Full wwPDB X-ray Structure Validation Report

Aug 8, 2020 – 09:54 AM BST

PDB ID	:	1G7Y
Title	:	THE CRYSTAL STRUCTURE OF THE 58KD VEGETATIVE LECTIN FROM THE TROPICAL LEGUME DOLICHOS BIFLORUS
Authors	:	Buts, L.; Hamelryck, T.W.; Loris, R.; Dao-Thi, M.-H.; Wyns, L.; Etzler, M.E.
Deposited on	:	2000-11-15
Resolution	:	2.50 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 (1)) were used in the production of this report:

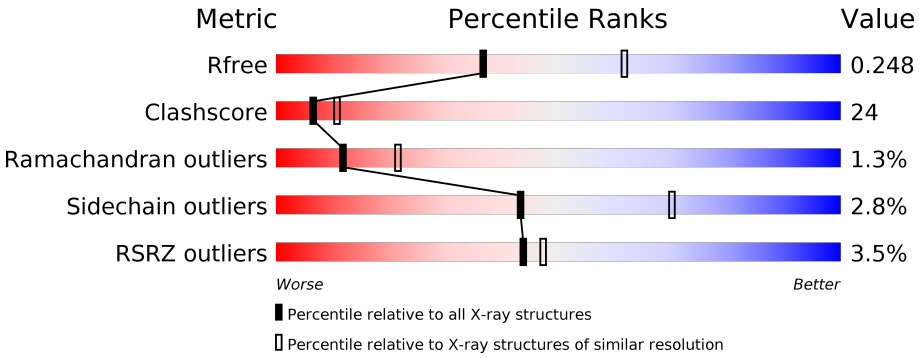
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	253	3% 74% 23%
1	B	253	5% 77% 18%
1	C	253	% 74% 23%
1	D	253	5% 76% 21%
1	E	253	3% 71% 25%
1	F	253	4% 75% 20%

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Mol	Chain	Length	Quality of chain
2	G	3	100%
2	I	3	100%
3	H	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
2	FUC	G	2	-	-	-	X
3	FUL	H	2	-	-	-	X
3	NAG	H	3	-	-	-	X

2 Entry composition

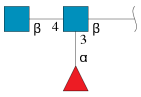
There are 6 unique types of molecules in this entry. The entry contains 11211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STEM/LEAF LECTIN DB58.

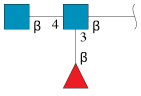
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	0	0	0
			1847	1168	299	380			
1	B	246	Total	C	N	O	0	0	0
			1823	1155	293	375			
1	C	251	Total	C	N	O	0	0	0
			1851	1169	298	384			
1	D	253	Total	C	N	O	0	0	0
			1866	1179	300	387			
1	E	249	Total	C	N	O	0	0	0
			1833	1159	297	377			
1	F	246	Total	C	N	O	0	0	0
			1824	1155	294	375			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mn 1 1	0	0
5	E	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0
5	A	1	Total Mn 1 1	0	0
5	F	1	Total Mn 1 1	0	0

- Molecule 6 is water.

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

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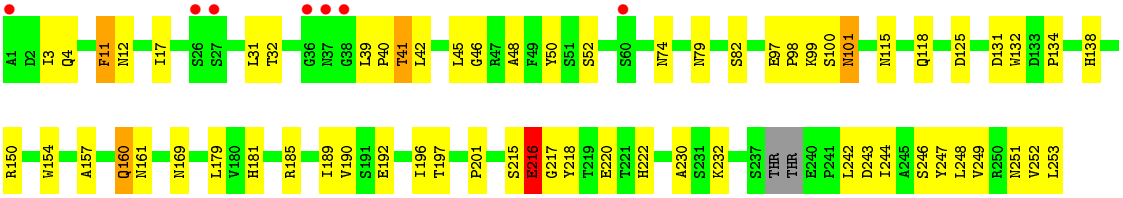
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	7	Total O 7 7	0	0
6	D	5	Total O 5 5	0	0
6	E	8	Total O 8 8	0	0
6	F	8	Total O 8 8	0	0

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.

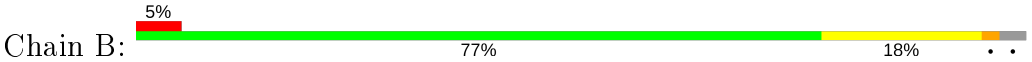
- Molecule 1: STEM/LEAF LECTIN DB58

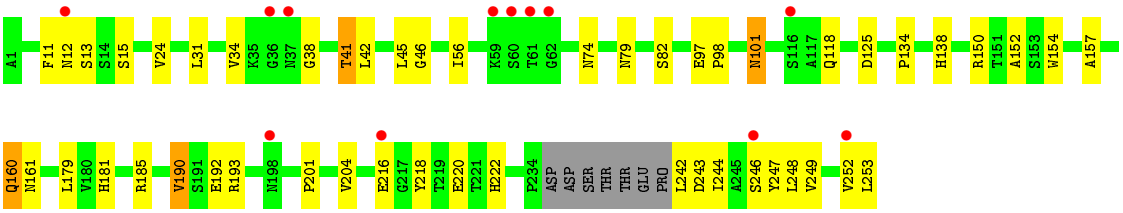
Chain A:



- Molecule 1: STEM/LEAF LECTIN DB58

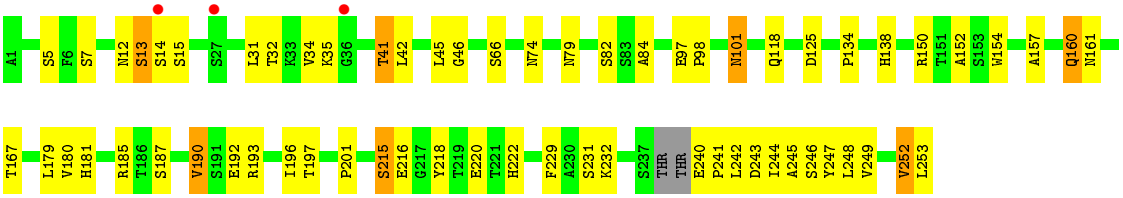
Chain B:





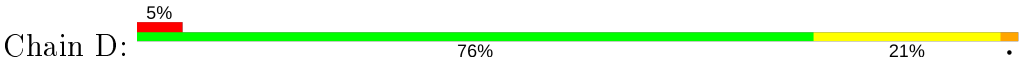
- Molecule 1: STEM/LEAF LECTIN DB58

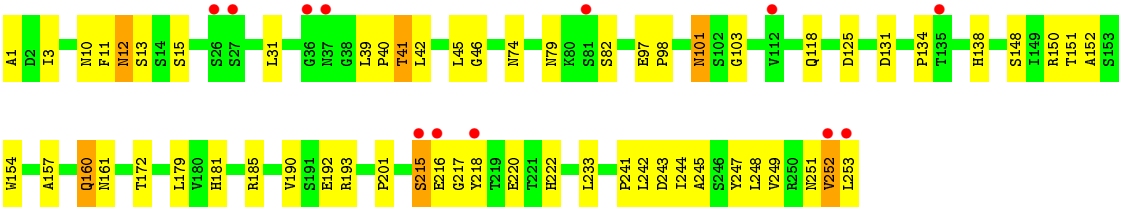
Chain C:



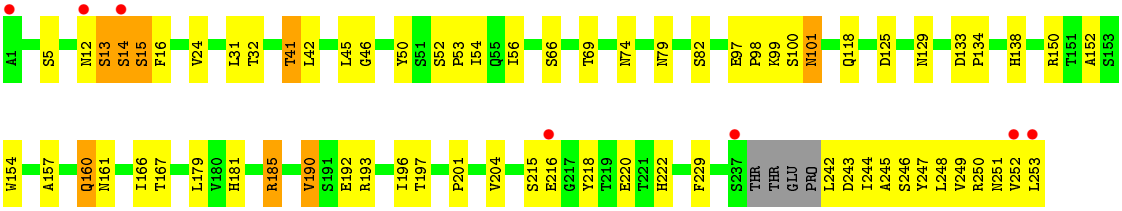
- Molecule 1: STEM/LEAF LECTIN DB58

Chain D:

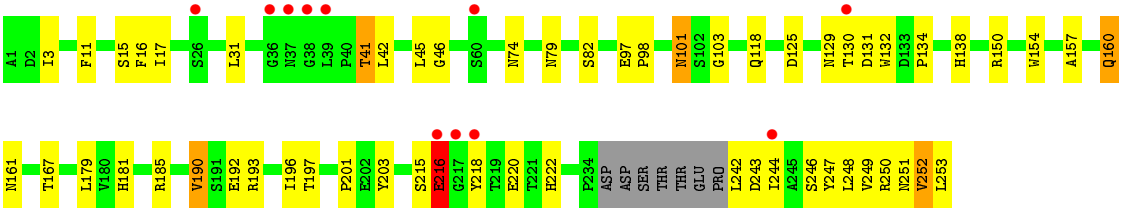




• Molecule 1: STEM/LEAF LECTIN DB58



• Molecule 1: STEM/LEAF LECTIN DB58



• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose


NAG1
FUL2
NAG3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.94Å 130.27Å 137.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-2.50) 93.7 (19.95-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.247 0.222 , 0.248	Depositor DCC
R_{free} test set	5994 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11211	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 3.80% 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, MN, NAG, FUL, 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	0.41	0/1887	0.67	0/2579
1	B	0.38	0/1862	0.69	0/2548
1	C	0.42	0/1890	0.71	1/2585 (0.0%)
1	D	0.40	0/1907	0.67	0/2612
1	E	0.40	0/1873	0.71	2/2561 (0.1%)
1	F	0.39	0/1864	0.69	2/2550 (0.1%)
All	All	0.40	0/11283	0.69	5/15435 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	185	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	185	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	84	ALA	C-N-CA	5.65	135.83	121.70
1	F	190	VAL	CB-CA-C	-5.34	101.25	111.40
1	F	17	ILE	N-CA-C	-5.16	97.06	111.00

