Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:18 PM BST

PDB ID	:	1RER
Title	:	Crystal structure of the homotrimer of fusion glycoprotein E1 from Semliki Forest Virus.
Authors	:	Gibbons, D.L.; Vaney, M.C.; Roussel, A.; Vigouroux, A.; Reilly, B.; Kielian, M.; Rey, F.A.
Deposited on	:	2003-11-07
Resolution	:	3.20 Å(reported)

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

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

The following versions of software and data (see references ①) were used in the production of this report:

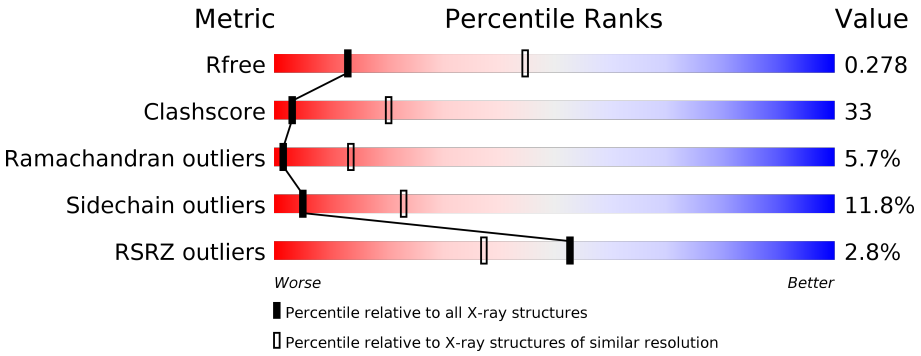
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	391	2% 51% 39% 9%
1	B	391	5% 49% 41% 9%
1	C	391	2% 53% 39% 7%
2	D	6	50% 50%
3	E	7	29% 71%
4	F	2	100%

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	BMA	D	4	-	-	-	X
3	NAG	E	1	X	-	-	-
3	MAN	E	4	-	-	-	X
3	NAG	E	5	-	-	-	X
3	MAN	E	6	-	-	-	X
3	FUC	E	7	X	-	-	-
4	NAG	F	2	-	-	-	X

2 Entry composition

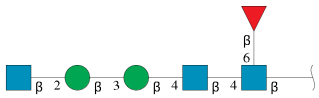
There are 8 unique types of molecules in this entry. The entry contains 9317 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Structural polyprotein.

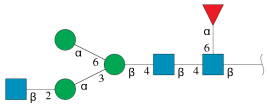
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2993	1891	501	578	23			
1	B	391	Total	C	N	O	S	0	0	0
			2993	1891	501	578	23			
1	C	391	Total	C	N	O	S	0	0	0
			2993	1891	501	578	23			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	0
			74	42	3	29			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
3	E	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	2	Total C N O 28 16 2 10	0	0	0

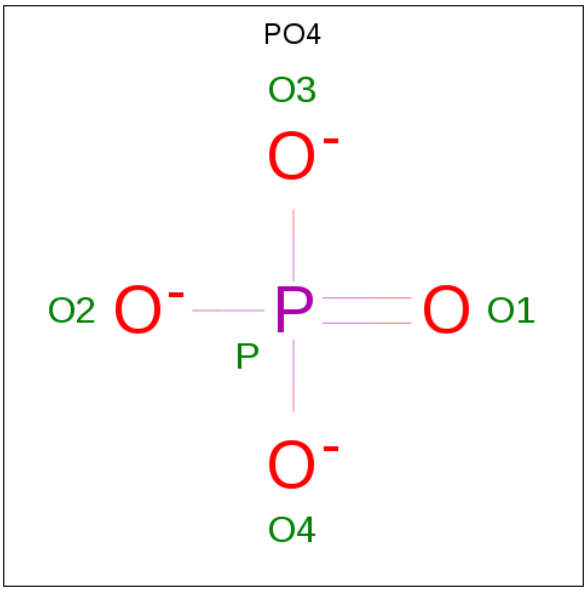
- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Br 1 1	0	0
5	A	1	Total Br 1 1	0	0
5	C	1	Total Br 1 1	0	0

- Molecule 6 is HOLMIUM ATOM (three-letter code: HO) (formula: Ho).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ho 1 1	0	0
6	A	2	Total Ho 2 2	0	0
6	C	1	Total Ho 1 1	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

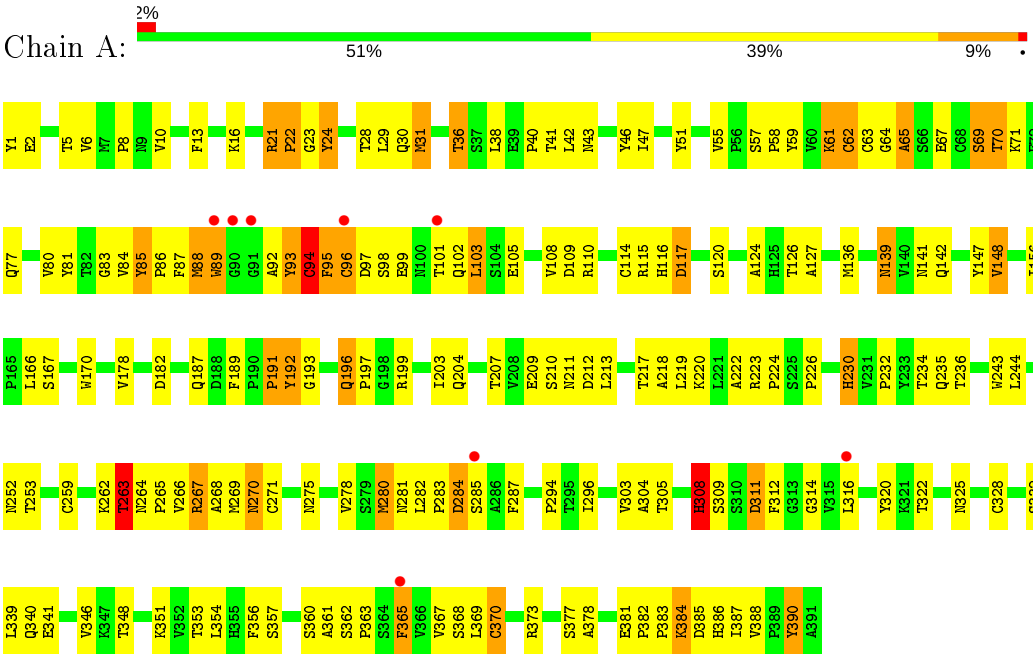
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	54	Total O 54 54	0	0
8	B	46	Total O 46 46	0	0
8	C	39	Total O 39 39	0	0

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.

