:E:303:THR:HB	2:E:330:THR:HA	1.92	0.50
3:F:206:LYS:HD2	3:F:210:GLN:CD	2.31	0.50
2:B:265:LYS:HD3	2:B:378:TYR:CE1	2.47	0.50
3:F:119:GLN:NE2	3:F:119:GLN:CA	2.74	0.49
2:B:361:MET:O	5:K:1:NAG:H81	2.12	0.49
3:F:172:LEU:H	3:F:239:GLN:NE2	1.97	0.49
3:C:325:ASN:C	3:C:325:ASN:HD22	2.14	0.49
2:B:265:LYS:HD3	2:B:378:TYR:CZ	2.47	0.49
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.95	0.49
5:L:1:NAG:C6	5:L:3:FUC:H5	2.34	0.49
1:D:136:LEU:O	1:D:137:GLN:C	2.51	0.49
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.48	0.49
3:F:155:ASP:O	3:F:159:LYS:HG3	2.13	0.49
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.47	0.49
3:F:197:ARG:HB2	3:F:382:THR:HB	1.95	0.49
2:E:271:GLN:HE21	2:E:271:GLN:HA	1.78	0.49
3:F:254:ASN:ND2	3:F:256:ARG:HH21	2.11	0.49
4:G:3:ARG:CG	4:G:4:PRO:HD2	2.35	0.48
5:L:1:NAG:C6	5:L:3:FUC:H3	2.41	0.48
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.95	0.48
1:D:144:LEU:CD2	1:D:182:GLN:HG2	2.42	0.48
2:E:165:LEU:HG	2:E:165:LEU:O	2.13	0.48
2:E:167:VAL:HG12	2:E:167:VAL:O	2.12	0.48
2:E:321:LYS:NZ	2:E:321:LYS:CB	2.76	0.48
3:F:365:ASN:HD22	3:F:365:ASN:N	2.06	0.48
3:F:393:THR:O	3:F:394:ILE:C	2.51	0.48
2:E:385:TRP:CZ2	4:J:3:ARG:HG2	2.48	0.48
2:B:161:ILE:HD12	2:B:161:ILE:N	2.28	0.48
2:B:217:LYS:HB3	3:C:213:GLU:HG3	1.95	0.48
3:F:254:ASN:ND2	3:F:256:ARG:NH2	2.61	0.48
3:F:325:ASN:HD22	3:F:325:ASN:C	2.17	0.48
1:A:153:ASP:O	1:A:157:LYS:HG2	2.14	0.48
1:D:135:LEU:HD13	1:D:135:LEU:C	2.34	0.48
3:F:295:PHE:CD2	4:I:2:PRO:HD3	2.48	0.48
3:C:263:ALA:HB1	3:C:264:MET:CE	2.43	0.48
3:C:138:PRO:HG3	7:C:413:HOH:O	2.14	0.48
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:SER:HA	3:C:285:ASP:OD2	2.13	0.48
1:D:144:LEU:HD23	1:D:144:LEU:O	2.13	0.48
1:A:175:LEU:N	1:A:175:LEU:HD22	2.28	0.47
2:B:364:ASN:ND2	5:K:1:NAG:C7	2.77	0.47
1:A:127:ILE:HG22	1:A:130:VAL:CB	2.44	0.47
1:D:144:LEU:HD22	1:D:182:GLN:HG2	1.95	0.47
2:E:172:LEU:O	3:F:113:ILE:HG22	2.14	0.47
2:E:201:CYS:O	3:F:143:VAL:HG21	2.14	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.12	0.47
2:E:266:TRP:HA	2:E:377:THR:HG21	1.97	0.47
3:C:153:CYS:HB2	3:C:192:THR:OG1	2.15	0.47
2:E:431:THR:HG21	4:J:3:ARG:HH12	1.79	0.47
1:D:140:VAL:C	1:D:142:ALA:N	2.68	0.47
1:A:154:ILE:HD12	2:B:182:LEU:HD13	1.97	0.47
2:B:172:LEU:HB3	3:C:113:ILE:HD11	1.97	0.47
2:B:332:GLN:O	2:B:338:TYR:HA	2.14	0.47
2:B:363:GLU:O	2:B:367:MET:HG2	2.14	0.47
3:F:205:LYS:HB3	3:F:205:LYS:HZ3	1.78	0.47
2:B:298:LYS:HG3	7:B:480:HOH:O	2.14	0.47
2:E:406:ARG:N	2:E:407:CYS:HA	2.27	0.47
2:B:258:GLY:HA2	7:B:462:HOH:O	2.15	0.47
3:C:363:TYR:HB3	4:G:3:ARG:NH2	2.30	0.47
1:A:183:LYS:O	1:A:187:GLN:HG3	2.15	0.47
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.96	0.47
2:B:393:GLN:O	2:B:397:GLU:HG3	2.14	0.47
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.29	0.46
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.97	0.46
2:B:434:GLY:O	2:B:436:VAL:N	2.47	0.46
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.49	0.46
1:A:162:ARG:NH1	1:A:162:ARG:HG2	2.30	0.46
2:B:162:PRO:HG2	3:C:97:GLU:OE1	2.15	0.46
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.51	0.46
1:D:162:ARG:NH1	1:D:162:ARG:HG2	2.30	0.46
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.97	0.46
5:L:2:NAG:C1	5:L:2:NAG:H83	2.45	0.46
2:B:351:ASN:HD21	2:B:354:MET:N	2.12	0.46
3:C:97:GLU:OE2	3:C:97:GLU:HA	2.15	0.46
3:C:261:ASP:CB	3:C:282:ALA:HB3	2.45	0.46
3:C:292:GLY:O	3:C:302:LYS:HD2	2.16	0.46
3:C:307:HIS:HD2	3:C:335:TRP:O	1.99	0.46
1:D:166:SER:N	2:E:195:THR:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:O	1:A:184:GLN:HB3	2.15	0.46
2:B:381:ASP:HB2	2:B:393:GLN:OE1	2.16	0.46