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	1847	0	1714	123	0
1	B	1823	0	1699	116	0
1	C	1851	0	1708	123	0
1	D	1866	0	1733	123	0
1	E	1833	0	1706	150	0
1	F	1824	0	1707	149	0
2	G	38	0	34	1	0
2	I	38	0	34	0	0
3	H	38	0	34	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	7	0	0	0	0
6	D	5	0	0	1	0
6	E	8	0	0	1	0
6	F	8	0	0	0	0
All	All	11211	0	10369	511	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 24.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:CG1	1:C:244:ILE:H	1.19	1.55
1:A:251:ASN:ND2	1:C:246:SER:CB	1.70	1.54
1:A:244:ILE:H	1:C:252:VAL:CG1	1.25	1.49
1:E:248:LEU:CB	1:F:244:ILE:HD13	1.15	1.46
1:A:252:VAL:HG12	1:C:244:ILE:N	1.20	1.40
1:E:242:LEU:CB	1:F:253:LEU:HB2	1.45	1.38
1:E:248:LEU:HB3	1:F:244:ILE:CD1	1.00	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:ND2	1:C:246:SER:HB3	1.31	1.31
1:B:246:SER:CB	1:D:251:ASN:HD21	1.42	1.31
1:E:242:LEU:O	1:F:252:VAL:N	1.63	1.28
1:B:252:VAL:CG1	1:D:242:LEU:O	1.79	1.27
1:A:244:ILE:N	1:C:252:VAL:CG1	1.94	1.26
1:B:244:ILE:HG12	1:D:252:VAL:CG1	1.66	1.26
1:E:242:LEU:C	1:F:252:VAL:H	1.40	1.24
1:B:242:LEU:O	1:D:252:VAL:CG1	1.85	1.24
1:B:252:VAL:HG13	1:D:242:LEU:O	1.35	1.23
1:A:244:ILE:N	1:C:252:VAL:HG13	1.47	1.22
1:E:253:LEU:N	1:F:242:LEU:O	1.72	1.22
1:B:244:ILE:N	1:D:252:VAL:HG12	1.53	1.22
1:B:246:SER:CB	1:D:251:ASN:ND2	2.03	1.21
1:B:242:LEU:O	1:D:252:VAL:HG13	1.04	1.18
1:E:252:VAL:N	1:F:243:ASP:HA	1.55	1.17
1:B:253:LEU:HD12	1:D:242:LEU:HB3	1.17	1.17
1:B:247:TYR:CB	1:D:248:LEU:H	1.56	1.16
1:A:247:TYR:CB	1:C:248:LEU:N	2.09	1.15
1:A:249:VAL:O	1:C:242:LEU:HA	1.46	1.15
1:B:247:TYR:HB3	1:D:248:LEU:H	1.06	1.13
1:A:253:LEU:HB2	1:C:242:LEU:CB	1.61	1.12
1:B:253:LEU:HD12	1:D:242:LEU:CB	1.80	1.12
1:B:244:ILE:H	1:D:252:VAL:CG1	1.63	1.12
1:E:244:ILE:HG12	1:F:252:VAL:CG1	1.79	1.12
1:A:247:TYR:HD1	1:C:246:SER:CA	1.17	1.11
1:A:248:LEU:N	1:C:247:TYR:HB3	1.47	1.11
1:E:247:TYR:CB	1:F:244:ILE:O	1.91	1.10
1:A:247:TYR:CB	1:C:248:LEU:H	1.64	1.10
1:B:252:VAL:HG12	1:D:244:ILE:N	1.66	1.10
1:E:248:LEU:HD13	1:F:244:ILE:HD12	1.31	1.09
1:A:251:ASN:ND2	1:C:246:SER:HB2	1.43	1.09
1:E:242:LEU:HB2	1:F:253:LEU:HB2	1.20	1.08
1:E:243:ASP:H	1:F:250:ARG:N	1.49	1.08
1:E:244:ILE:HG12	1:F:252:VAL:HG11	1.25	1.07
1:B:247:TYR:CB	1:D:248:LEU:N	2.10	1.07
1:B:242:LEU:HB3	1:D:253:LEU:HD12	1.07	1.07
1:B:252:VAL:CG1	1:D:244:ILE:H	1.66	1.06
1:B:246:SER:HB2	1:D:251:ASN:ND2	1.66	1.06
1:B:252:VAL:HG12	1:D:244:ILE:H	0.95	1.05
1:A:247:TYR:HB3	1:C:248:LEU:N	1.51	1.04
1:E:249:VAL:O	1:F:242:LEU:CA	2.01	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:HB3	1:C:248:LEU:H	0.87	1.02
1:E:247:TYR:HB3	1:F:244:ILE:O	1.21	1.01
1:B:242:LEU:HB3	1:D:253:LEU:CD1	1.90	1.01
1:B:247:TYR:HB3	1:D:248:LEU:N	1.66	1.01
1:B:246:SER:HB2	1:D:251:ASN:HD21	0.86	1.01
1:B:244:ILE:HG12	1:D:252:VAL:HG11	1.05	1.00
1:E:252:VAL:H	1:F:242:LEU:C	1.64	1.00
1:E:243:ASP:HA	1:F:252:VAL:N	1.56	1.00
1:A:248:LEU:N	1:C:247:TYR:CB	2.23	1.00
1:E:242:LEU:CB	1:F:253:LEU:CB	2.39	0.99
1:B:248:LEU:N	1:D:247:TYR:HB3	1.71	0.99
1:B:246:SER:HB3	1:D:251:ASN:ND2	1.76	0.99
1:E:252:VAL:N	1:F:243:ASP:CA	2.26	0.98
1:B:248:LEU:H	1:D:247:TYR:HB3	1.20	0.98
1:A:253:LEU:HB2	1:C:242:LEU:HB2	1.47	0.97
1:E:244:ILE:CG1	1:F:252:VAL:HG11	1.93	0.97
1:E:243:ASP:CA	1:F:252:VAL:N	2.27	0.97
1:E:242:LEU:HB3	1:F:253:LEU:HB2	1.47	0.96
1:E:253:LEU:H	1:F:242:LEU:C	1.69	0.96
1:B:247:TYR:HB2	1:D:248:LEU:N	1.76	0.95
1:B:242:LEU:CB	1:D:253:LEU:HD12	1.97	0.94
1:E:249:VAL:O	1:F:242:LEU:HA	1.12	0.94
1:A:248:LEU:H	1:C:247:TYR:HB3	1.02	0.94
1:B:242:LEU:C	1:D:253:LEU:N	2.21	0.94
1:B:252:VAL:HG12	1:D:242:LEU:O	1.65	0.93
1:A:252:VAL:CG1	1:C:242:LEU:O	2.18	0.92
1:B:244:ILE:CG2	1:D:244:ILE:HG22	1.99	0.92
1:B:244:ILE:CG1	1:D:252:VAL:HG11	1.98	0.91
1:E:248:LEU:HB3	1:F:244:ILE:HD12	1.50	0.90
1:B:242:LEU:O	1:D:253:LEU:N	2.04	0.90
1:E:248:LEU:CD1	1:F:244:ILE:HD12	1.88	0.90
1:E:244:ILE:O	1:F:247:TYR:HB3	1.70	0.90
1:A:252:VAL:HG13	1:C:242:LEU:O	1.69	0.90
1:A:253:LEU:HB2	1:C:242:LEU:HB3	1.53	0.89
1:B:253:LEU:CD1	1:D:242:LEU:CB	2.42	0.89
1:B:244:ILE:H	1:D:252:VAL:HG12	0.74	0.88
1:A:242:LEU:HB3	1:C:253:LEU:HD12	1.54	0.88
1:E:253:LEU:HB2	1:F:242:LEU:N	1.89	0.87
1:E:247:TYR:HB3	1:F:248:LEU:H	1.38	0.87
1:A:247:TYR:HB2	1:C:248:LEU:N	1.90	0.86
1:E:252:VAL:H	1:F:243:ASP:CA	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:N	1:F:243:ASP:H	1.71	0.86
1:E:253:LEU:HB2	1:F:242:LEU:CB	2.05	0.86
1:E:242:LEU:C	1:F:252:VAL:N	2.18	0.86
1:A:244:ILE:H	1:C:252:VAL:HG13	0.70	0.85
1:B:252:VAL:HG11	1:D:244:ILE:HG12	1.56	0.85
1:B:252:VAL:CG1	1:D:244:ILE:HG12	2.07	0.85
1:B:242:LEU:HA	1:D:249:VAL:O	1.77	0.85
1:E:248:LEU:CB	1:F:244:ILE:CD1	1.75	0.84
1:E:248:LEU:CB	1:F:244:ILE:HD12	1.97	0.84
1:B:253:LEU:CD1	1:D:242:LEU:HB2	2.06	0.83
1:E:252:VAL:H	1:F:243:ASP:HA	1.39	0.83
1:E:243:ASP:N	1:F:252:VAL:H	1.75	0.83
1:A:249:VAL:O	1:C:242:LEU:CA	2.27	0.82
1:E:252:VAL:H	1:F:243:ASP:N	1.76	0.82
1:A:244:ILE:N	1:C:252:VAL:HG12	1.92	0.82
1:E:248:LEU:CA	1:F:244:ILE:HD13	2.09	0.82
1:A:249:VAL:C	1:C:243:ASP:H	1.83	0.81
1:B:248:LEU:N	1:D:247:TYR:CB	2.40	0.81
1:A:252:VAL:HG12	1:C:243:ASP:C	2.01	0.81
1:A:242:LEU:HB3	1:C:253:LEU:CD1	2.11	0.80
1:A:243:ASP:HA	1:C:252:VAL:CG1	2.06	0.80
1:E:193:ARG:NH1	1:E:193:ARG:HB2	1.97	0.80
1:E:242:LEU:O	1:F:252:VAL:CG1	2.30	0.79
1:B:253:LEU:CD1	1:D:242:LEU:HB3	1.96	0.79
1:B:242:LEU:C	1:D:253:LEU:H	1.80	0.79
1:E:246:SER:HB3	1:F:247:TYR:HA	1.65	0.78
1:B:244:ILE:HG22	1:D:244:ILE:CG2	2.14	0.78
1:B:246:SER:H	1:D:251:ASN:HD22	1.32	0.78
1:E:248:LEU:H	1:F:247:TYR:HB3	1.48	0.77
1:E:244:ILE:H	1:F:252:VAL:CG1	1.95	0.77
1:E:247:TYR:HA	1:F:246:SER:CB	2.16	0.76
1:E:253:LEU:N	1:F:242:LEU:N	2.27	0.76
1:E:252:VAL:HG13	1:F:244:ILE:N	2.01	0.76