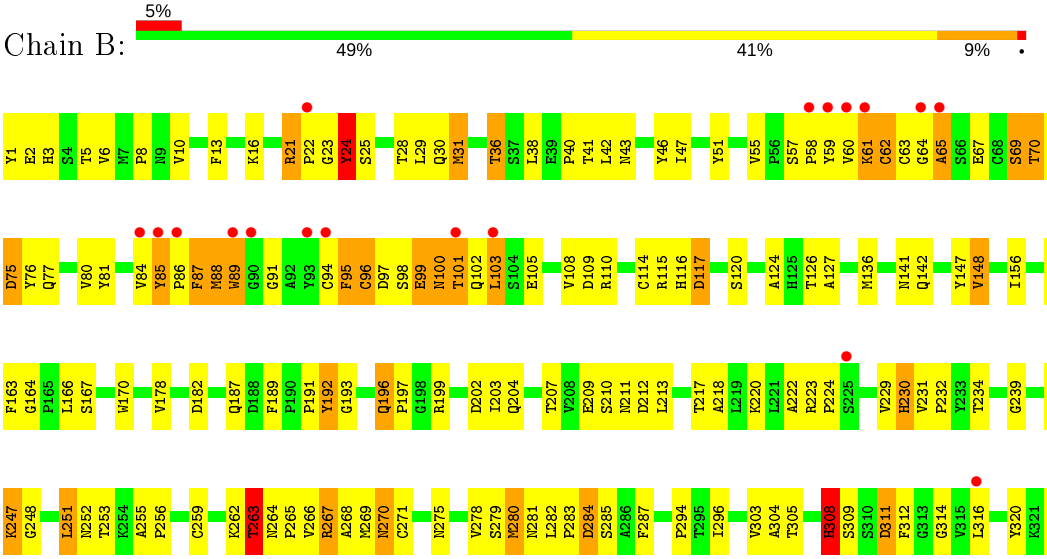
- Molecule 1: Structural polyprotein

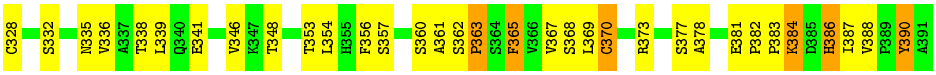
Chain A:



- Molecule 1: Structural polyprotein

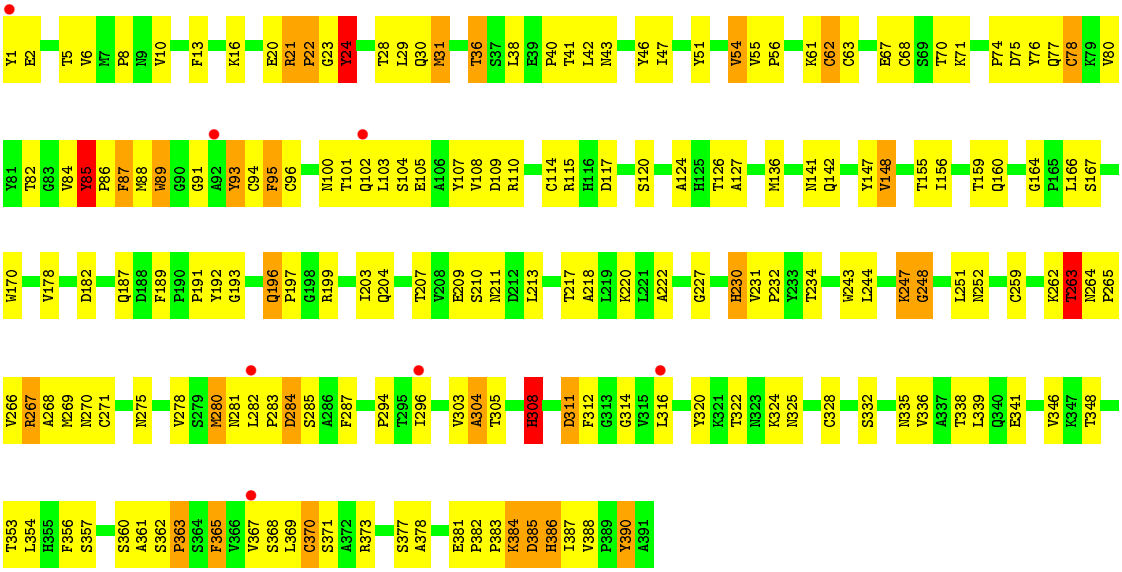
Chain B:





• Molecule 1: Structural polyprotein

Chain C:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.20Å 198.20Å 116.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 171.64 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-3.20) 93.8 (171.64-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.285 0.261 , 0.278	Depositor DCC
R_{free} test set	2204 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9317	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: BMA, NAG, PO4, HO, BR, FUL, MAN, 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	0.70	0/3073	0.76	3/4193 (0.1%)
1	B	0.73	0/3073	0.75	2/4193 (0.0%)
1	C	0.69	0/3073	0.74	2/4193 (0.0%)
All	All	0.71	0/9219	0.75	7/12579 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	A	21	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	C	21	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	94	CYS	CA-CB-SG	5.74	124.34	114.00
1	B	263	THR	N-CA-C	5.34	125.42	111.00
1	A	263	THR	N-CA-C	5.29	125.29	111.00
1	C	263	THR	N-CA-C	5.24	125.15	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	2993	0	2889	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2993	0	2888	225	1
1	C	2993	0	2889	184	0
2	D	74	0	64	5	0
3	E	85	0	73	6	0
4	F	28	0	25	5	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	5	0	0	0	0
8	A	54	0	0	2	0
8	B	46	0	0	8	0
8	C	39	0	0	5	0
All	All	9317	0	8828	600	1

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 33.