2:E:280:THR:O	2:E:281:ASP:C	2.54	0.46
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.51	0.46
2:E:406:ARG:O	2:E:406:ARG:HG2	2.16	0.46
2:B:164:ASN:HD22	2:B:164:ASN:HA	1.60	0.45
2:B:408:HIS:O	4:H:1:GLY:N	2.39	0.45
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.16	0.45
3:C:365:ASN:ND2	3:C:365:ASN:N	2.61	0.45
2:B:181:LYS:O	2:B:184:SER:HB2	2.16	0.45
3:C:344:LEU:HD23	3:C:344:LEU:N	2.31	0.45
2:E:172:LEU:HD22	3:F:113:ILE:HB	1.98	0.45
3:F:234:HIS:NE2	3:F:269:PRO:HB3	2.31	0.45
1:A:127:ILE:HG22	1:A:130:VAL:HB	1.99	0.45
2:B:351:ASN:CG	2:B:354:MET:HB2	2.37	0.45
1:D:140:VAL:C	1:D:142:ALA:H	2.18	0.45
1:D:143:GLN:HB2	3:F:114:TYR:CE1	2.52	0.45
3:F:239:GLN:O	3:F:240:SER:C	2.54	0.45
3:C:96:TYR:CG	3:C:97:GLU:N	2.85	0.45
1:D:140:VAL:HA	3:F:114:TYR:CE1	2.51	0.45
3:F:231:GLU:O	3:F:235:LEU:HG	2.15	0.45
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.98	0.45
3:F:230:ASN:HB3	3:F:274:TYR:CG	2.52	0.45
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.85	0.45
2:E:238:VAL:HG22	2:E:239:TYR:N	2.32	0.45
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.84	0.45
2:E:385:TRP:CE2	4:J:3:ARG:HG2	2.52	0.45
3:F:121:ILE:O	3:F:125:LYS:HG3	2.17	0.45
2:B:211:CYS:SG	2:B:250:THR:HA	2.57	0.44
3:F:229:GLY:O	3:F:233:ILE:HG13	2.17	0.44
3:C:123:ASN:O	3:C:126:GLU:HB2	2.18	0.44
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.82	0.44
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.99	0.44
2:E:176:ARG:HD2	2:E:176:ARG:C	2.37	0.44
2:E:397:GLU:OE1	4:J:3:ARG:NH1	2.51	0.44
2:B:212:GLU:O	2:B:215:ILE:HG22	2.17	0.44
3:C:206:LYS:HB3	3:C:210:GLN:HB2	1.98	0.44
3:C:259:THR:O	3:C:286:ALA:HB3	2.17	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.81	0.44
3:F:248:VAL:HG13	3:F:344:LEU:HD11	1.99	0.44
3:F:389:PHE:C	3:F:391:ARG:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:2:NAG:O7	5:L:2:NAG:O4	2.32	0.44
2:B:212:GLU:OE2	2:B:216:ARG:HD3	2.17	0.44
2:E:172:LEU:HB3	3:F:113:ILE:CG2	2.43	0.44
2:B:202:ASN:HD21	2:B:284:ASN:HB2	1.78	0.44
2:E:279:ASN:O	2:E:281:ASP:N	2.51	0.43
3:F:110:LEU:N	3:F:110:LEU:HD23	2.33	0.43
3:F:322:PHE:HD1	3:F:338:LYS:HD2	1.83	0.43
4:I:3:ARG:CG	4:I:4:PRO:HD2	2.45	0.43
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.80	0.43
3:C:203:ASP:O	3:C:206:LYS:HE3	2.18	0.43
3:F:365:ASN:ND2	3:F:365:ASN:N	2.66	0.43
2:B:182:LEU:HB3	3:C:124:LEU:HD21	2.01	0.43
3:F:206:LYS:HB3	3:F:210:GLN:HB2	1.99	0.43
1:A:189:ILE:HG22	1:A:189:ILE:O	2.18	0.43
2:B:310:LEU:HB3	2:B:326:TYR:HB2	1.99	0.43
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.16	0.43
1:D:137:GLN:O	1:D:140:VAL:HG22	2.18	0.43
4:H:3:ARG:HA	4:H:3:ARG:HD3	1.86	0.43
3:F:249:GLU:CB	3:F:383:THR:HG23	2.45	0.43
3:C:294:ASP:C	3:C:296:GLY:H	2.22	0.43
1:D:177:ASP:O	1:D:181:GLN:HG3	2.18	0.43
2:E:179:ILE:O	2:E:183:GLU:HB2	2.19	0.43
2:B:161:ILE:H	2:B:161:ILE:CD1	2.31	0.43
1:D:143:GLN:HB2	3:F:114:TYR:HE1	1.84	0.43
2:E:165:LEU:HD21	3:F:110:LEU:HD12	2.00	0.43
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.48	0.43
2:B:385:TRP:CZ3	4:H:3:ARG:HG3	2.54	0.43
3:F:364:ASP:HB3	3:F:375:ARG:HG3	2.01	0.43
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.31	0.42
2:E:218:GLY:HA3	3:F:210:GLN:HG2	2.01	0.42
2:E:351:ASN:ND2	2:E:354:MET:H	2.17	0.42
2:E:422:TYR:HA	2:E:426:MET:CE	2.49	0.42
3:F:221:THR:O	3:F:223:THR:HG23	2.19	0.42
3:F:320:ASP:HB3	3:F:336:MET:HB2	2.00	0.42
1:A:185:LEU:HD22	1:A:189:ILE:CG1	2.49	0.42
3:F:206:LYS:HD2	3:F:210:GLN:OE1	2.19	0.42
3:F:217:HIS:O	3:F:224:THR:CG2	2.67	0.42
1:A:127:ILE:CG2	1:A:130:VAL:HG23	2.47	0.42
2:B:209:LYS:HD2	2:B:305:MET:HE1	2.01	0.42
2:B:367:MET:HE2	2:B:406:ARG:HD3	2.02	0.42