1:E:244:ILE:HG23	1:F:244:ILE:HG22	1.67	0.76
1:E:253:LEU:HB2	1:F:242:LEU:HB3	1.67	0.76
1:D:252:VAL:HG13	1:D:253:LEU:H	1.49	0.75
1:E:247:TYR:HA	1:F:246:SER:HB2	1.66	0.75
1:B:244:ILE:HG22	1:D:244:ILE:HG22	1.68	0.75
1:E:252:VAL:N	1:F:242:LEU:O	2.19	0.75
1:E:243:ASP:H	1:F:249:VAL:C	1.88	0.75
1:A:242:LEU:O	1:C:252:VAL:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:SER:HB2	1:F:251:ASN:ND2	2.02	0.74
1:A:243:ASP:HA	1:C:252:VAL:HG12	1.69	0.73
1:E:185:ARG:HD2	1:F:192:GLU:OE2	1.87	0.73
1:A:252:VAL:CG1	1:C:244:ILE:HG12	2.17	0.73
1:E:252:VAL:HG13	1:F:243:ASP:HA	1.71	0.73
1:B:152:ALA:HB2	1:B:190:VAL:HG13	1.70	0.72
1:D:152:ALA:HB3	1:D:190:VAL:HG22	1.71	0.72
1:C:152:ALA:HB2	1:C:190:VAL:HG13	1.71	0.72
1:E:248:LEU:N	1:F:247:TYR:HB3	2.03	0.71
1:A:252:VAL:CG1	1:C:244:ILE:N	2.04	0.71
1:E:152:ALA:HB2	1:E:190:VAL:HG13	1.72	0.71
1:E:244:ILE:O	1:F:247:TYR:CB	2.30	0.71
1:E:242:LEU:HB2	1:F:253:LEU:CB	2.11	0.71
1:E:244:ILE:H	1:F:252:VAL:HG12	1.54	0.71
1:A:248:LEU:C	1:C:243:ASP:C	2.38	0.71
1:E:249:VAL:C	1:F:243:ASP:H	1.94	0.70
1:A:242:LEU:HD12	1:A:243:ASP:H	1.57	0.70
1:E:244:ILE:N	1:F:252:VAL:HG12	2.06	0.70
1:E:242:LEU:HB3	1:F:253:LEU:CB	2.16	0.69
1:E:243:ASP:N	1:F:250:ARG:N	2.34	0.69
1:A:243:ASP:CA	1:C:252:VAL:CG1	2.71	0.69
1:E:193:ARG:HH11	1:E:193:ARG:HB2	1.58	0.69
1:C:42:LEU:HD13	1:C:215:SER:O	1.94	0.68
1:E:249:VAL:C	1:F:243:ASP:N	2.48	0.67
1:E:245:ALA:O	1:F:247:TYR:HB2	1.95	0.66
1:B:246:SER:H	1:D:251:ASN:ND2	1.92	0.66
1:A:185:ARG:HD2	1:C:192:GLU:OE2	1.96	0.66
1:A:243:ASP:HB3	1:C:247:TYR:O	1.96	0.65
1:A:252:VAL:HG13	1:C:244:ILE:HG12	1.79	0.65
1:C:152:ALA:CB	1:C:190:VAL:HG13	2.26	0.65
1:A:247:TYR:CD1	1:C:246:SER:CA	2.05	0.65
1:F:129:ASN:HD22	1:F:132:TRP:HZ2	1.41	0.65
1:E:242:LEU:O	1:F:252:VAL:HG12	1.95	0.64
1:B:185:ARG:HD2	1:D:192:GLU:OE2	1.98	0.64
1:B:249:VAL:O	1:D:242:LEU:HD12	1.97	0.64
1:A:252:VAL:HG12	1:C:244:ILE:H	0.47	0.63
1:E:247:TYR:CB	1:F:248:LEU:H	2.10	0.63
1:A:189:ILE:HD13	1:C:187:SER:HB2	1.81	0.63
1:E:246:SER:CB	1:F:247:TYR:HA	2.13	0.63
1:A:247:TYR:HD1	1:C:246:SER:HA	1.49	0.62
1:E:253:LEU:HD12	1:F:242:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASP:CA	1:C:252:VAL:HG12	2.28	0.62
1:C:150:ARG:NH1	1:C:192:GLU:OE1	2.33	0.62
1:B:246:SER:N	1:D:251:ASN:ND2	2.47	0.62
1:A:252:VAL:HG11	1:C:244:ILE:HB	1.81	0.61
1:A:243:ASP:C	1:C:252:VAL:CG1	2.65	0.61
1:E:252:VAL:CA	1:F:242:LEU:O	2.48	0.61
1:D:152:ALA:CB	1:D:190:VAL:HG22	2.29	0.61
1:F:3:ILE:HD12	1:F:3:ILE:N	2.16	0.61
1:B:244:ILE:CG2	1:D:244:ILE:CG2	2.71	0.61
1:B:247:TYR:O	1:D:243:ASP:HB3	2.00	0.61
1:A:252:VAL:HG11	1:C:244:ILE:CB	2.31	0.60
1:E:252:VAL:CG1	1:F:243:ASP:HA	2.31	0.60
1:E:242:LEU:HB3	1:F:253:LEU:CG	2.32	0.60
1:D:42:LEU:HD13	1:D:215:SER:O	2.02	0.60
1:B:244:ILE:CG1	1:D:252:VAL:CG1	2.61	0.60
1:E:251:ASN:ND2	1:F:246:SER:HB2	2.17	0.59
1:C:97:GLU:HG3	1:C:98:PRO:HD2	1.85	0.59
1:F:248:LEU:O	1:F:252:VAL:HG12	2.02	0.59
1:D:42:LEU:HD11	1:D:216:GLU:HA	1.83	0.59
1:A:248:LEU:HD23	1:A:252:VAL:HG11	1.84	0.59
1:C:180:VAL:HG22	1:C:187:SER:HB3	1.85	0.59
1:E:97:GLU:HG3	1:E:98:PRO:HD2	1.85	0.59
1:A:243:ASP:C	1:C:252:VAL:HG12	2.24	0.58
1:E:253:LEU:HB2	1:F:242:LEU:CA	2.33	0.58
1:E:243:ASP:CG	1:F:247:TYR:O	2.40	0.58
1:A:252:VAL:HG12	1:C:243:ASP:CA	2.34	0.58
1:F:97:GLU:HG3	1:F:98:PRO:HD2	1.86	0.58
1:B:252:VAL:HG12	1:D:243:ASP:CA	2.34	0.58
1:B:243:ASP:C	1:D:251:ASN:HB2	2.24	0.57
1:E:247:TYR:HB3	1:F:248:LEU:N	2.11	0.57
1:A:97:GLU:HG3	1:A:98:PRO:HD2	1.86	0.57
1:A:192:GLU:OE2	1:C:185:ARG:HD2	2.04	0.57
1:B:97:GLU:HG3	1:B:98:PRO:HD2	1.86	0.57
1:A:216:GLU:OE1	1:A:216:GLU:HA	2.04	0.57
1:A:243:ASP:CB	1:C:247:TYR:O	2.52	0.57
1:D:248:LEU:HD23	1:D:252:VAL:HG11	1.84	0.56
1:E:250:ARG:N	1:F:243:ASP:N	2.47	0.56
1:D:97:GLU:HG3	1:D:98:PRO:HD2	1.87	0.56
1:B:13:SER:C	1:B:15:SER:H	2.09	0.55
1:E:152:ALA:CB	1:E:190:VAL:HG13	2.35	0.55
1:E:244:ILE:C	1:F:247:TYR:C	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:C	1:C:243:ASP:N	2.57	0.55
1:B:246:SER:CB	1:D:251:ASN:HD22	2.12	0.55
1:A:248:LEU:H	1:C:247:TYR:CB	1.92	0.55
1:E:252:VAL:N	1:F:243:ASP:N	2.51	0.55
1:E:13:SER:HA	1:E:24:VAL:HG21	1.90	0.54
1:B:246:SER:HB3	1:D:251:ASN:HD22	1.71	0.54
1:E:192:GLU:OE2	1:F:185:ARG:HD2	2.08	0.54
1:E:250:ARG:CA	1:F:243:ASP:H	2.20	0.54
1:A:253:LEU:HB3	1:C:66:SER:HB3	1.89	0.54
1:D:103:GLY:HA2	6:D:4255:HOH:O	2.08	0.54
1:E:242:LEU:HA	1:F:249:VAL:O	2.06	0.54
1:C:13:SER:O	1:C:14:SER:HB2	2.08	0.54
1:E:244:ILE:CG2	1:F:244:ILE:HG22	2.36	0.54
1:E:252:VAL:C	1:F:242:LEU:O	2.41	0.54
1:A:249:VAL:HG13	1:C:232:LYS:HB2	1.90	0.53
1:E:251:ASN:ND2	1:F:246:SER:CB	2.71	0.53
1:B:246:SER:N	1:D:251:ASN:HD22	2.01	0.53
1:E:243:ASP:N	1:F:249:VAL:C	2.62	0.53
1:D:252:VAL:HG22	1:D:253:LEU:N	2.24	0.53
1:F:129:ASN:ND2	1:F:132:TRP:CZ2	2.71	0.53
1:A:11:PHE:CD1	1:A:11:PHE:N	2.77	0.53
1:A:249:VAL:C	1:C:242:LEU:CA	2.77	0.52
1:A:74:ASN:HD22	1:A:161:ASN:HD22	1.57	0.52
1:A:247:TYR:CD1	1:C:246:SER:C	2.78	0.52
1:A:246:SER:HB3	1:C:247:TYR:HA	1.91	0.52
1:B:244:ILE:HG22	1:D:244:ILE:HG23	1.88	0.52
1:F:150:ARG:NH1	1:F:192:GLU:OE1	2.43	0.52
1:A:242:LEU:HD12	1:A:243:ASP:N	2.22	0.52
1:B:242:LEU:HB3	1:D:253:LEU:CG	2.38	0.52
1:B:244:ILE:C	1:D:247:TYR:C	2.66	0.52
1:C:74:ASN:HD22	1:C:161:ASN:HD22	1.57	0.52
1:E:251:ASN:ND2	1:F:246:SER:OG	2.42	0.52
1:E:252:VAL:N	1:F:242:LEU:C	2.48	0.52
1:B:248:LEU:HD22	1:B:252:VAL:HG11	1.91	0.52
1:C:152:ALA:HB2	1:C:190:VAL:CG1	2.38	0.52
1:B:243:ASP:H	1:D:249:VAL:C	2.13	0.52
1:E:12:ASN:O	1:E:14:SER:N	2.43	0.51
1:E:150:ARG:NH1	1:E:192:GLU:OE1	2.44	0.51
1:F:74:ASN:HD22	1:F:161:ASN:HD22	1.58	0.51
1:A:253:LEU:OXT	1:C:240:GLU:O	2.22	0.51
1:E:253:LEU:CB	1:F:242:LEU:HB3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:O	1:D:241:PRO:HG2	2.11	0.51