All (600) 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:C:21:ARG:NH2	1:C:24:TYR:CE2	2.08	1.19
1:C:21:ARG:NH2	1:C:24:TYR:CZ	2.17	1.10
1:C:21:ARG:NH2	1:C:24:TYR:OH	1.84	1.09
1:B:65:ALA:HA	1:B:101:THR:HG21	1.39	1.04
1:A:65:ALA:HA	1:A:101:THR:HG21	1.41	1.02
1:B:84:VAL:HG13	1:B:223:ARG:HH11	1.17	1.01
1:B:61:LYS:HZ2	1:B:62:CYS:H	1.00	0.99
1:B:265:PRO:HG2	1:B:267:ARG:HD2	1.44	0.99
1:C:265:PRO:HG2	1:C:267:ARG:HD2	1.43	0.99
2:D:1:NAG:H61	2:D:2:NAG:HN2	1.28	0.98
1:A:265:PRO:HG2	1:A:267:ARG:HD2	1.45	0.97
1:A:61:LYS:HZ2	1:A:62:CYS:H	1.00	0.97
1:C:316:LEU:HD11	1:C:365:PHE:CZ	2.01	0.96
1:C:5:THR:HG22	1:C:6:VAL:H	1.30	0.96
1:A:316:LEU:HD11	1:A:365:PHE:CZ	2.01	0.95
1:A:5:THR:HG22	1:A:6:VAL:H	1.31	0.94
1:C:303:VAL:HG22	1:C:316:LEU:CD2	1.97	0.94
1:A:316:LEU:HD11	1:A:365:PHE:CE1	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HD11	1:B:365:PHE:CZ	2.03	0.93
1:B:303:VAL:HG22	1:B:316:LEU:CD2	1.97	0.92
1:B:5:THR:HG22	1:B:6:VAL:H	1.33	0.92
1:C:316:LEU:HD11	1:C:365:PHE:CE1	2.05	0.92
1:A:303:VAL:HG22	1:A:316:LEU:CD2	1.99	0.92
1:B:316:LEU:HD11	1:B:365:PHE:CE1	2.06	0.91
1:C:21:ARG:NH2	1:C:24:TYR:HE2	1.66	0.90
1:A:59:TYR:HB3	1:A:103:LEU:HD23	1.54	0.89
1:B:59:TYR:HB3	1:B:103:LEU:HD23	1.53	0.89
1:C:61:LYS:HB2	1:C:101:THR:O	1.75	0.86
1:B:303:VAL:HG22	1:B:316:LEU:HD23	1.59	0.84
1:C:303:VAL:HG22	1:C:316:LEU:HD23	1.59	0.84
1:A:303:VAL:HG22	1:A:316:LEU:HD23	1.60	0.83
1:C:332:SER:HB2	1:C:339:LEU:HD13	1.61	0.83
1:B:61:LYS:NZ	1:B:62:CYS:H	1.78	0.82
1:B:384:LYS:H	1:B:384:LYS:HD3	1.43	0.82
2:D:1:NAG:H61	2:D:2:NAG:N2	1.94	0.82
1:A:61:LYS:HB3	1:A:101:THR:HG23	1.62	0.82
1:B:84:VAL:HG13	1:B:223:ARG:NH1	1.95	0.81
1:C:141:ASN:HB2	4:F:1:NAG:H83	1.63	0.81
1:C:304:ALA:HB2	8:C:436:HOH:O	1.79	0.81
1:A:160:GLN:H	1:A:281:ASN:ND2	1.79	0.81
1:B:160:GLN:H	1:B:281:ASN:ND2	1.79	0.80
1:C:160:GLN:H	1:C:281:ASN:ND2	1.79	0.80
1:B:61:LYS:HB3	1:B:101:THR:HG23	1.64	0.79
1:B:332:SER:HB2	1:B:339:LEU:HD13	1.64	0.79
1:C:54:VAL:HG21	1:C:107:TYR:CE1	2.18	0.78
1:A:332:SER:HB2	1:A:339:LEU:HD13	1.65	0.77
1:B:100:ASN:HD22	1:B:100:ASN:N	1.80	0.77
3:E:2:NAG:H5	3:E:7:FUC:H5	1.66	0.76
1:B:84:VAL:HG11	1:B:224:PRO:HD2	1.66	0.76
1:C:104:SER:HB2	1:C:231:VAL:HG13	1.67	0.76
1:A:61:LYS:NZ	1:A:62:CYS:H	1.81	0.76
1:C:187:GLN:HE22	1:C:243:TRP:HE1	1.31	0.76
1:C:294:PRO:HA	1:C:324:LYS:HE2	1.68	0.75
1:B:187:GLN:HE22	1:B:243:TRP:HE1	1.34	0.74
1:A:126:THR:HB	1:B:170:TRP:CH2	2.23	0.74
1:B:265:PRO:HG2	1:B:267:ARG:CD	2.18	0.74
1:B:10:VAL:HA	8:B:450:HOH:O	1.87	0.74
1:A:265:PRO:HG2	1:A:267:ARG:CD	2.18	0.73
4:F:1:NAG:H62	4:F:2:NAG:N2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TRP:CH2	1:C:126:THR:HB	2.23	0.73
1:A:187:GLN:HE22	1:A:243:TRP:HE1	1.34	0.73
1:C:54:VAL:HG23	1:C:107:TYR:O	1.87	0.73
1:C:308:HIS:HB3	1:C:383:PRO:HD3	1.71	0.73
1:B:308:HIS:HB3	1:B:383:PRO:HD3	1.71	0.72
1:A:16:LYS:HE3	1:A:30:GLN:NE2	2.04	0.72
1:B:141:ASN:CG	3:E:1:NAG:HN2	1.91	0.72
1:C:265:PRO:HG2	1:C:267:ARG:CD	2.19	0.72
1:A:126:THR:HB	1:B:170:TRP:CZ3	2.25	0.71
1:B:16:LYS:HE3	1:B:30:GLN:NE2	2.05	0.71
1:C:16:LYS:HE3	1:C:30:GLN:NE2	2.04	0.71
1:C:384:LYS:HZ2	1:C:385:ASP:H	1.38	0.71
1:A:308:HIS:HB3	1:A:383:PRO:HD3	1.71	0.71
1:B:61:LYS:HZ1	1:B:62:CYS:HB2	1.55	0.71
1:C:86:PRO:HG2	1:C:227:GLY:H	1.55	0.71
1:C:21:ARG:O	1:C:21:ARG:HG3	1.90	0.71
1:B:110:ARG:HB2	1:B:114:CYS:SG	2.31	0.70
1:B:142:GLN:HB3	1:B:156:ILE:HD12	1.72	0.70
1:B:21:ARG:HG3	1:B:21:ARG:O	1.92	0.70
1:C:142:GLN:HB3	1:C:156:ILE:HD12	1.74	0.70
1:A:170:TRP:CZ3	1:C:126:THR:HB	2.26	0.70
1:B:316:LEU:HG	1:B:356:PHE:CD2	2.28	0.69
1:A:142:GLN:HB3	1:A:156:ILE:HD12	1.73	0.69
1:B:86:PRO:HG2	1:B:229:VAL:CG1	2.22	0.69
1:A:5:THR:HG22	1:A:6:VAL:N	2.08	0.69
1:C:316:LEU:HG	1:C:356:PHE:CD2	2.28	0.69
1:A:61:LYS:HB3	1:A:101:THR:CG2	2.23	0.69
1:A:61:LYS:HZ2	1:A:62:CYS:N	1.84	0.69
1:A:88:MET:HG3	1:A:89:TRP:H	1.57	0.69
1:C:308:HIS:HB2	1:C:382:PRO:HA	1.76	0.68
1:C:110:ARG:HB2	1:C:114:CYS:SG	2.33	0.68
1:A:88:MET:HG2	1:A:92:ALA:HA	1.75	0.68
1:B:84:VAL:O	1:B:86:PRO:HD3	1.92	0.68
1:B:63:CYS:HA	1:B:100:ASN:HA	1.76	0.68
1:B:84:VAL:CG1	1:B:224:PRO:HD2	2.23	0.68
1:A:316:LEU:HG	1:A:356:PHE:CD2	2.29	0.67
1:A:88:MET:CG	1:A:92:ALA:HA	2.24	0.67
1:B:5:THR:HG22	1:B:6:VAL:N	2.09	0.67
1:C:267:ARG:HH11	1:C:267:ARG:HG3	1.58	0.67