3:C:251:GLU:HG3	3:C:257:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.55	0.42
1:A:127:ILE:HG12	1:A:128:GLU:CD	2.40	0.42
1:A:134:GLN:O	1:A:138:LYS:HG3	2.19	0.42
2:B:159:SER:C	2:B:162:PRO:HD2	2.40	0.42
2:B:264:ARG:HB3	7:B:466:HOH:O	2.19	0.42
1:D:168:ALA:HA	2:E:189:GLN:NE2	2.24	0.42
5:K:1:NAG:H4	5:K:3:FUC:H5	2.02	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
2:B:383:ASP:OD1	2:B:383:ASP:C	2.57	0.42
3:C:143:VAL:HA	7:C:419:HOH:O	2.19	0.42
2:E:253:GLN:HB3	2:E:452:MET:HB2	2.01	0.42
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.84	0.42
2:E:212:GLU:HB2	2:E:456:PRO:HD2	2.02	0.42
2:E:245:GLU:O	2:E:246:ASN:HB2	2.19	0.42
2:B:411:ASN:N	2:B:412:PRO:HD3	2.35	0.42
2:E:169:ARG:O	2:E:173:GLU:HB2	2.19	0.42
2:B:345:TYR:CB	2:B:354:MET:HE3	2.44	0.41
3:C:113:ILE:HG13	3:C:114:TYR:N	2.34	0.41
1:D:165:CYS:HB3	2:E:193:CYS:HA	2.02	0.41
2:E:411:ASN:N	2:E:412:PRO:HD3	2.36	0.41
3:C:197:ARG:HG2	3:C:382:THR:CG2	2.50	0.41
2:E:271:GLN:HA	2:E:271:GLN:NE2	2.34	0.41
2:E:389:ASP:HA	2:E:390:PRO:HD2	1.94	0.41
3:F:273:LYS:HE3	3:F:319:ASN:ND2	2.35	0.41
2:B:212:GLU:HB2	2:B:456:PRO:HD2	2.02	0.41
2:B:406:ARG:N	2:B:407:CYS:HA	2.33	0.41
2:B:434:GLY:O	2:B:436:VAL:HG23	2.20	0.41
1:D:139:ASN:O	1:D:142:ALA:HB3	2.20	0.41
2:E:351:ASN:C	2:E:351:ASN:HD22	2.23	0.41
3:F:124:LEU:O	3:F:127:LYS:HB3	2.20	0.41
1:A:150:LEU:HD21	3:C:124:LEU:HD23	2.03	0.41
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.41
3:C:261:ASP:HB3	3:C:282:ALA:HB3	2.02	0.41
3:C:286:ALA:O	3:C:372:TRP:HB2	2.20	0.41
2:B:183:GLU:HG2	3:C:124:LEU:HD13	2.03	0.41
3:C:263:ALA:HB1	3:C:264:MET:HE2	2.01	0.41
1:D:148:LYS:HE3	1:D:175:LEU:HD12	2.01	0.41
1:D:162:ARG:HG2	1:D:162:ARG:HH11	1.85	0.41
2:B:217:LYS:CB	3:C:213:GLU:HG3	2.51	0.41
3:C:141:ASP:OD1	3:C:143:VAL:HG13	2.20	0.41
1:A:185:LEU:HD22	1:A:189:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:VAL:HG11	2:B:440:TRP:NE1	2.36	0.41
3:C:131:LEU:O	3:C:134:GLN:HB2	2.20	0.41
2:E:253:GLN:HE22	2:E:451:SER:HA	1.84	0.41
3:F:292:GLY:C	3:F:302:LYS:HD3	2.41	0.41
2:B:224:MET:CE	2:B:237:ARG:HD3	2.48	0.41
2:B:315:GLU:HA	2:B:320:ASP:O	2.20	0.41
2:B:263:GLY:HA2	2:B:400:GLY:HA2	2.03	0.41
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.56	0.41
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.56	0.41
3:F:197:ARG:HD3	3:F:204:PHE:CZ	2.55	0.41
2:B:168:LEU:HB3	3:C:110:LEU:HD13	2.02	0.41
3:C:196:LYS:HD2	3:C:383:THR:HB	2.02	0.41
3:C:266:LYS:HE3	3:C:266:LYS:HB2	1.82	0.40
3:C:393:THR:O	3:C:393:THR:HG22	2.21	0.40
2:E:234:LYS:HA	2:E:235:PRO:HD3	1.95	0.40
3:F:344:LEU:HA	3:F:367:ILE:HG23	2.03	0.40
3:C:275:ARG:NH2	3:C:311:GLN:HE21	2.19	0.40
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.51	0.40
3:F:307:HIS:CE1	3:F:342:GLY:H	2.39	0.40
1:A:133:ILE:HD11	2:B:164:ASN:HB3	2.02	0.40
2:B:172:LEU:CB	3:C:113:ILE:HD11	2.51	0.40
2:B:302:LEU:HD13	2:B:454:ILE:HD11	2.04	0.40
3:F:304:PHE:O	3:F:337:ASN:HB3	2.21	0.40
3:F:391:ARG:HD2	3:F:391:ARG:HA	1.89	0.40
1:A:158:ILE:HG23	2:B:189:GLN:NE2	2.33	0.40
2:B:417:TYR:HB2	2:B:446:SER:HB3	2.03	0.40
3:F:315:TRP:CZ3	3:F:316:ASP:HB3	2.56	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%)	59 (94%)	4 (6%)	0	100 100
1	D	54/66 (82%)	44 (82%)	9 (17%)	1 (2%)	8 20
2	B	299/313 (96%)	266 (89%)	30 (10%)	3 (1%)	15 37
2	E	292/313 (93%)	268 (92%)	21 (7%)	3 (1%)	15 37
3	C	297/311 (96%)	269 (91%)	23 (8%)	5 (2%)	9 23
3	F	283/311 (91%)	262 (93%)	17 (6%)	4 (1%)	11 28
4	G	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	I	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	J	2/4 (50%)	2 (100%)	0	0	100 100
All	All	1296/1396 (93%)	1173 (90%)	107 (8%)	16 (1%)	13 32