1:D:74:ASN:HD22	1:D:161:ASN:HD22	1.58	0.51
1:B:118:GLN:HB3	1:B:201:PRO:HD3	1.93	0.50
1:A:246:SER:CB	1:C:247:TYR:HA	2.41	0.50
1:E:245:ALA:O	1:F:247:TYR:CB	2.27	0.50
1:A:216:GLU:O	1:A:218:TYR:N	2.42	0.50
1:B:243:ASP:N	1:D:249:VAL:C	2.65	0.50
1:E:13:SER:O	1:E:15:SER:N	2.44	0.50
1:E:74:ASN:HD22	1:E:161:ASN:HD22	1.58	0.50
1:A:248:LEU:CD2	1:A:252:VAL:HG11	2.40	0.50
1:B:192:GLU:HG3	1:B:193:ARG:N	2.27	0.50
1:E:244:ILE:CB	1:F:252:VAL:HG11	2.40	0.50
1:A:118:GLN:HB3	1:A:201:PRO:HD3	1.94	0.50
1:E:253:LEU:H	1:F:242:LEU:CA	2.24	0.50
1:B:74:ASN:HD22	1:B:161:ASN:HD22	1.57	0.49
1:A:248:LEU:HD13	1:C:167:THR:HG21	1.93	0.49
1:F:11:PHE:CE2	1:F:16:PHE:HZ	2.30	0.49
1:A:247:TYR:O	1:C:243:ASP:HB3	2.11	0.49
1:E:118:GLN:HB3	1:E:201:PRO:HD3	1.94	0.49
1:A:50:TYR:CE2	1:A:52:SER:HB3	2.47	0.49
1:B:249:VAL:O	1:D:242:LEU:HA	2.12	0.49
1:B:249:VAL:C	1:D:243:ASP:H	2.15	0.49
1:A:243:ASP:C	1:C:252:VAL:HG13	2.24	0.49
1:A:45:LEU:HD23	1:A:45:LEU:C	2.33	0.49
1:D:118:GLN:HB3	1:D:201:PRO:HD3	1.94	0.49
1:E:167:THR:HG21	1:F:248:LEU:HD13	1.93	0.49
1:C:118:GLN:HB3	1:C:201:PRO:HD3	1.93	0.49
1:C:34:VAL:HG12	1:C:35:LYS:O	2.13	0.49
1:D:172:THR:O	1:D:193:ARG:NH1	2.46	0.49
1:E:45:LEU:HD23	1:E:45:LEU:C	2.34	0.48
1:F:41:THR:CG2	1:F:42:LEU:N	2.76	0.48
1:B:246:SER:CA	1:D:251:ASN:ND2	2.74	0.48
1:F:74:ASN:HD22	1:F:161:ASN:ND2	2.11	0.48
1:E:41:THR:CG2	1:E:42:LEU:N	2.77	0.48
2:G:2:FUC:H5	2:G:3:NAG:O5	2.13	0.48
1:A:74:ASN:HD22	1:A:161:ASN:ND2	2.11	0.48
1:A:41:THR:CG2	1:A:42:LEU:N	2.76	0.48
1:E:74:ASN:HD22	1:E:161:ASN:ND2	2.11	0.48
1:D:82:SER:O	1:D:218:TYR:HA	2.14	0.48
1:F:16:PHE:CD2	1:F:16:PHE:N	2.78	0.48
1:F:118:GLN:HB3	1:F:201:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:SER:O	1:F:218:TYR:HA	2.13	0.48
1:E:244:ILE:N	1:F:252:VAL:CG1	2.67	0.48
1:B:74:ASN:HD22	1:B:161:ASN:ND2	2.12	0.48
1:D:45:LEU:C	1:D:45:LEU:HD23	2.34	0.48
1:B:45:LEU:C	1:B:45:LEU:HD23	2.34	0.48
1:B:247:TYR:O	1:D:243:ASP:CB	2.62	0.48
1:D:185:ARG:NH2	1:D:185:ARG:HB2	2.29	0.48
1:F:248:LEU:CA	1:F:252:VAL:HG12	2.43	0.48
1:A:252:VAL:HG11	1:C:244:ILE:CG1	2.44	0.48
1:F:45:LEU:C	1:F:45:LEU:HD23	2.33	0.47
1:A:248:LEU:N	1:C:247:TYR:HB2	2.22	0.47
1:C:32:THR:OG1	1:C:222:HIS:HD2	1.98	0.47
1:C:45:LEU:HD23	1:C:45:LEU:C	2.35	0.47
1:D:41:THR:CG2	1:D:42:LEU:N	2.77	0.47
1:E:66:SER:HB3	1:F:253:LEU:HB3	1.96	0.47
1:A:244:ILE:O	1:C:248:LEU:HG	2.12	0.47
1:E:13:SER:H	1:E:24:VAL:HG11	1.80	0.47
1:B:82:SER:O	1:B:218:TYR:HA	2.15	0.47
1:D:74:ASN:HD22	1:D:161:ASN:ND2	2.11	0.47
1:E:82:SER:O	1:E:218:TYR:HA	2.14	0.47
1:E:253:LEU:CG	1:F:242:LEU:HB3	2.45	0.47
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.79	0.47
1:B:101:ASN:C	1:B:101:ASN:HD22	2.18	0.47
1:B:160:GLN:HE21	1:B:160:GLN:HA	1.80	0.47
1:C:160:GLN:HE21	1:C:160:GLN:HA	1.79	0.47
1:E:245:ALA:O	1:E:249:VAL:HG23	2.15	0.47
1:B:41:THR:CG2	1:B:42:LEU:N	2.77	0.47
1:C:74:ASN:HD22	1:C:161:ASN:ND2	2.12	0.47
1:C:252:VAL:HG22	1:C:253:LEU:N	2.30	0.47
1:F:215:SER:HB3	1:F:218:TYR:CD1	2.50	0.47
1:C:157:ALA:H	1:C:181:HIS:CE1	2.33	0.46
1:C:41:THR:CG2	1:C:42:LEU:N	2.77	0.46
1:D:160:GLN:HE21	1:D:160:GLN:HA	1.80	0.46
1:E:246:SER:HB2	1:F:251:ASN:HD21	1.77	0.46
1:A:115:ASN:ND2	1:F:203:TYR:OH	2.48	0.46
1:B:179:LEU:HD23	1:B:179:LEU:C	2.36	0.46
1:B:242:LEU:O	1:D:253:LEU:HG	2.15	0.46
1:B:252:VAL:HG12	1:D:243:ASP:C	2.30	0.46
1:A:82:SER:O	1:A:218:TYR:HA	2.13	0.46
1:A:253:LEU:CB	1:C:242:LEU:HB3	2.36	0.46
1:C:97:GLU:HG3	1:C:98:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:GLN:HE21	1:F:160:GLN:HA	1.80	0.46
1:A:243:ASP:CA	1:C:252:VAL:HG13	2.42	0.46
1:E:97:GLU:HG3	1:E:98:PRO:CD	2.45	0.46
1:F:42:LEU:HD13	1:F:215:SER:O	2.16	0.46
1:F:15:SER:C	1:F:16:PHE:HD2	2.19	0.46
1:B:97:GLU:HG3	1:B:98:PRO:CD	2.46	0.46
1:C:82:SER:O	1:C:218:TYR:HA	2.15	0.46
1:D:11:PHE:O	1:D:12:ASN:CB	2.64	0.46
1:A:101:ASN:HD22	1:A:101:ASN:C	2.19	0.46
1:C:179:LEU:HD23	1:C:179:LEU:C	2.37	0.46
1:E:160:GLN:HE21	1:E:160:GLN:HA	1.81	0.46
1:E:5:SER:HA	1:E:229:PHE:O	2.16	0.46
1:B:152:ALA:CB	1:B:190:VAL:HG13	2.44	0.45
1:F:16:PHE:HD2	1:F:16:PHE:N	2.13	0.45
1:E:242:LEU:HB3	1:F:248:LEU:C	2.36	0.45
1:F:248:LEU:CD2	1:F:252:VAL:HG11	2.41	0.45
1:A:252:VAL:CG1	1:C:244:ILE:CB	2.94	0.45
1:D:157:ALA:H	1:D:181:HIS:CE1	2.34	0.45
1:E:129:ASN:O	1:E:133:ASP:HB2	2.16	0.45
1:B:252:VAL:CA	1:D:242:LEU:O	2.58	0.45
1:F:101:ASN:C	1:F:101:ASN:HD22	2.19	0.45
1:D:97:GLU:HG3	1:D:98:PRO:CD	2.46	0.45
1:E:16:PHE:N	1:E:16:PHE:CD2	2.82	0.45
1:E:16:PHE:N	1:E:16:PHE:HD2	2.14	0.45
1:E:79:ASN:HB3	1:E:82:SER:HB3	1.98	0.45
1:F:154:TRP:HE1	1:F:181:HIS:CE1	2.35	0.45
1:A:179:LEU:HD23	1:A:179:LEU:C	2.37	0.45
1:C:7:SER:HB3	1:D:3:ILE:HB	1.99	0.45
1:D:179:LEU:C	1:D:179:LEU:HD23	2.37	0.45
1:E:179:LEU:HD23	1:E:179:LEU:C	2.37	0.45
1:E:246:SER:CB	1:F:251:ASN:ND2	2.75	0.45
1:A:154:TRP:HE1	1:A:181:HIS:CE1	2.35	0.45
1:A:252:VAL:HG11	1:C:244:ILE:HG12	1.96	0.45
1:E:101:ASN:C	1:E:101:ASN:HD22	2.20	0.45
1:A:32:THR:OG1	1:A:222:HIS:HD2	2.00	0.45
1:C:79:ASN:HB3	1:C:82:SER:HB3	1.99	0.45
1:F:97:GLU:HG3	1:F:98:PRO:CD	2.45	0.45
1:A:252:VAL:CG1	1:C:244:ILE:CG1	2.90	0.45
1:B:157:ALA:H	1:B:181:HIS:CE1	2.35	0.45
1:C:193:ARG:HH11	1:C:193:ARG:HG3	1.80	0.45
1:E:157:ALA:H	1:E:181:HIS:CE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:LEU:HD13	1:F:167:THR:HG21	1.99	0.45
1:A:79:ASN:HB3	1:A:82:SER:HB3	1.98	0.44
1:F:154:TRP:HE1	1:F:181:HIS:HE1	1.65	0.44
1:A:249:VAL:O	1:C:243:ASP:N	2.49	0.44
1:B:242:LEU:CA	1:D:249:VAL:C	2.85	0.44
1:E:253:LEU:CB	1:F:242:LEU:N	2.41	0.44
1:A:17:ILE:O	1:A:48:ALA:HA	2.18	0.44
1:A:157:ALA:H	1:A:181:HIS:CE1	2.35	0.44
1:A:31:LEU:O	1:A:46:GLY:HA3	2.18	0.44
1:D:79:ASN:HB3	1:D:82:SER:HB3	1.98	0.44
1:F:31:LEU:O	1:F:46:GLY:HA3	2.17	0.44