1:B:84:VAL:HG22	1:B:223:ARG:HD2	1.77	0.67
1:A:267:ARG:N	1:A:267:ARG:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HE3	8:A:446:HOH:O	1.94	0.67
1:A:43:ASN:HB2	1:B:311:ASP:OD1	1.95	0.67
1:B:308:HIS:HB2	1:B:382:PRO:HA	1.76	0.67
1:C:160:GLN:H	1:C:281:ASN:HD21	1.42	0.67
1:C:267:ARG:N	1:C:267:ARG:HD3	2.10	0.67
1:A:88:MET:SD	1:A:92:ALA:HA	2.35	0.67
1:C:5:THR:HG22	1:C:6:VAL:N	2.07	0.67
1:A:308:HIS:HB2	1:A:382:PRO:HA	1.76	0.67
1:B:267:ARG:N	1:B:267:ARG:HD3	2.10	0.67
1:B:316:LEU:HD11	1:B:365:PHE:HZ	1.59	0.67
1:B:61:LYS:HB3	1:B:101:THR:CG2	2.26	0.66
1:C:148:VAL:HG13	1:C:166:LEU:HB2	1.77	0.66
1:B:126:THR:HB	1:C:170:TRP:CH2	2.30	0.66
1:B:160:GLN:H	1:B:281:ASN:HD21	1.42	0.66
1:A:384:LYS:HZ2	1:A:385:ASP:H	1.42	0.66
1:C:89:TRP:HE1	1:C:100:ASN:HD21	1.44	0.66
1:B:148:VAL:HG13	1:B:166:LEU:HB2	1.78	0.65
1:C:89:TRP:HE1	1:C:100:ASN:ND2	1.94	0.65
1:C:84:VAL:C	1:C:86:PRO:HD3	2.16	0.65
1:A:73:LYS:HB2	1:A:76:TYR:HB2	1.78	0.65
1:A:83:GLY:HA2	1:A:98:SER:O	1.96	0.65
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.61	0.65
1:A:311:ASP:OD1	1:C:43:ASN:HB2	1.97	0.65
1:B:222:ALA:O	1:B:232:PRO:HG2	1.97	0.64
1:B:267:ARG:HH11	1:B:267:ARG:HG3	1.61	0.64
1:B:29:LEU:HD12	1:B:30:GLN:H	1.62	0.64
1:B:384:LYS:HD3	1:B:384:LYS:N	2.09	0.64
1:A:160:GLN:H	1:A:281:ASN:HD21	1.43	0.64
1:C:104:SER:HB2	1:C:231:VAL:CG1	2.27	0.64
1:C:1:TYR:O	1:C:281:ASN:HA	1.97	0.64
1:A:316:LEU:HD11	1:A:365:PHE:HZ	1.58	0.64
1:B:81:TYR:HB3	1:B:84:VAL:HG21	1.78	0.64
1:A:110:ARG:HB2	1:A:114:CYS:SG	2.37	0.64
1:A:222:ALA:O	1:A:232:PRO:HG2	1.97	0.64
1:C:316:LEU:HD11	1:C:365:PHE:HZ	1.56	0.64
1:B:100:ASN:ND2	1:B:100:ASN:N	2.46	0.64
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.63	0.64
1:C:56:PRO:HD2	1:C:105:GLU:O	1.97	0.64
1:B:202:ASP:HB2	8:B:435:HOH:O	1.96	0.64
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.63	0.64
1:B:61:LYS:HZ2	1:B:62:CYS:N	1.84	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:HB	1:C:270:ASN:HA	1.80	0.63
1:A:59:TYR:CB	1:A:103:LEU:HD23	2.28	0.63
1:A:148:VAL:HG13	1:A:166:LEU:HB2	1.80	0.63
1:B:264:ASN:HB3	1:B:265:PRO:HD3	1.80	0.63
1:A:367:VAL:HG12	1:A:368:SER:N	2.14	0.63
1:C:86:PRO:CG	1:C:227:GLY:H	2.11	0.63
1:C:74:PRO:O	1:C:75:ASP:OD2	2.17	0.63
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.63	0.63
1:A:61:LYS:HE3	1:A:64:GLY:CA	2.29	0.63
1:A:1:TYR:O	1:A:281:ASN:HA	1.98	0.63
1:B:67:GLU:HA	1:B:80:VAL:HG11	1.81	0.63
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.64	0.63
1:A:2:GLU:HA	1:A:280:MET:O	1.99	0.63
1:B:36:THR:HB	1:B:270:ASN:HA	1.81	0.62
1:B:73:LYS:HB2	1:B:76:TYR:HB2	1.79	0.62
1:C:222:ALA:O	1:C:232:PRO:HG2	1.98	0.62
1:B:94:CYS:SG	1:B:100:ASN:OD1	2.58	0.62
1:C:325:ASN:OD1	1:C:348:THR:N	2.33	0.62
1:C:264:ASN:HB3	1:C:265:PRO:HD3	1.80	0.62
1:A:325:ASN:OD1	1:A:348:THR:N	2.32	0.62
1:C:85:TYR:N	1:C:86:PRO:HD3	2.14	0.62
1:B:81:TYR:HB3	1:B:84:VAL:CG2	2.29	0.62
1:C:2:GLU:HA	1:C:280:MET:O	2.00	0.62
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.64	0.62
1:B:2:GLU:HA	1:B:280:MET:O	1.99	0.61
1:C:29:LEU:HD12	1:C:30:GLN:H	1.65	0.61
1:A:264:ASN:HB3	1:A:265:PRO:HD3	1.82	0.61
1:C:316:LEU:HD11	1:C:365:PHE:HE1	1.64	0.61
1:A:191:PRO:HA	5:A:417:BR:BR	2.56	0.61
1:A:316:LEU:CD1	1:A:365:PHE:CE1	2.83	0.61
1:A:94:CYS:O	1:A:95:PHE:HB2	2.00	0.61
1:C:367:VAL:HG12	1:C:368:SER:N	2.16	0.61
1:B:29:LEU:HD12	1:B:30:GLN:N	2.16	0.61
1:B:325:ASN:OD1	1:B:348:THR:N	2.33	0.61
1:C:21:ARG:CZ	1:C:24:TYR:CE2	2.84	0.61
1:B:24:TYR:HD1	8:B:445:HOH:O	1.83	0.60
1:A:71:LYS:H	1:A:76:TYR:HE2	1.48	0.60
1:B:247:LYS:O	1:B:247:LYS:HG3	2.02	0.60
1:B:61:LYS:HE3	1:B:64:GLY:CA	2.30	0.60
1:A:85:TYR:CE2	1:A:87:PHE:HB3	2.36	0.60
1:B:71:LYS:H	1:B:76:TYR:HE2	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:HA	1:A:357:SER:HB2	1.84	0.60
1:A:67:GLU:HA	1:A:80:VAL:HG11	1.82	0.60
1:B:1:TYR:O	1:B:281:ASN:HA	2.00	0.60
1:A:316:LEU:HD11	1:A:365:PHE:HE1	1.63	0.60
1:B:196:GLN:HA	1:B:196:GLN:HE21	1.66	0.60
1:C:85:TYR:O	8:C:438:HOH:O	2.16	0.60
1:B:367:VAL:HG12	1:B:368:SER:N	2.17	0.60
1:B:59:TYR:CB	1:B:103:LEU:HD23	2.29	0.60
1:B:61:LYS:HD3	1:B:62:CYS:N	2.17	0.60
1:C:320:TYR:CE1	1:C:346:VAL:HG13	2.37	0.60
1:A:88:MET:HG3	1:A:89:TRP:N	2.18	0.59
1:A:36:THR:HB	1:A:270:ASN:HA	1.83	0.59