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	435	VAL
3	C	97	GLU
3	C	301	ALA
1	D	137	GLN
2	E	281	ASP
3	F	241	ALA
2	B	281	ASP
3	C	198	LEU
3	F	240	SER
2	B	256	GLN
2	E	256	GLN
3	F	199	ASP
2	E	280	THR
3	F	390	ASN
3	C	241	ALA
3	C	303	PHE

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%)	57 (95%)	3 (5%)	24 51
1	D	52/61 (85%)	49 (94%)	3 (6%)	20 43
2	B	259/271 (96%)	252 (97%)	7 (3%)	44 74
2	E	252/271 (93%)	244 (97%)	8 (3%)	39 68
3	C	250/257 (97%)	238 (95%)	12 (5%)	25 53
3	F	237/257 (92%)	227 (96%)	10 (4%)	30 58
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%)	2 (67%)	1 (33%)	0 0
All	All	1122/1190 (94%)	1076 (96%)	46 (4%)	30 59

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	144	LEU
1	A	185	LEU
2	B	164	ASN
2	B	196	PRO
2	B	210	GLU
2	B	253	GLN
2	B	301	GLN
2	B	304	ARG
2	B	351	ASN
3	C	96	TYR
3	C	104	ASP
3	C	118	ASN
3	C	143	VAL
3	C	163	GLN
3	C	250	LEU
3	C	302	LYS
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	382	THR
3	C	383	THR
1	D	138	LYS
1	D	172	GLU

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Mol	Chain	Res	Type
1	D	176	LYS
2	E	190	MET
2	E	210	GLU
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	301	GLN
2	E	321	LYS
2	E	351	ASN
3	F	113	ILE
3	F	172	LEU
3	F	176	GLN
3	F	250	LEU
3	F	302	LYS
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR
4	G	3	ARG
4	I	3	ARG
4	J	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	139	ASN
1	A	181	GLN
1	A	187	GLN
2	B	164	ASN
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	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	408	HIS

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Mol	Chain	Res	Type
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	163	GLN
3	C	176	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
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	143	GLN
1	D	187	GLN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	123	ASN
3	F	144	GLN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN

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Mol	Chain	Res	Type
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	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	5,2	14,14,15	0.70	0	17,19,21	0.74	1 (5%)
5	NAG	K	2	5	14,14,15	0.66	0	17,19,21	0.62	0
5	FUC	K	3	5	10,10,11	0.61	0	14,14,16	0.40	0
5	NAG	L	1	5,2	14,14,15	0.62	0	17,19,21	1.30	3 (17%)
5	NAG	L	2	5	14,14,15	0.75	0	17,19,21	0.74	0
5	FUC	L	3	5	10,10,11	0.62	0	14,14,16	0.81	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	5,2	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	5,2	-	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 (5) 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	114.84	110.24
5	L	1	NAG	C2-N2-C7	-2.48	119.37	122.90
5	L	1	NAG	O5-C1-C2	-2.30	107.66	111.29
5	K	1	NAG	C2-N2-C7	-2.16	119.83	122.90
5	L	3	FUC	C1-C2-C3	2.05	112.19	109.67

There are no chirality outliers.