1:A:249:VAL:C	1:C:242:LEU:HA	2.28	0.44
1:B:244:ILE:HG23	1:D:244:ILE:HG22	1.92	0.44
1:D:243:ASP:OD1	1:D:245:ALA:HB3	2.17	0.44
1:E:31:LEU:O	1:E:46:GLY:HA3	2.18	0.44
1:C:31:LEU:O	1:C:46:GLY:HA3	2.16	0.44
1:C:5:SER:HA	1:C:229:PHE:O	2.18	0.44
1:B:242:LEU:CA	1:D:249:VAL:O	2.58	0.44
1:E:154:TRP:HE1	1:E:181:HIS:CE1	2.35	0.44
1:E:243:ASP:H	1:F:250:ARG:CA	2.24	0.44
1:E:248:LEU:N	1:F:247:TYR:CB	2.77	0.44
1:F:125:ASP:HB3	1:F:138:HIS:CE1	2.52	0.44
1:F:179:LEU:C	1:F:179:LEU:HD23	2.37	0.44
1:A:216:GLU:C	1:A:218:TYR:H	2.20	0.44
1:A:97:GLU:HG3	1:A:98:PRO:CD	2.46	0.44
1:B:79:ASN:HB3	1:B:82:SER:HB3	1.99	0.44
1:C:101:ASN:C	1:C:101:ASN:HD22	2.21	0.44
1:D:154:TRP:HE1	1:D:181:HIS:CE1	2.36	0.44
1:B:253:LEU:HD13	1:D:242:LEU:HB2	1.95	0.44
1:B:12:ASN:HA	1:B:24:VAL:HG11	2.00	0.44
1:F:244:ILE:HG22	1:F:248:LEU:CD1	2.47	0.44
1:B:242:LEU:HD12	1:B:243:ASP:N	2.32	0.44
1:C:12:ASN:O	1:C:13:SER:O	2.35	0.44
1:D:148:SER:HB2	1:D:151:THR:CG2	2.48	0.44
1:E:125:ASP:HB3	1:E:138:HIS:CE1	2.53	0.43
1:F:157:ALA:H	1:F:181:HIS:CE1	2.36	0.43
1:A:169:ASN:HA	1:C:253:LEU:HD22	1.99	0.43
1:F:79:ASN:HB3	1:F:82:SER:HB3	1.99	0.43
1:B:252:VAL:HG12	1:D:243:ASP:HA	1.97	0.43
1:B:31:LEU:O	1:B:46:GLY:HA3	2.18	0.43
1:A:115:ASN:CB	1:F:203:TYR:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:O	1:B:181:HIS:HD2	2.01	0.43
1:D:101:ASN:HD22	1:D:101:ASN:C	2.19	0.43
1:D:125:ASP:HB3	1:D:138:HIS:CE1	2.53	0.43
1:E:56:ILE:HG23	6:E:5260:HOH:O	2.19	0.43
1:C:154:TRP:HE1	1:C:181:HIS:CE1	2.36	0.43
1:C:248:LEU:HD23	1:C:252:VAL:HG11	2.01	0.43
1:D:31:LEU:O	1:D:46:GLY:HA3	2.17	0.43
1:A:134:PRO:HD2	1:A:138:HIS:CE1	2.53	0.43
1:D:13:SER:C	1:D:15:SER:H	2.22	0.43
1:E:154:TRP:HE1	1:E:181:HIS:HE1	1.67	0.43
1:A:161:ASN:O	1:A:181:HIS:HD2	2.01	0.43
1:B:242:LEU:CA	1:D:253:LEU:O	2.65	0.43
1:C:42:LEU:HD21	1:C:216:GLU:O	2.19	0.43
1:E:252:VAL:HG13	1:F:243:ASP:CA	2.45	0.43
1:A:154:TRP:HE1	1:A:181:HIS:HE1	1.67	0.43
1:D:1:ALA:HA	1:D:233:LEU:O	2.19	0.43
1:E:53:PRO:C	1:E:54:ILE:HD12	2.39	0.43
1:A:3:ILE:HG22	1:A:4:GLN:N	2.34	0.43
1:B:244:ILE:N	1:D:252:VAL:CG1	2.45	0.43
1:E:251:ASN:HD22	1:F:246:SER:HB2	1.81	0.43
1:B:150:ARG:NH1	1:B:192:GLU:OE1	2.52	0.43
1:B:154:TRP:HE1	1:B:181:HIS:CE1	2.36	0.43
1:E:161:ASN:O	1:E:181:HIS:HD2	2.02	0.43
1:E:50:TYR:CE2	1:E:52:SER:HB3	2.54	0.43
1:B:11:PHE:O	1:B:12:ASN:CB	2.67	0.42
1:A:246:SER:CA	1:C:247:TYR:HA	2.28	0.42
1:E:99:LYS:HB3	1:E:100:SER:H	1.71	0.42
1:C:134:PRO:HD2	1:C:138:HIS:CE1	2.54	0.42
1:B:220:GLU:OE2	1:B:222:HIS:HE1	2.02	0.42
1:E:247:TYR:CB	1:F:248:LEU:N	2.73	0.42
1:F:220:GLU:OE2	1:F:222:HIS:HE1	2.02	0.42
1:A:150:ARG:NH1	1:A:192:GLU:OE1	2.53	0.42
1:F:42:LEU:HD21	1:F:216:GLU:O	2.19	0.42
1:C:125:ASP:HB3	1:C:138:HIS:CE1	2.54	0.42
1:F:103:GLY:HA3	1:F:129:ASN:HD21	1.83	0.42
1:F:161:ASN:O	1:F:181:HIS:HD2	2.02	0.42
1:F:252:VAL:HG13	1:F:253:LEU:N	2.33	0.42
1:B:242:LEU:CB	1:D:253:LEU:CD1	2.78	0.42
1:A:99:LYS:HB3	1:A:100:SER:H	1.73	0.42
1:B:244:ILE:HG23	1:D:244:ILE:O	2.20	0.42
1:C:220:GLU:OE2	1:C:222:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASP:OD1	1:C:247:TYR:CE1	2.73	0.42
1:B:125:ASP:HB3	1:B:138:HIS:CE1	2.54	0.42
1:A:232:LYS:HB2	1:C:249:VAL:CG1	2.50	0.42
1:A:242:LEU:O	1:C:252:VAL:HG22	2.20	0.42
1:F:3:ILE:H	1:F:3:ILE:HD12	1.84	0.42
1:B:157:ALA:HB1	1:B:160:GLN:HG3	2.02	0.42
1:C:161:ASN:O	1:C:181:HIS:HD2	2.03	0.42
1:D:252:VAL:HG13	1:D:253:LEU:N	2.25	0.42
1:A:157:ALA:HB1	1:A:160:GLN:HG3	2.02	0.41
1:A:252:VAL:HG13	1:A:253:LEU:N	2.31	0.41
1:B:134:PRO:HD2	1:B:138:HIS:CE1	2.54	0.41
1:F:244:ILE:HG22	1:F:248:LEU:HD11	2.01	0.41
1:D:154:TRP:HE1	1:D:181:HIS:HE1	1.67	0.41
1:A:220:GLU:OE2	1:A:222:HIS:HE1	2.03	0.41
1:B:12:ASN:CA	1:B:24:VAL:HG11	2.50	0.41
1:D:220:GLU:OE2	1:D:222:HIS:HE1	2.04	0.41
1:F:196:ILE:CG2	1:F:197:THR:N	2.83	0.41
1:E:253:LEU:CD1	1:F:242:LEU:HB3	2.46	0.41
1:A:242:LEU:O	1:C:252:VAL:CG1	2.62	0.41
1:B:253:LEU:HD23	1:D:241:PRO:CB	2.50	0.41
1:C:154:TRP:HE1	1:C:181:HIS:HE1	1.67	0.41
1:B:34:VAL:HG12	1:B:38:GLY:HA2	2.03	0.41
1:C:243:ASP:OD1	1:C:245:ALA:HB3	2.21	0.41
1:E:220:GLU:OE2	1:E:222:HIS:HE1	2.03	0.41
1:B:13:SER:C	1:B:15:SER:N	2.73	0.41
1:B:247:TYR:HB3	1:D:247:TYR:HB3	1.65	0.41
1:A:249:VAL:CG1	1:C:232:LYS:HB2	2.48	0.41
1:D:134:PRO:HD2	1:D:138:HIS:CE1	2.55	0.41
1:D:150:ARG:NH1	1:D:192:GLU:OE1	2.54	0.41
1:B:56:ILE:HG12	1:B:204:VAL:HG22	2.03	0.41
1:E:244:ILE:HG22	1:E:248:LEU:CD1	2.50	0.41
1:E:134:PRO:HD2	1:E:138:HIS:CE1	2.55	0.41
1:A:247:TYR:O	1:C:243:ASP:CB	2.65	0.41
1:C:157:ALA:HB1	1:C:160:GLN:HG3	2.02	0.41
1:C:196:ILE:CG2	1:C:197:THR:N	2.84	0.41
1:D:82:SER:OG	1:D:217:GLY:O	2.35	0.41
1:A:196:ILE:CG2	1:A:197:THR:N	2.84	0.41
1:D:10:ASN:OD1	1:D:10:ASN:C	2.59	0.41
1:A:125:ASP:HB3	1:A:138:HIS:CE1	2.55	0.40
1:B:243:ASP:CA	1:D:252:VAL:HG12	2.50	0.40
1:E:32:THR:OG1	1:E:222:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:PRO:HD2	1:F:138:HIS:CE1	2.56	0.40
1:A:39:LEU:HA	1:A:40:PRO:HD3	1.84	0.40
1:D:39:LEU:HA	1:D:40:PRO:HD3	1.84	0.40
1:D:82:SER:HG	1:D:217:GLY:C	2.23	0.40
1:E:69:THR:HG22	1:E:166:ILE:HB	2.03	0.40
1:E:53:PRO:O	1:E:54:ILE:HD12	2.21	0.40
1:B:101:ASN:C	1:B:101:ASN:ND2	2.75	0.40
1:E:196:ILE:CG2	1:E:197:THR:N	2.85	0.40
1:F:157:ALA:HB1	1:F:160:GLN:HG3	2.02	0.40
1:C:229:PHE:CE1	1:C:231:SER:HB2	2.56	0.40
1:A:230:ALA:HB3	1:C:249:VAL:HG21	2.03	0.40
1:E:56:ILE:HG12	1:E:204:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	247/253 (98%)	225 (91%)	17 (7%)	5 (2%)	7 12
1	B	242/253 (96%)	224 (93%)	17 (7%)	1 (0%)	34 54
1	C	247/253 (98%)	229 (93%)	15 (6%)	3 (1%)	13 24
1	D	251/253 (99%)	234 (93%)	14 (6%)	3 (1%)	13 24
1	E	245/253 (97%)	224 (91%)	17 (7%)	4 (2%)	9 17
1	F	242/253 (96%)	224 (93%)	15 (6%)	3 (1%)	13 24
All	All	1474/1518 (97%)	1360 (92%)	95 (6%)	19 (1%)	12 21