1:C:247:LYS:O	1:C:247:LYS:HG3	2.01	0.59
1:A:247:LYS:O	1:A:247:LYS:HG3	2.01	0.59
1:A:373:ARG:HH11	1:A:373:ARG:HG3	1.66	0.59
1:B:126:THR:HB	1:C:170:TRP:CZ3	2.36	0.59
1:C:316:LEU:CD1	1:C:365:PHE:CE1	2.83	0.59
1:C:187:GLN:NE2	1:C:243:TRP:HE1	1.97	0.59
1:C:264:ASN:HB3	1:C:265:PRO:CD	2.33	0.59
1:C:312:PHE:HA	1:C:357:SER:HB2	1.85	0.59
1:B:187:GLN:NE2	1:B:243:TRP:HE1	2.00	0.59
1:B:312:PHE:HA	1:B:357:SER:HB2	1.84	0.59
1:B:61:LYS:NZ	1:B:62:CYS:HB2	2.16	0.59
1:A:61:LYS:HD3	1:A:62:CYS:N	2.18	0.59
1:B:84:VAL:HG11	1:B:223:ARG:HG3	1.84	0.59
1:B:294:PRO:HG2	1:B:328:CYS:SG	2.43	0.59
1:B:43:ASN:HB2	1:C:311:ASP:OD1	2.01	0.59
1:B:264:ASN:HB3	1:B:265:PRO:CD	2.33	0.59
1:C:54:VAL:HG21	1:C:107:TYR:CZ	2.36	0.59
1:A:80:VAL:HG12	1:A:103:LEU:HD12	1.85	0.58
1:B:80:VAL:HG12	1:B:103:LEU:HD12	1.85	0.58
1:C:294:PRO:HG2	1:C:328:CYS:SG	2.43	0.58
1:A:61:LYS:NZ	1:A:62:CYS:HB2	2.18	0.58
1:A:42:LEU:HD23	1:A:124:ALA:HB2	1.86	0.58
1:A:61:LYS:HZ1	1:A:62:CYS:HB2	1.67	0.58
1:A:29:LEU:HD12	1:A:30:GLN:H	1.67	0.58
1:B:58:PRO:HG3	1:B:231:VAL:HG22	1.85	0.58
1:B:373:ARG:HG3	1:B:373:ARG:HH11	1.68	0.58
1:A:187:GLN:NE2	1:A:243:TRP:HE1	1.99	0.58
1:A:294:PRO:HG2	1:A:328:CYS:SG	2.43	0.58
1:C:193:GLY:N	8:C:426:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TYR:CE1	1:A:346:VAL:HG13	2.38	0.58
1:C:42:LEU:HD23	1:C:124:ALA:HB2	1.85	0.58
1:B:10:VAL:HG23	1:B:10:VAL:O	2.04	0.57
1:B:320:TYR:CE1	1:B:346:VAL:HG13	2.39	0.57
1:C:21:ARG:CZ	1:C:24:TYR:HE2	2.17	0.57
1:A:264:ASN:HB3	1:A:265:PRO:CD	2.35	0.57
1:B:86:PRO:HB3	8:B:447:HOH:O	2.04	0.57
1:B:316:LEU:HD11	1:B:365:PHE:HE1	1.64	0.57
1:C:68:CYS:HB3	1:C:103:LEU:HD21	1.86	0.57
1:C:29:LEU:HD12	1:C:30:GLN:N	2.18	0.57
1:B:207:THR:HG22	1:B:210:SER:HB2	1.86	0.57
1:B:84:VAL:O	1:B:86:PRO:CD	2.52	0.57
1:B:65:ALA:HA	1:B:101:THR:CG2	2.26	0.57
1:C:373:ARG:HG3	1:C:373:ARG:HH11	1.71	0.56
1:C:341:GLU:HG3	1:C:354:LEU:HD22	1.87	0.56
1:A:29:LEU:HD12	1:A:30:GLN:N	2.20	0.56
1:B:98:SER:C	1:B:99:GLU:HG3	2.25	0.56
1:B:167:SER:HB3	1:B:275:ASN:OD1	2.06	0.56
1:B:341:GLU:HG3	1:B:354:LEU:HD22	1.88	0.56
1:A:207:THR:HG22	1:A:210:SER:HB2	1.88	0.56
1:A:341:GLU:HG3	1:A:354:LEU:HD22	1.88	0.56
1:C:36:THR:O	1:C:269:MET:HA	2.05	0.56
1:B:308:HIS:CB	1:B:382:PRO:HA	2.36	0.55
1:C:167:SER:HB3	1:C:275:ASN:OD1	2.06	0.55
1:A:167:SER:HB3	1:A:275:ASN:OD1	2.04	0.55
1:A:284:ASP:CG	1:C:284:ASP:OD1	2.44	0.55
1:B:42:LEU:HD23	1:B:124:ALA:HB2	1.87	0.55
1:C:5:THR:CG2	1:C:6:VAL:H	2.13	0.55
1:A:308:HIS:CB	1:A:382:PRO:HA	2.36	0.55
1:A:63:CYS:C	1:A:65:ALA:H	2.10	0.55
1:A:63:CYS:SG	1:A:94:CYS:O	2.65	0.55
1:B:36:THR:O	1:B:269:MET:HA	2.06	0.55
1:C:308:HIS:CB	1:C:382:PRO:HA	2.36	0.55
1:C:203:ILE:O	1:C:204:GLN:HG3	2.07	0.54
1:B:203:ILE:O	1:B:204:GLN:HG3	2.06	0.54
1:A:207:THR:O	1:A:210:SER:HB3	2.06	0.54
1:A:36:THR:O	1:A:269:MET:HA	2.07	0.54
1:A:353:THR:O	1:A:354:LEU:HD23	2.07	0.54
1:A:203:ILE:O	1:A:204:GLN:HG3	2.08	0.54
1:A:212:ASP:OD2	1:B:386:HIS:HB2	2.08	0.54
1:C:21:ARG:CG	1:C:21:ARG:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:C	1:A:139:ASN:HD22	2.12	0.54
1:B:141:ASN:CG	3:E:1:NAG:N2	2.61	0.53
1:B:353:THR:O	1:B:354:LEU:HD23	2.06	0.53
1:B:63:CYS:C	1:B:65:ALA:H	2.11	0.53
1:A:108:VAL:HG12	1:A:109:ASP:N	2.23	0.53
1:A:41:THR:OG1	1:A:127:ALA:HB2	2.08	0.53
1:C:207:THR:HG22	1:C:210:SER:HB2	1.89	0.53
1:C:207:THR:O	1:C:210:SER:HB3	2.08	0.53
1:C:294:PRO:CA	1:C:324:LYS:HE2	2.37	0.53
1:B:207:THR:O	1:B:210:SER:HB3	2.08	0.53
1:B:31:MET:HE2	1:B:278:VAL:HG11	1.91	0.53
1:B:46:TYR:CD1	1:B:46:TYR:C	2.80	0.53
1:A:63:CYS:SG	1:A:94:CYS:C	2.87	0.53
1:B:21:ARG:CG	1:B:21:ARG:O	2.57	0.53
1:B:316:LEU:CD1	1:B:365:PHE:CE1	2.85	0.53
1:C:41:THR:OG1	1:C:127:ALA:HB2	2.08	0.53
1:C:353:THR:O	1:C:354:LEU:HD23	2.09	0.53
1:A:283:PRO:C	1:A:285:SER:H	2.12	0.53
1:A:85:TYR:HD1	1:A:226:PRO:HB3	1.74	0.53
1:C:332:SER:HB2	1:C:339:LEU:CD1	2.35	0.53
1:C:365:PHE:HD2	1:C:365:PHE:H	1.56	0.53
1:A:46:TYR:C	1:A:46:TYR:CD1	2.82	0.53
1:B:108:VAL:HG12	1:B:109:ASP:N	2.24	0.53
1:C:10:VAL:O	1:C:10:VAL:HG23	2.09	0.52
1:C:387:ILE:N	1:C:387:ILE:HD12	2.25	0.52
1:C:108:VAL:HG12	1:C:109:ASP:N	2.23	0.52
1:C:104:SER:CB	1:C:231:VAL:HG13	2.37	0.52
1:A:31:MET:HE1	1:A:278:VAL:HG11	1.91	0.52
1:A:63:CYS:HB2	1:A:96:CYS:O	2.09	0.52
1:C:207:THR:H	1:C:210:SER:HB2	1.74	0.52