All (13) 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	C1-C2-N2-C7
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	L	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	L	2	NAG	C1-C2-N2-C7
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C3-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	3	FUC	1	0
5	L	1	NAG	9	0

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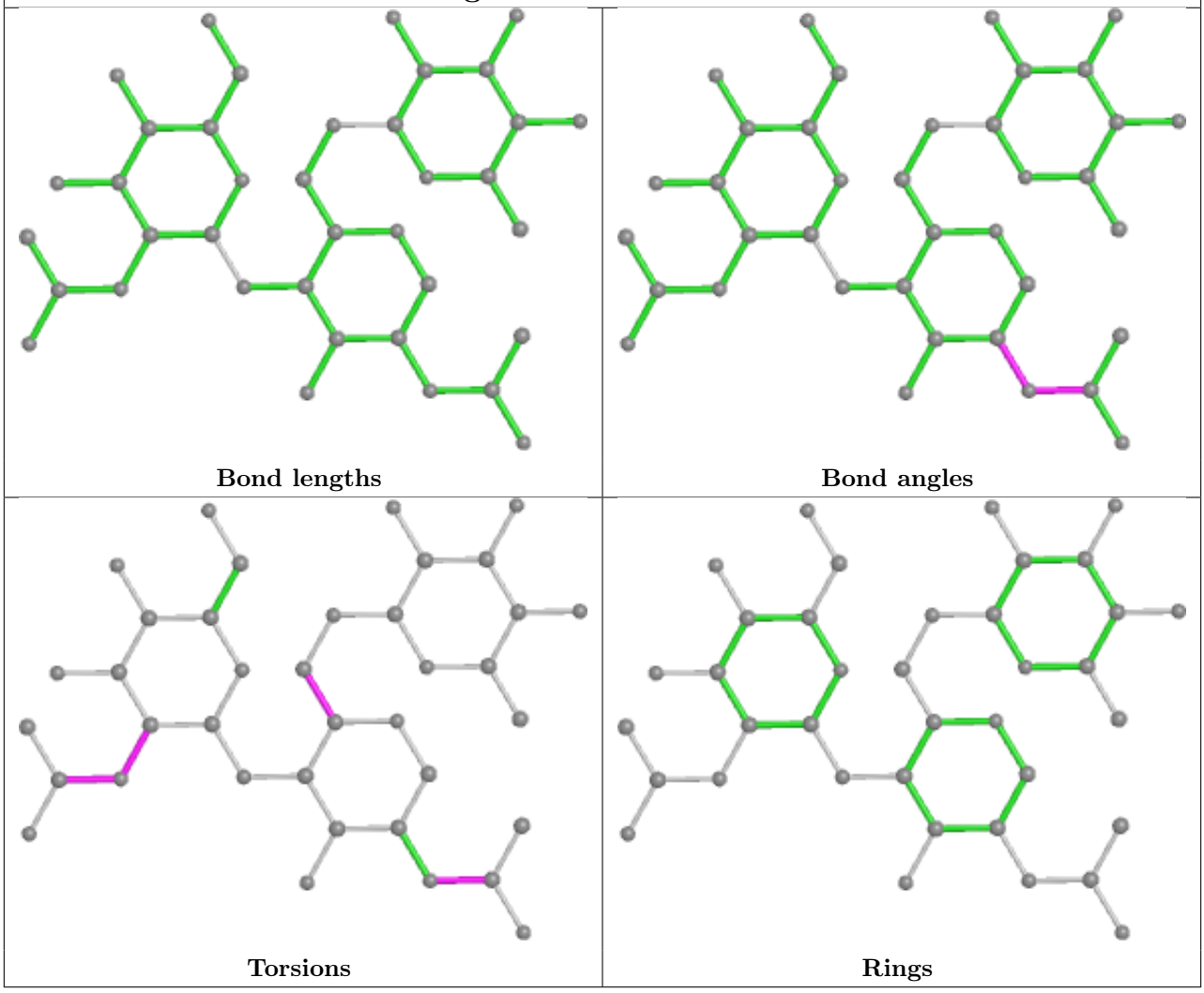
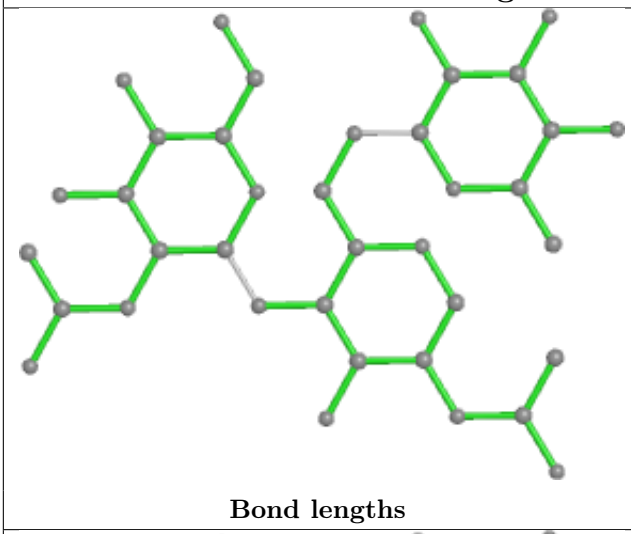
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	NAG	5	0
5	K	1	NAG	5	0
5	L	3	FUC	6	0