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU

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Mol	Chain	Res	Type
1	C	13	SER
1	E	14	SER
1	A	12	ASN
1	A	215	SER
1	A	217	GLY
1	B	216	GLU
1	C	215	SER
1	D	215	SER
1	E	13	SER
1	E	15	SER
1	F	130	THR
1	A	132	TRP
1	D	12	ASN
1	E	215	SER
1	F	216	GLU
1	F	252	VAL
1	D	252	VAL
1	C	241	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	198/216 (92%)	191 (96%)	7 (4%)	36	62
1	B	197/216 (91%)	193 (98%)	4 (2%)	55	79
1	C	199/216 (92%)	193 (97%)	6 (3%)	41	68
1	D	202/216 (94%)	198 (98%)	4 (2%)	55	79
1	E	197/216 (91%)	192 (98%)	5 (2%)	47	73
1	F	198/216 (92%)	191 (96%)	7 (4%)	36	62
All	All	1191/1296 (92%)	1158 (97%)	33 (3%)	43	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	41	THR
1	A	101	ASN
1	A	131	ASP
1	A	160	GLN
1	A	190	VAL
1	A	216	GLU
1	B	41	THR
1	B	101	ASN
1	B	160	GLN
1	B	190	VAL
1	C	15	SER
1	C	41	THR
1	C	101	ASN
1	C	160	GLN
1	C	190	VAL
1	C	252	VAL
1	D	41	THR
1	D	101	ASN
1	D	131	ASP
1	D	160	GLN
1	E	41	THR
1	E	101	ASN
1	E	160	GLN
1	E	190	VAL
1	E	216	GLU
1	F	41	THR
1	F	101	ASN
1	F	131	ASP
1	F	160	GLN
1	F	190	VAL
1	F	193	ARG
1	F	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	115	ASN
1	A	160	GLN
1	A	161	ASN
1	A	181	HIS
1	A	222	HIS

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Mol	Chain	Res	Type
1	B	101	ASN
1	B	115	ASN
1	B	160	GLN
1	B	161	ASN
1	B	181	HIS
1	B	222	HIS
1	C	101	ASN
1	C	160	GLN
1	C	161	ASN
1	C	181	HIS
1	C	222	HIS
1	D	101	ASN
1	D	160	GLN
1	D	161	ASN
1	D	181	HIS
1	D	222	HIS
1	D	251	ASN
1	E	101	ASN
1	E	160	GLN
1	E	161	ASN
1	E	181	HIS
1	E	222	HIS
1	E	251	ASN
1	F	101	ASN
1	F	160	GLN
1	F	161	ASN
1	F	181	HIS
1	F	222	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

9 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	$\#\|Z\| > 2$
2	NAG	G	1	1,2	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
2	FUC	G	2	2	10,10,11	0.81	0	14,14,16	0.53	0
2	NAG	G	3	2	14,14,15	0.73	0	17,19,21	0.70	0
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	0.94	2 (11%)
3	FUL	H	2	3	10,10,11	0.54	0	14,14,16	0.39	0
3	NAG	H	3	3	14,14,15	0.56	0	17,19,21	0.97	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.52	0	17,19,21	0.64	0
2	FUC	I	2	2	10,10,11	0.67	0	14,14,16	0.50	0
2	NAG	I	3	2	14,14,15	0.57	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUL	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
2	NAG	I	3	2	-	2/6/23/26	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})
3	H	1	NAG	C2-N2-C7	-2.61	119.19	122.90
3	H	3	NAG	C2-N2-C7	-2.31	119.61	122.90
2	G	1	NAG	C4-C3-C2	2.07	114.06	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	O3-C3-C2	-2.00	105.32	109.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

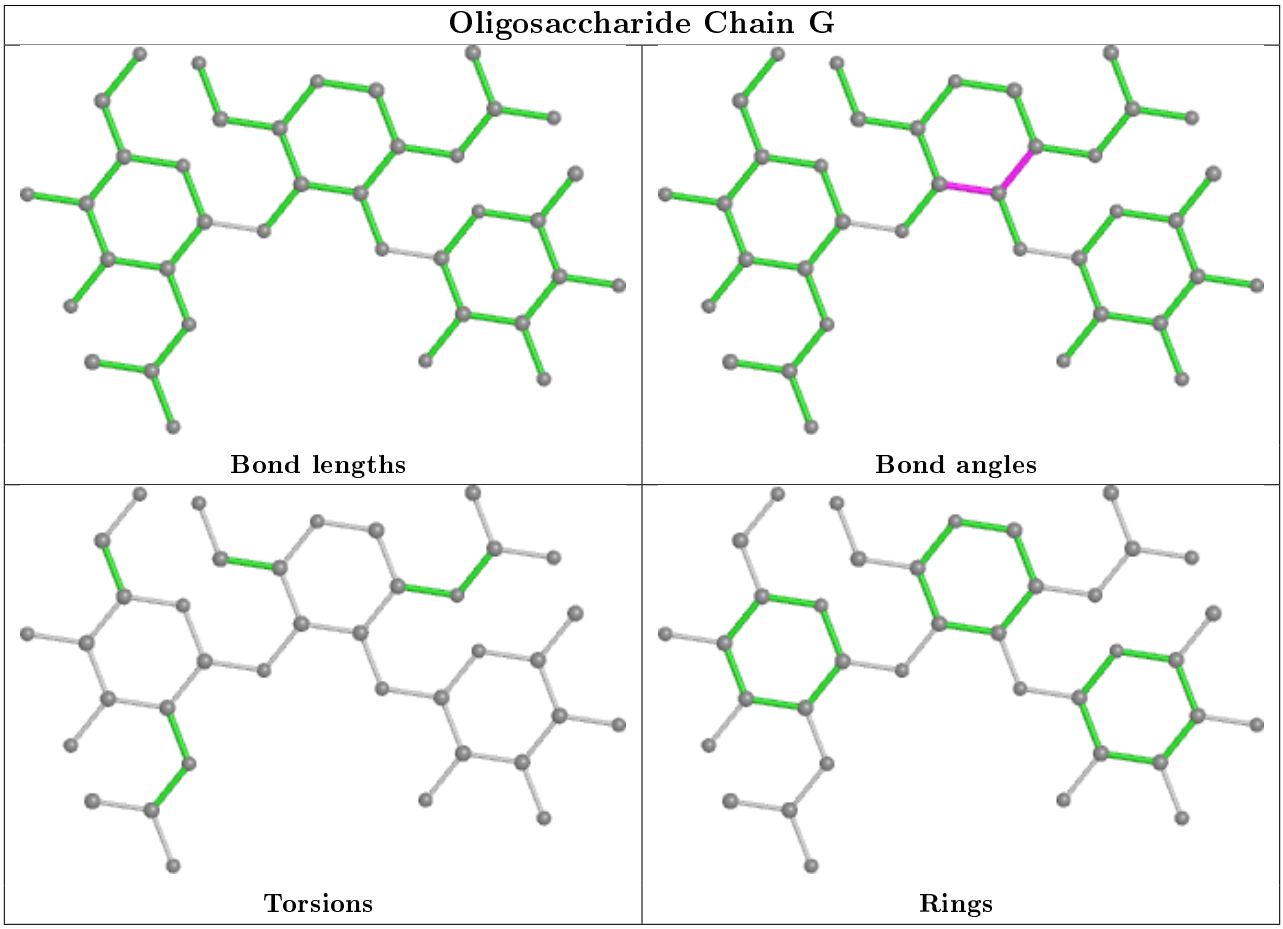
Mol	Chain	Res	Type	Atoms
2	I	3	NAG	C4-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6

There are no ring outliers.