1:B:387:ILE:N	1:B:387:ILE:HD12	2.24	0.52
1:A:85:TYR:CD1	1:A:226:PRO:HB3	2.45	0.52
1:B:41:THR:OG1	1:B:127:ALA:HB2	2.09	0.52
1:C:78:CYS:SG	1:C:78:CYS:O	2.67	0.52
1:A:10:VAL:HG23	1:A:10:VAL:O	2.09	0.52
1:A:387:ILE:HD12	1:A:387:ILE:N	2.25	0.51
1:C:31:MET:HE2	1:C:278:VAL:HG11	1.91	0.51
1:A:207:THR:H	1:A:210:SER:HB2	1.75	0.51
1:C:40:PRO:HB2	1:C:124:ALA:HB1	1.93	0.51
1:A:311:ASP:H	1:C:43:ASN:HD22	1.58	0.51
1:C:46:TYR:CD1	1:C:46:TYR:C	2.82	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PRO:HG2	1:B:229:VAL:HG12	1.92	0.51
1:C:71:LYS:HD3	1:C:76:TYR:CE1	2.45	0.51
1:B:332:SER:HB2	1:B:339:LEU:CD1	2.36	0.51
1:C:54:VAL:CG2	1:C:107:TYR:O	2.58	0.51
2:D:3:BMA:H5	2:D:5:NAG:HN2	1.76	0.51
1:A:367:VAL:CG1	1:A:368:SER:N	2.73	0.51
1:A:51:TYR:CD1	1:A:51:TYR:C	2.83	0.51
1:B:88:MET:O	1:B:89:TRP:HB3	2.11	0.51
1:B:25:SER:HB3	8:B:445:HOH:O	2.11	0.51
1:B:84:VAL:O	1:B:86:PRO:N	2.44	0.51
1:A:62:CYS:O	1:A:101:THR:HG22	2.11	0.50
1:A:5:THR:CG2	1:A:6:VAL:H	2.13	0.50
1:B:43:ASN:HD22	1:C:311:ASP:H	1.58	0.50
1:C:93:TYR:CD1	1:C:93:TYR:N	2.79	0.50
1:A:88:MET:HG2	1:A:92:ALA:CA	2.41	0.50
1:A:40:PRO:HB2	1:A:124:ALA:HB1	1.93	0.50
1:A:81:TYR:O	1:A:101:THR:HA	2.11	0.50
1:B:100:ASN:O	1:B:101:THR:HB	2.10	0.50
1:A:116:HIS:HB3	8:A:451:HOH:O	2.12	0.50
1:B:220:LYS:HB3	1:B:234:THR:OG1	2.12	0.50
1:B:51:TYR:CD1	1:B:51:TYR:C	2.84	0.50
1:A:109:ASP:HA	1:A:213:LEU:CD2	2.42	0.50
1:A:365:PHE:HD2	1:A:365:PHE:H	1.57	0.50
1:B:283:PRO:C	1:B:285:SER:H	2.14	0.50
1:A:332:SER:HB2	1:A:339:LEU:CD1	2.38	0.49
1:C:220:LYS:HB3	1:C:234:THR:OG1	2.12	0.49
1:C:283:PRO:C	1:C:285:SER:H	2.14	0.49
1:C:362:SER:HA	1:C:378:ALA:O	2.12	0.49
1:B:202:ASP:CB	8:B:435:HOH:O	2.55	0.49
1:C:316:LEU:CD1	1:C:365:PHE:HE1	2.24	0.49
1:B:95:PHE:CD2	1:B:95:PHE:N	2.79	0.49
1:C:267:ARG:HG3	1:C:267:ARG:NH1	2.26	0.49
1:B:267:ARG:HG3	1:B:267:ARG:NH1	2.27	0.49
1:B:316:LEU:CD1	1:B:365:PHE:HE1	2.25	0.49
1:A:362:SER:HA	1:A:378:ALA:O	2.13	0.49
1:B:365:PHE:H	1:B:365:PHE:HD2	1.55	0.49
1:C:51:TYR:C	1:C:51:TYR:CD1	2.86	0.49
4:F:1:NAG:H62	4:F:2:NAG:C7	2.42	0.49
1:A:316:LEU:HD21	1:A:365:PHE:HZ	1.78	0.49
1:A:84:VAL:HG21	1:A:224:PRO:HB2	1.94	0.49
1:B:296:ILE:HD11	1:B:369:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:NH1	1:B:335:ASN:HD22	2.10	0.49
1:A:61:LYS:HE3	1:A:64:GLY:HA3	1.94	0.49
1:C:217:THR:O	1:C:218:ALA:HB3	2.13	0.49
1:B:207:THR:H	1:B:210:SER:HB2	1.77	0.49
1:C:109:ASP:HA	1:C:213:LEU:CD2	2.43	0.49
1:C:365:PHE:CD2	1:C:365:PHE:N	2.81	0.49
1:C:67:GLU:OE1	1:C:80:VAL:HG11	2.13	0.49
1:B:40:PRO:HB2	1:B:124:ALA:HB1	1.95	0.48
1:A:160:GLN:HB3	1:A:281:ASN:HD21	1.78	0.48
1:B:81:TYR:O	1:B:101:THR:HA	2.13	0.48
1:B:160:GLN:HB3	1:B:281:ASN:HD21	1.77	0.48
1:A:365:PHE:N	1:A:365:PHE:CD2	2.82	0.48
1:B:62:CYS:O	1:B:101:THR:HG22	2.14	0.48
1:A:296:ILE:HD11	1:A:369:LEU:HB3	1.96	0.48
1:B:85:TYR:HB3	1:B:100:ASN:HB2	1.95	0.48
1:B:85:TYR:O	1:B:85:TYR:CD2	2.67	0.48
1:B:316:LEU:HD21	1:B:365:PHE:HZ	1.78	0.48
1:C:20:GLU:O	1:C:22:PRO:HD3	2.13	0.48
1:C:160:GLN:HB3	1:C:281:ASN:HD21	1.78	0.48
1:A:217:THR:O	1:A:218:ALA:HB3	2.13	0.48
1:B:109:ASP:HA	1:B:213:LEU:CD2	2.44	0.48
1:B:21:ARG:NH2	8:B:461:HOH:O	2.38	0.48
1:B:281:ASN:C	1:B:282:LEU:HG	2.35	0.48
1:B:1:TYR:CD1	1:B:283:PRO:HB3	2.49	0.48
1:B:136:MET:HG2	1:B:141:ASN:ND2	2.29	0.47
1:B:61:LYS:HE3	1:B:64:GLY:HA3	1.96	0.47
1:C:85:TYR:C	8:C:438:HOH:O	2.53	0.47
1:A:65:ALA:HA	1:A:101:THR:CG2	2.29	0.47
1:B:362:SER:HA	1:B:378:ALA:O	2.13	0.47
1:C:367:VAL:CG1	1:C:368:SER:N	2.76	0.47
1:A:189:PHE:O	1:A:189:PHE:CD1	2.67	0.47
1:A:243:TRP:CE3	1:A:244:LEU:HD12	2.50	0.47
1:B:182:ASP:C	1:B:263:THR:HG21	2.34	0.47
1:C:189:PHE:CD1	1:C:189:PHE:O	2.67	0.47
1:C:243:TRP:CE3	1:C:244:LEU:HD12	2.50	0.47
1:A:243:TRP:HE3	1:A:244:LEU:HD12	1.80	0.47
1:A:88:MET:CE	1:A:92:ALA:HA	2.44	0.47
1:B:24:TYR:CD2	1:B:24:TYR:N	2.81	0.47
1:A:93:TYR:O	1:A:94:CYS:C	2.53	0.47
1:B:75:ASP:O	1:B:77:GLN:HG2	2.15	0.47
1:C:93:TYR:HD1	1:C:93:TYR:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:HB3	1:A:234:THR:OG1	2.14	0.47
1:A:314:GLY:HA3	1:A:356:PHE:CE2	2.50	0.47
1:B:367:VAL:CG1	1:B:368:SER:N	2.77	0.47
1:B:63:CYS:CA	1:B:100:ASN:HA	2.45	0.47
1:B:95:PHE:HD2	1:B:96:CYS:N	2.13	0.47
1:C:316:LEU:HD21	1:C:365:PHE:HZ	1.80	0.47
1:A:147:TYR:O	1:A:166:LEU:HG	2.15	0.46