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

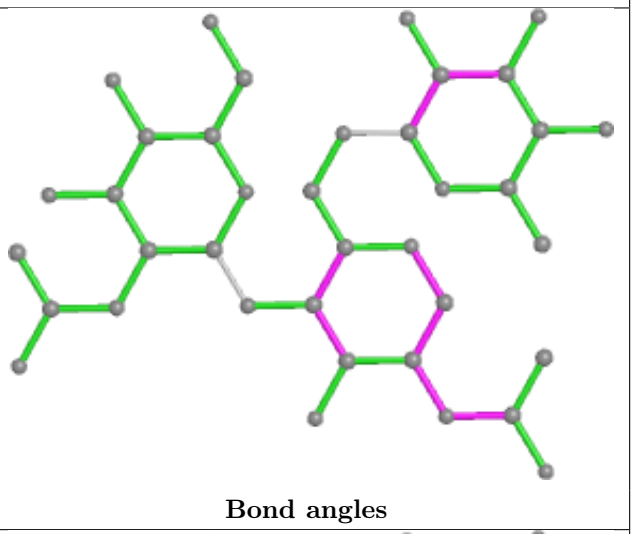
Oligosaccharide Chain K



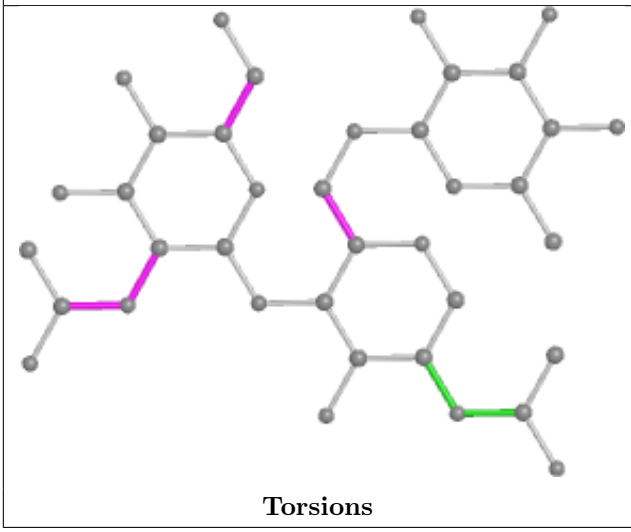
Oligosaccharide Chain L



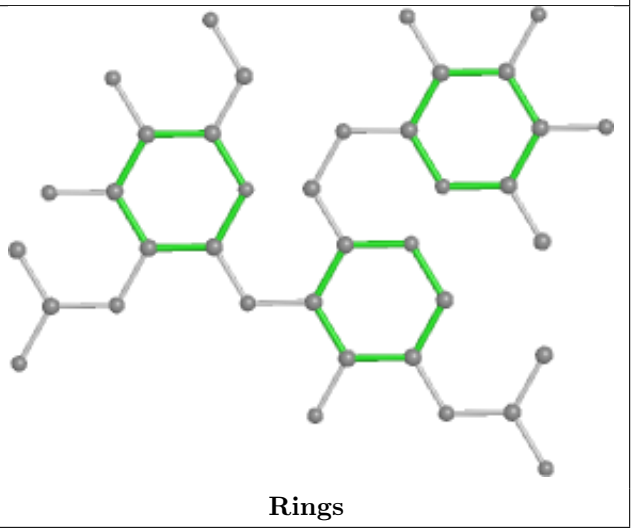
Bond lengths



Bond angles



Torsions



Rings

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

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	65/66 (98%)	0.27	5 (7%) 13 11	24, 57, 85, 99	0
1	D	56/66 (84%)	0.73	10 (17%) 1 1	24, 68, 110, 115	0
2	B	301/313 (96%)	-0.10	7 (2%) 60 62	22, 41, 69, 96	0
2	E	294/313 (93%)	-0.40	5 (1%) 70 72	13, 26, 64, 105	0
3	C	299/311 (96%)	-0.06	10 (3%) 46 46	25, 44, 70, 86	0
3	F	285/311 (91%)	-0.24	12 (4%) 36 35	16, 30, 66, 113	0
4	G	4/4 (100%)	0.65	0 100 100	63, 64, 65, 70	0
4	H	4/4 (100%)	0.57	0 100 100	62, 62, 65, 66	0
4	I	4/4 (100%)	-0.03	0 100 100	36, 38, 40, 43	0
4	J	4/4 (100%)	-0.02	0 100 100	34, 37, 38, 41	0
All	All	1316/1396 (94%)	-0.13	49 (3%) 41 41	13, 37, 80, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	VAL	6.8
3	F	394	ILE	5.9
3	C	394	ILE	5.4
1	D	133	ILE	4.8
3	F	110	LEU	4.6
1	D	138	LYS	4.5
3	C	240	SER	4.2
3	F	393	THR	3.8