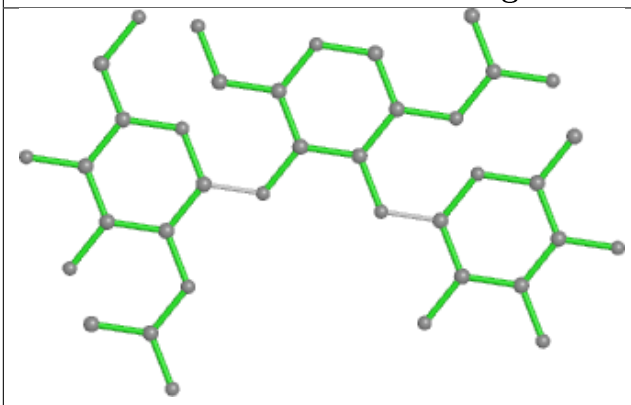
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FUC	1	0
2	G	3	NAG	1	0

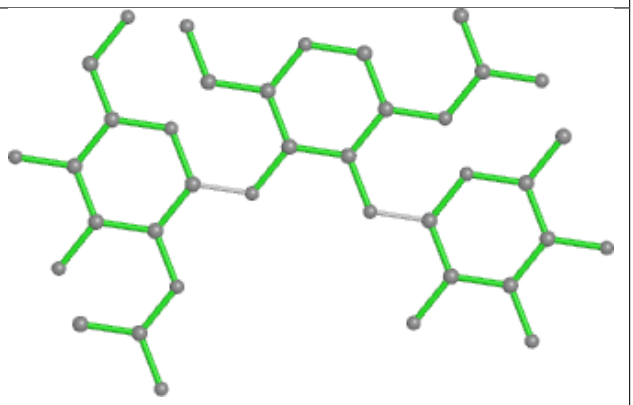
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



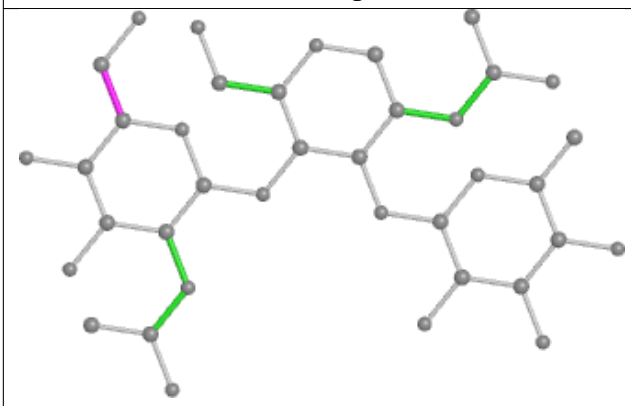
Oligosaccharide Chain I



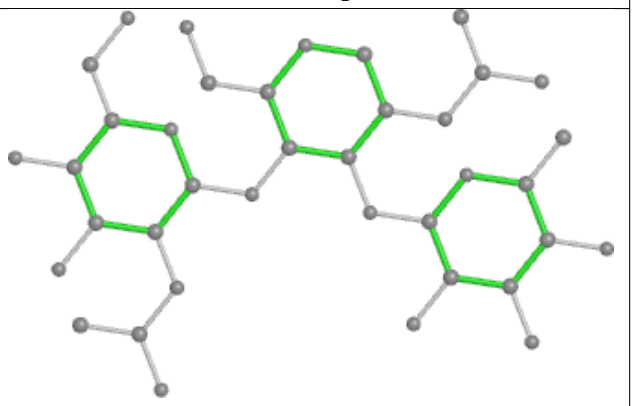
Bond lengths



Bond angles

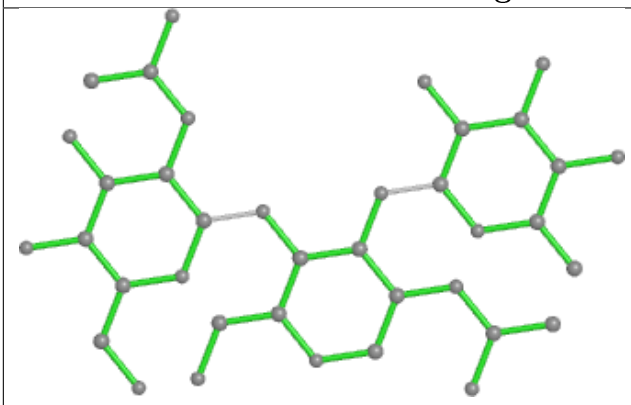


Torsions

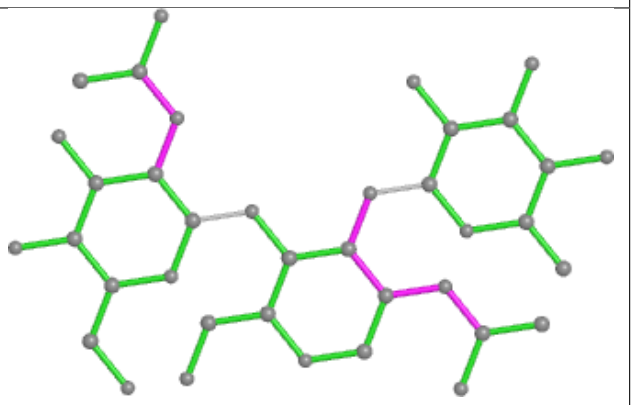


Rings

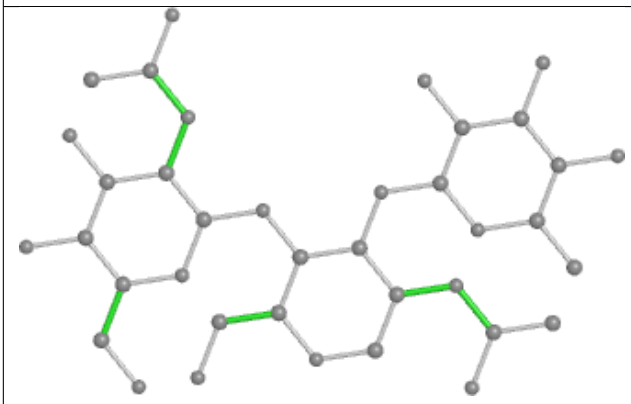
Oligosaccharide Chain H



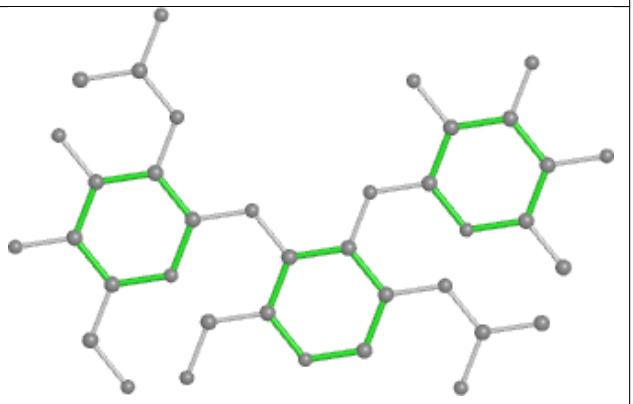
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	251/253 (99%)	-0.10	7 (2%) 53 56	22, 36, 62, 81	17 (6%)
1	B	246/253 (97%)	-0.03	12 (4%) 29 31	24, 36, 59, 82	12 (4%)
1	C	251/253 (99%)	-0.13	3 (1%) 79 80	21, 34, 60, 78	17 (6%)
1	D	253/253 (100%)	0.08	12 (4%) 31 33	22, 37, 63, 87	19 (7%)
1	E	249/253 (98%)	-0.18	7 (2%) 53 56	21, 34, 62, 86	15 (6%)
1	F	246/253 (97%)	-0.06	11 (4%) 33 36	18, 37, 63, 88	12 (4%)
All	All	1496/1518 (98%)	-0.07	52 (3%) 44 47	18, 36, 62, 88	92 (6%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	5.6
1	D	36	GLY	5.3
1	B	60	SER	5.0
1	D	216	GLU	4.9
1	F	37	ASN	4.5
1	A	36	GLY	4.5
1	D	215	SER	4.0
1	F	217	GLY	3.7
1	D	27	SER	3.6
1	F	39	LEU	3.5
1	E	1	ALA	3.5
1	D	252	VAL	3.4
1	F	216	GLU	3.4
1	F	36	GLY	3.3
1	A	1	ALA	3.3
1	A	37	ASN	3.2
1	D	37	ASN	3.2
1	D	112	VAL	3.2
1	F	218	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	38	GLY	3.0
1	A	27	SER	3.0
1	E	252	VAL	3.0
1	F	60	SER	2.9
1	A	26	SER	2.9
1	C	27	SER	2.9
1	E	216	GLU	2.7
1	B	62	GLY	2.7
1	B	59	LYS	2.6
1	E	12	ASN	2.6
1	B	116	SER	2.6
1	D	135	THR	2.6
1	D	253	LEU	2.6
1	C	36	GLY	2.5
1	A	38	GLY	2.4
1	F	130	THR	2.4
1	E	237	SER	2.4
1	D	26	SER	2.3
1	F	244	ILE	2.3
1	B	198	ASN	2.3
1	D	218	TYR	2.3
1	E	253	LEU	2.2
1	B	37	ASN	2.2
1	B	61	THR	2.2
1	B	216	GLU	2.2
1	B	12	ASN	2.2
1	D	81	SER	2.2
1	E	14	SER	2.2
1	F	26	SER	2.1
1	B	36	GLY	2.1
1	B	246	SER	2.1
1	A	60	SER	2.1
1	C	14	SER	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)

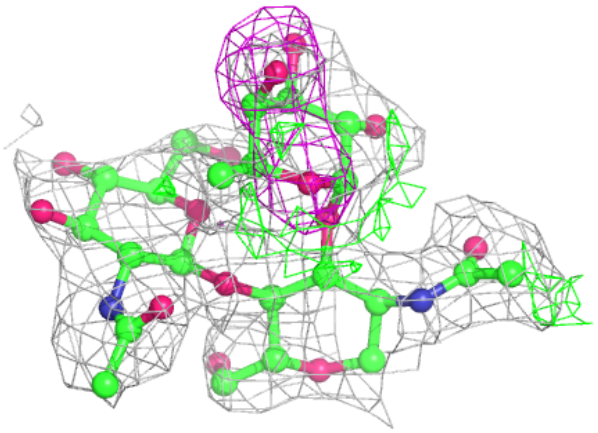
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