1:A:63:CYS:SG	1:A:96:CYS:N	2.88	0.46
1:B:110:ARG:NH1	1:B:110:ARG:HG2	2.30	0.46
1:C:1:TYR:CD1	1:C:283:PRO:HB3	2.49	0.46
1:C:87:PHE:O	1:C:89:TRP:CD1	2.68	0.46
1:A:103:LEU:HD22	1:A:103:LEU:H	1.81	0.46
1:A:281:ASN:C	1:A:282:LEU:HG	2.35	0.46
1:B:85:TYR:O	1:B:85:TYR:CG	2.68	0.46
1:A:81:TYR:CD2	1:A:223:ARG:HG3	2.50	0.46
1:C:281:ASN:C	1:C:282:LEU:HG	2.36	0.46
1:B:189:PHE:CD1	1:B:189:PHE:O	2.69	0.46
1:B:217:THR:O	1:B:218:ALA:HB3	2.15	0.46
1:B:84:VAL:CG1	1:B:223:ARG:CG	2.94	0.46
1:C:296:ILE:HD11	1:C:369:LEU:HB3	1.98	0.46
1:C:361:ALA:O	1:C:362:SER:HB2	2.16	0.46
1:C:61:LYS:HB2	1:C:101:THR:C	2.36	0.46
1:B:84:VAL:HG13	1:B:223:ARG:HG2	1.98	0.46
1:A:203:ILE:C	1:A:204:GLN:HG3	2.36	0.46
1:A:336:VAL:HG22	1:A:336:VAL:O	2.16	0.46
1:B:84:VAL:CG2	1:B:223:ARG:HD2	2.44	0.46
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.27	0.46
1:B:239:GLY:N	8:B:435:HOH:O	2.48	0.46
1:B:55:VAL:HG23	1:B:105:GLU:O	2.15	0.46
1:B:81:TYR:HB3	1:B:84:VAL:CB	2.46	0.46
1:C:182:ASP:C	1:C:263:THR:HG21	2.36	0.46
1:A:1:TYR:CD1	1:A:283:PRO:HB3	2.51	0.46
1:A:361:ALA:O	1:A:362:SER:HB2	2.16	0.46
1:B:203:ILE:C	1:B:204:GLN:HG3	2.36	0.46
1:B:58:PRO:HG3	1:B:231:VAL:CG2	2.46	0.46
1:B:80:VAL:HG23	1:B:80:VAL:O	2.15	0.46
1:C:243:TRP:HE3	1:C:244:LEU:HD12	1.81	0.46
1:B:120:SER:O	1:B:178:VAL:HA	2.16	0.46
1:A:120:SER:O	1:A:178:VAL:HA	2.16	0.45
1:A:182:ASP:C	1:A:263:THR:HG21	2.36	0.45
1:A:80:VAL:HG23	1:A:80:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TRP:CE3	1:B:244:LEU:HD12	2.51	0.45
1:B:96:CYS:C	1:B:98:SER:H	2.19	0.45
1:C:147:TYR:O	1:C:166:LEU:HG	2.15	0.45
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.76	0.45
1:C:259:CYS:SG	1:C:268:ALA:HB1	2.57	0.45
1:B:10:VAL:CG2	1:B:10:VAL:O	2.64	0.45
1:B:314:GLY:HA3	1:B:356:PHE:CE2	2.51	0.45
1:C:110:ARG:NH1	1:C:110:ARG:HG2	2.31	0.45
1:C:203:ILE:C	1:C:204:GLN:HG3	2.36	0.45
1:C:341:GLU:CG	1:C:354:LEU:HD22	2.45	0.45
1:A:259:CYS:SG	1:A:268:ALA:HB1	2.57	0.45
1:C:67:GLU:OE2	1:C:80:VAL:HG11	2.16	0.45
1:A:316:LEU:CD1	1:A:365:PHE:HE1	2.23	0.45
1:B:243:TRP:HE3	1:B:244:LEU:HD12	1.81	0.45
1:B:5:THR:CG2	1:B:6:VAL:H	2.15	0.45
1:A:85:TYR:HA	1:A:86:PRO:HD3	1.62	0.45
1:B:212:ASP:OD2	1:C:386:HIS:HB2	2.17	0.45
1:A:103:LEU:HD22	1:A:103:LEU:N	2.32	0.45
1:A:8:PRO:HG3	1:A:13:PHE:CD2	2.51	0.45
1:B:262:LYS:HD3	1:B:262:LYS:HA	1.77	0.45
1:B:341:GLU:CG	1:B:354:LEU:HD22	2.46	0.45
1:B:61:LYS:HD3	1:B:62:CYS:O	2.16	0.45
1:C:55:VAL:HG21	1:C:231:VAL:HG21	1.97	0.45
1:C:68:CYS:SG	1:C:103:LEU:HD11	2.56	0.45
1:A:61:LYS:HE3	1:A:64:GLY:C	2.37	0.45
1:A:136:MET:HG2	1:A:141:ASN:ND2	2.32	0.45
1:C:136:MET:HG2	1:C:141:ASN:ND2	2.32	0.45
1:C:314:GLY:HA3	1:C:356:PHE:CE2	2.52	0.45
1:C:336:VAL:O	1:C:336:VAL:HG22	2.17	0.45
1:A:110:ARG:NH1	1:A:110:ARG:HG2	2.30	0.44
1:A:284:ASP:OD2	1:C:284:ASP:OD1	2.35	0.44
1:B:283:PRO:C	1:B:285:SER:N	2.71	0.44
1:C:55:VAL:CG2	1:C:231:VAL:HG21	2.47	0.44
1:B:8:PRO:HG3	1:B:13:PHE:CD2	2.53	0.44
3:E:4:MAN:C1	3:E:5:NAG:H2	2.48	0.44
1:A:77:GLN:NE2	1:A:219:LEU:O	2.51	0.44
1:A:283:PRO:C	1:A:285:SER:N	2.70	0.44
1:A:36:THR:HG22	1:A:36:THR:O	2.17	0.44
1:B:61:LYS:HE3	1:B:64:GLY:C	2.37	0.44
1:A:341:GLU:CG	1:A:354:LEU:HD22	2.47	0.44
1:B:369:LEU:O	1:B:370:CYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG13	1:B:223:ARG:CG	2.48	0.44
1:A:55:VAL:HG23	1:A:105:GLU:O	2.18	0.44
1:A:69:SER:O	1:A:70:THR:HG23	2.18	0.44
1:A:197:PRO:O	1:A:199:ARG:HG2	2.18	0.44
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.76	0.44
1:B:320:TYR:HE1	1:B:346:VAL:HG13	1.82	0.44
1:B:147:TYR:O	1:B:166:LEU:HG	2.19	0.43
1:C:247:LYS:O	1:C:248:GLY:O	2.36	0.43
1:C:369:LEU:O	1:C:370:CYS:HB2	2.17	0.43
1:A:247:LYS:O	1:A:248:GLY:O	2.36	0.43
1:A:284:ASP:OD1	1:B:284:ASP:CG	2.57	0.43
1:A:21:ARG:HA	1:A:22:PRO:HD3	1.90	0.43
1:C:68:CYS:SG	1:C:103:LEU:CD1	3.06	0.43
1:C:36:THR:O	1:C:36:THR:HG22	2.18	0.43
1:C:54:VAL:HG21	1:C:107:TYR:CD1	2.53	0.43
1:B:199:ARG:HG3	1:B:199:ARG:HH11	1.83	0.43
1:C:74:PRO:HG2	1:C:108:VAL:O	2.18	0.43
1:C:8:PRO:HG3	1:C:13:PHE:CD2	2.53	0.43
1:C:199:ARG:HH11	1:C:199:ARG:HG3	1.83	0.43
1:C:63:CYS:SG	1:C:94:CYS:HB3	2.59	0.43
1:A:243:TRP:CH2	1:A:247:LYS:HD3	2.54	0.43
1:B:230:HIS:N	1:B:230:HIS:CD2	2.85	0.43
1:B:21:ARG:NH2	1:B:24:TYR:CE2	2.86	0.43
1:B:114:CYS:O	1:B:115:ARG:C	2.57	0.43