3	F	113	ILE	3.6
3	C	393	THR	3.4
2	E	169	ARG	3.3
1	D	140	VAL	3.3
3	C	241	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	281	ASP	3.1
2	B	458	PHE	3.1
1	D	135	LEU	3.1
1	D	134	GLN	3.1
3	C	96	TYR	3.1
1	A	127	ILE	3.1
3	F	240	SER	3.0
2	B	162	PRO	2.9
3	F	297	ASP	2.9
2	E	281	ASP	2.9
2	E	458	PHE	2.9
3	F	114	TYR	2.9
3	F	241	ALA	2.9
3	F	120	LYS	2.8
1	D	187	GLN	2.6
3	C	109	TYR	2.6
1	D	184	GLN	2.5
1	A	128	GLU	2.5
3	C	360	PRO	2.5
2	B	158	ASN	2.4
2	B	280	THR	2.4
1	A	174	ASP	2.4
3	F	111	GLN	2.3
3	F	299	PRO	2.3
2	B	386	LEU	2.3
3	C	175	ASN	2.2
1	D	176	LYS	2.2
3	F	115	ASN	2.2
3	C	254	ASN	2.2
3	C	357	ALA	2.2
1	A	190	ALA	2.1
1	D	183	LYS	2.1
2	E	171	ILE	2.1
1	D	186	GLU	2.1
2	B	387	THR	2.1
2	E	318	LYS	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)

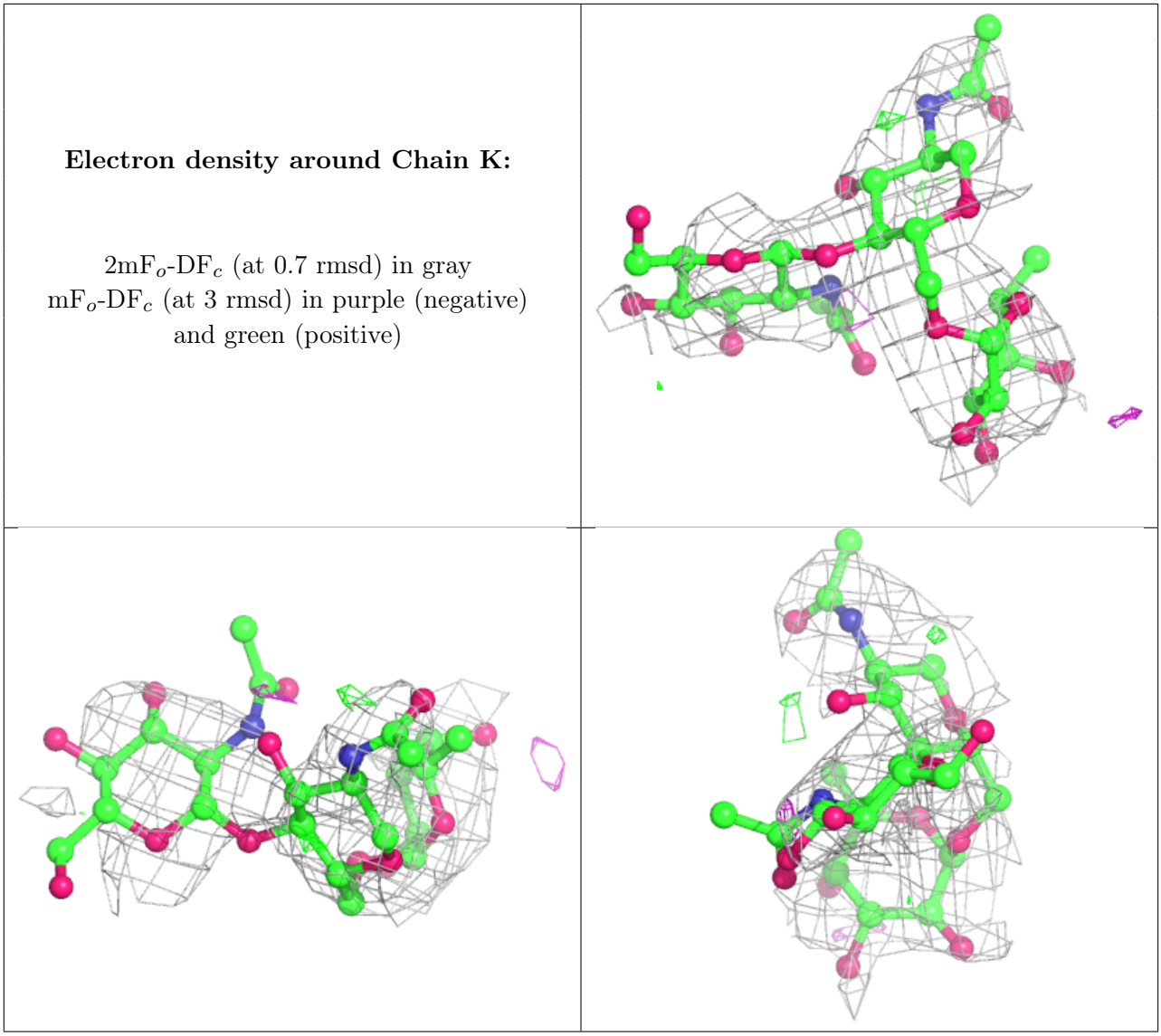
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	K	2	14/15	0.72	0.55	105,106,108,109	0
5	NAG	L	2	14/15	0.73	0.41	69,72,77,78	0
5	FUC	K	3	10/11	0.75	0.40	101,103,103,103	0
5	NAG	K	1	14/15	0.76	0.32	91,95,100,102	0
5	NAG	L	1	14/15	0.86	0.19	48,56,61,67	0
5	FUC	L	3	10/11	0.93	0.29	62,63,63,64	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.