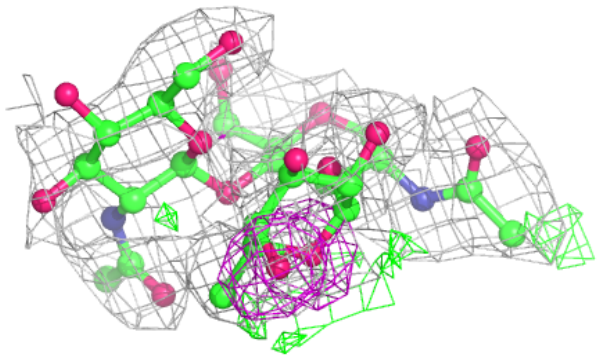
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUL	H	2	10/11	0.49	0.45	1,94,98,98	0
2	FUC	G	2	10/11	0.52	0.48	1,95,99,100	0
2	NAG	G	1	14/15	0.71	0.28	57,77,88,97	0
3	NAG	H	3	14/15	0.72	0.41	85,93,98,99	0
3	NAG	H	1	14/15	0.78	0.31	71,77,89,93	0
2	NAG	G	3	14/15	0.84	0.43	69,85,93,98	0
2	NAG	I	3	14/15	0.95	0.22	52,60,64,76	0
2	NAG	I	1	14/15	0.97	0.13	29,35,48,52	0
2	FUC	I	2	10/11	0.97	0.14	28,46,51,53	0

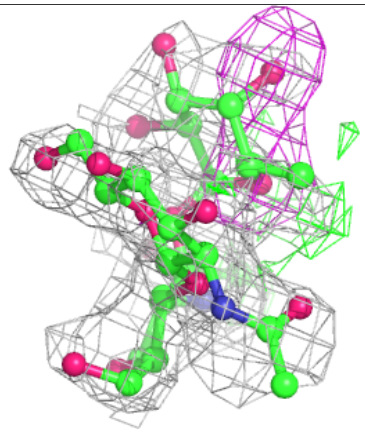
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

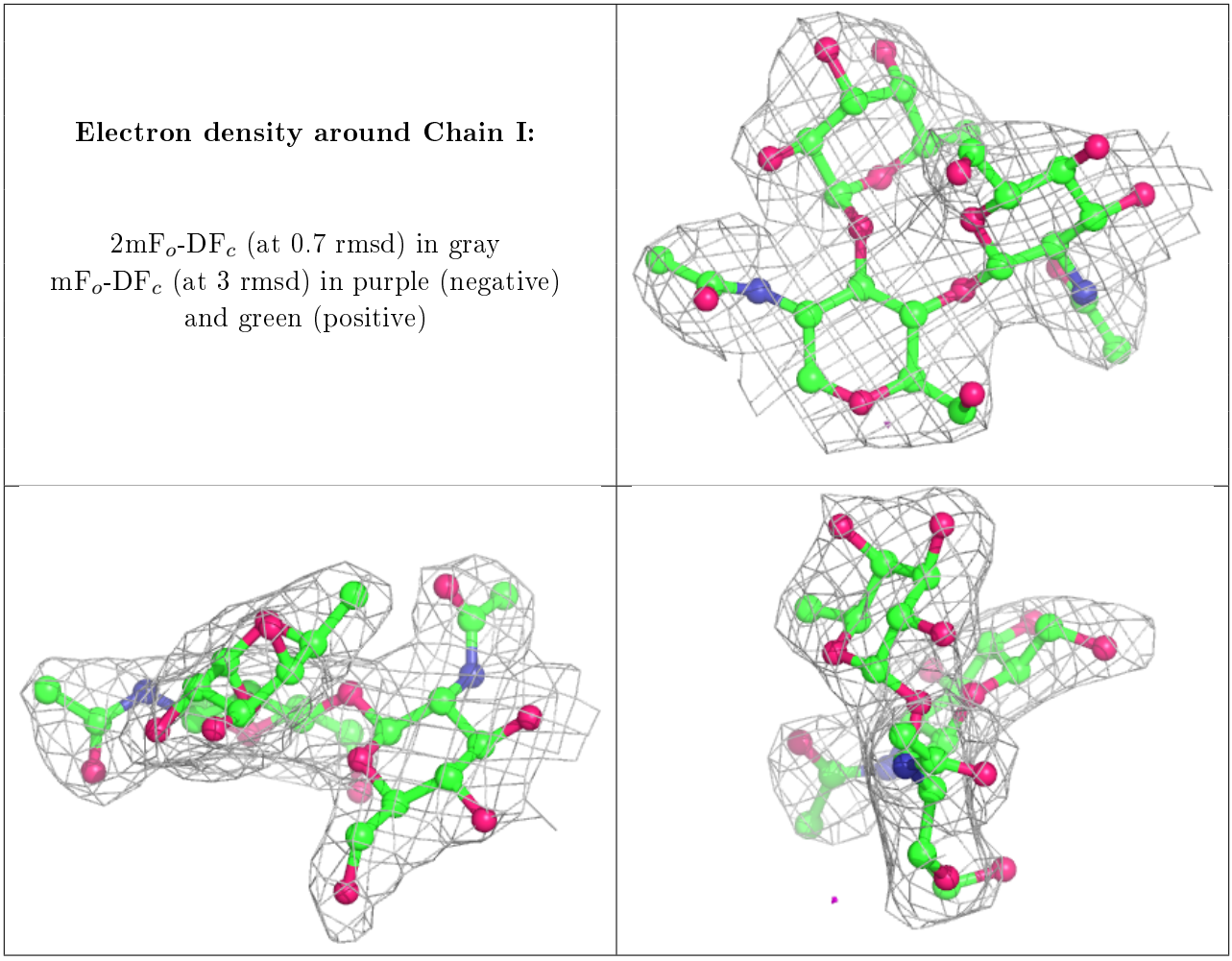






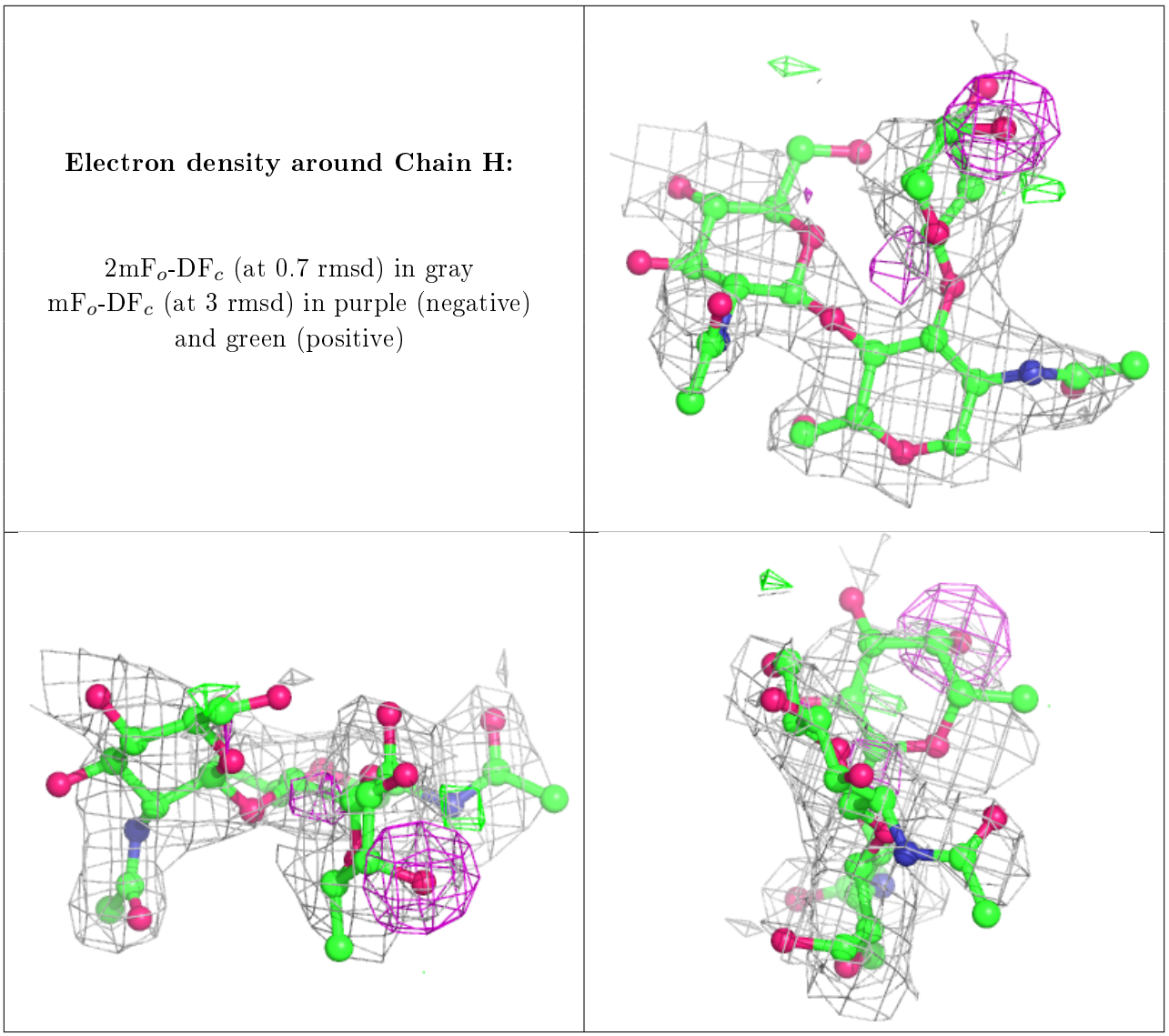
Electron density around Chain I:

$2mF_o$-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 H:

$2mF_o$-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
5	MN	B	257	1/1	0.93	0.10	29,29,29,29	0
4	CA	D	254	1/1	0.96	0.06	41,41,41,41	0
4	CA	F	254	1/1	0.96	0.09	54,54,54,54	0
4	CA	E	254	1/1	0.96	0.07	30,30,30,30	0
4	CA	A	254	1/1	0.97	0.08	43,43,43,43	0
5	MN	F	257	1/1	0.97	0.09	38,38,38,38	0
5	MN	D	257	1/1	0.98	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	254	1/1	0.98	0.04	31,31,31,31	0
4	CA	C	254	1/1	0.98	0.08	36,36,36,36	0
5	MN	E	257	1/1	0.99	0.05	23,23,23,23	0
5	MN	A	257	1/1	1.00	0.08	29,29,29,29	0
5	MN	C	257	1/1	1.00	0.08	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.