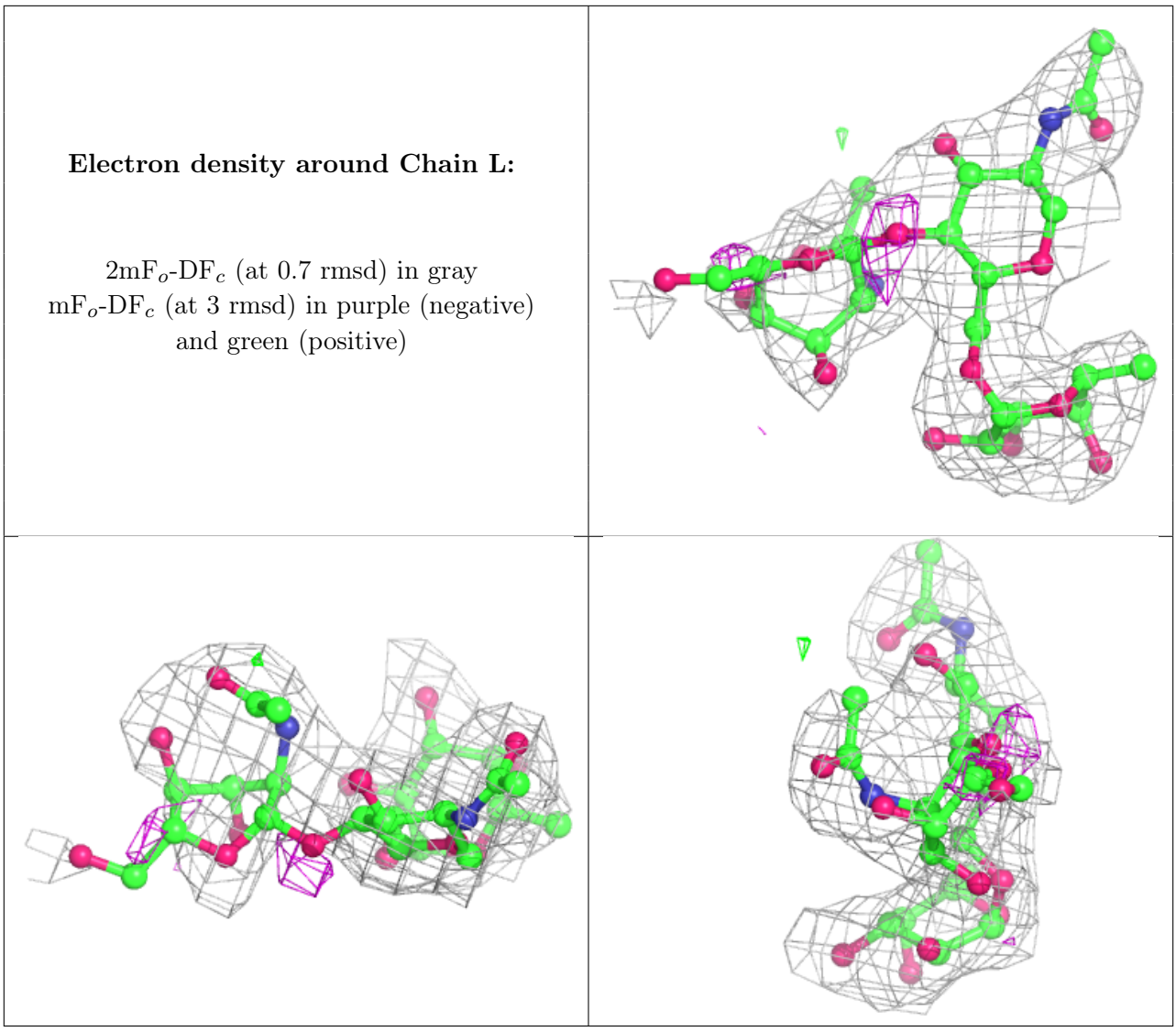
Electron density around Chain K:

$2mF_o$-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	E	2	1/1	0.91	0.10	29,29,29,29	0
6	CA	B	2	1/1	0.93	0.05	54,54,54,54	0
6	CA	F	1	1/1	0.96	0.05	29,29,29,29	0
6	CA	C	1	1/1	0.98	0.04	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.