1:B:361:ALA:O	1:B:362:SER:HB2	2.18	0.43
1:C:120:SER:O	1:C:178:VAL:HA	2.18	0.43
1:C:230:HIS:CD2	1:C:230:HIS:N	2.85	0.43
1:C:71:LYS:HD3	1:C:76:TYR:CZ	2.54	0.43
1:C:85:TYR:N	1:C:86:PRO:CD	2.81	0.43
1:A:170:TRP:CD1	1:A:170:TRP:C	2.92	0.43
1:A:230:HIS:N	1:A:230:HIS:CD2	2.85	0.43
1:A:235:GLN:HG2	1:A:236:THR:H	1.84	0.43
1:B:81:TYR:HB3	1:B:84:VAL:HB	2.01	0.43
1:A:88:MET:HG2	1:A:92:ALA:N	2.34	0.43
1:B:103:LEU:H	1:B:103:LEU:HD22	1.83	0.43
1:B:6:VAL:CG2	1:B:275:ASN:HB2	2.49	0.43
1:A:207:THR:HG23	1:A:210:SER:N	2.34	0.43
1:A:251:LEU:O	1:A:253:THR:N	2.52	0.43
1:A:84:VAL:HG22	1:A:85:TYR:N	2.34	0.42
1:B:267:ARG:NH1	1:C:335:ASN:HD22	2.17	0.42
1:B:259:CYS:SG	1:B:268:ALA:HB1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:HIS:HB3	1:B:309:SER:H	1.61	0.42
1:B:365:PHE:N	1:B:365:PHE:CD2	2.81	0.42
1:C:283:PRO:C	1:C:285:SER:N	2.72	0.42
3:E:4:MAN:H4	3:E:5:NAG:O6	2.19	0.42
1:B:207:THR:HG23	1:B:210:SER:N	2.34	0.42
1:C:243:TRP:CH2	1:C:247:LYS:HD3	2.54	0.42
1:A:139:ASN:C	1:A:139:ASN:ND2	2.72	0.42
1:A:57:SER:HA	1:A:58:PRO:HD3	1.83	0.42
1:B:69:SER:O	1:B:70:THR:HG23	2.20	0.42
1:C:141:ASN:CG	4:F:1:NAG:N2	2.73	0.42
1:C:197:PRO:O	1:C:199:ARG:HG2	2.19	0.42
1:A:369:LEU:O	1:A:370:CYS:HB2	2.18	0.42
1:B:59:TYR:O	1:B:103:LEU:CD2	2.68	0.42
1:B:115:ARG:HH12	1:B:209:GLU:HG3	1.83	0.42
1:B:74:PRO:HB2	1:B:108:VAL:O	2.20	0.42
1:A:6:VAL:CG2	1:A:275:ASN:HB2	2.49	0.42
1:A:88:MET:HG2	1:A:92:ALA:H	1.85	0.42
4:F:1:NAG:H62	4:F:2:NAG:HN2	1.82	0.42
1:B:255:ALA:HA	1:B:256:PRO:HD3	1.87	0.42
1:B:38:LEU:HD23	1:B:38:LEU:O	2.20	0.42
1:C:77:GLN:NE2	8:C:444:HOH:O	2.53	0.42
1:B:202:ASP:OD1	1:B:217:THR:HG22	2.20	0.42
1:B:210:SER:OG	1:B:211:ASN:N	2.52	0.42
1:B:99:GLU:N	1:B:99:GLU:OE1	2.52	0.42
1:A:115:ARG:HH12	1:A:209:GLU:HG3	1.85	0.42
1:B:360:SER:O	1:B:363:PRO:HD3	2.19	0.42
1:A:312:PHE:CD2	1:A:340:GLN:HB2	2.55	0.42
1:C:360:SER:O	1:C:363:PRO:HD3	2.19	0.42
1:A:320:TYR:HE1	1:A:346:VAL:HG13	1.82	0.41
1:A:312:PHE:CA	1:A:357:SER:HB2	2.50	0.41
1:C:210:SER:OG	1:C:211:ASN:N	2.53	0.41
1:C:320:TYR:HE1	1:C:346:VAL:HG13	1.81	0.41
1:A:316:LEU:HD13	1:A:367:VAL:HG21	2.01	0.41
1:B:251:LEU:O	1:B:253:THR:N	2.53	0.41
1:B:336:VAL:HG22	1:B:336:VAL:O	2.20	0.41
1:C:362:SER:N	1:C:363:PRO:CD	2.83	0.41
1:C:91:GLY:O	1:C:95:PHE:HD1	2.03	0.41
1:A:114:CYS:O	1:A:115:ARG:C	2.59	0.41
1:A:43:ASN:HD22	1:B:311:ASP:H	1.68	0.41
1:A:75:ASP:O	1:A:77:GLN:HG2	2.19	0.41
1:A:84:VAL:HG13	1:A:84:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:OE1	1:B:80:VAL:HG21	2.20	0.41
1:B:243:TRP:CH2	1:B:247:LYS:HD3	2.55	0.41
1:B:246:GLU:O	1:B:247:LYS:C	2.59	0.41
1:B:57:SER:HA	1:B:58:PRO:HD3	1.79	0.41
1:B:85:TYR:O	1:B:86:PRO:C	2.59	0.41
1:C:114:CYS:O	1:C:115:ARG:C	2.56	0.41
1:A:38:LEU:HD13	1:A:170:TRP:O	2.21	0.41
1:C:38:LEU:HD13	1:C:170:TRP:O	2.21	0.41
1:C:316:LEU:HD13	1:C:367:VAL:HG21	2.02	0.41
1:A:207:THR:HG23	1:A:210:SER:H	1.86	0.41
1:B:116:HIS:O	1:B:117:ASP:HB2	2.20	0.41
1:C:10:VAL:O	1:C:10:VAL:CG2	2.68	0.41
1:A:31:MET:CE	1:A:278:VAL:HG11	2.51	0.41
1:A:360:SER:O	1:A:363:PRO:HD3	2.21	0.41
1:B:207:THR:HG23	1:B:210:SER:H	1.86	0.41
1:B:3:HIS:O	1:B:279:SER:HA	2.21	0.41
1:C:115:ARG:HH12	1:C:209:GLU:HG3	1.85	0.41
2:D:3:BMA:H5	2:D:5:NAG:C7	2.51	0.41
1:A:61:LYS:HD3	1:A:62:CYS:O	2.21	0.41
1:B:108:VAL:CG1	1:B:109:ASP:N	2.84	0.41
1:C:108:VAL:CG1	1:C:109:ASP:N	2.84	0.41
1:B:161:PHE:HB3	1:B:163:PHE:CE1	2.56	0.41
1:B:38:LEU:HD13	1:B:170:TRP:O	2.21	0.41
1:C:6:VAL:CG2	1:C:275:ASN:HB2	2.50	0.41
1:A:59:TYR:O	1:A:103:LEU:CD2	2.69	0.41
1:C:101:THR:HG22	1:C:102:GLN:N	2.36	0.41
3:E:2:NAG:C5	3:E:7:FUC:H5	2.43	0.41
1:A:10:VAL:CG2	1:A:10:VAL:O	2.69	0.40
1:A:308:HIS:HB3	1:A:309:SER:H	1.62	0.40
1:B:312:PHE:CA	1:B:357:SER:HB2	2.50	0.40
1:B:362:SER:N	1:B:363:PRO:CD	2.84	0.40
1:A:362:SER:N	1:A:363:PRO:CD	2.84	0.40
1:C:170:TRP:C	1:C:170:TRP:CD1	2.93	0.40
1:A:284:ASP:CB	1:C:284:ASP:OD1	2.70	0.40
1:C:370:CYS:HB3	1:C:371:SER:H	1.61	0.40
1:A:192:TYR:CG	1:A:193:GLY:N	2.89	0.40
1:A:67:GLU:OE1	1:A:80:VAL:HG21	2.21	0.40
1:B:223:ARG:HA	1:B:224:PRO:HD3	1.94	0.40
1:B:36:THR:O	1:B:36:THR:HG22	2.20	0.40
1:B:84:VAL:CG1	1:B:223:ARG:HG3	2.49	0.40
1:C:243:TRP:CZ3	1:C:247:LYS:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:BMA:H5	2:D:5:NAG:N2	2.35	0.40
1:A:116:HIS:O	1:A:117:ASP:HB2	2.21	0.40
1:A:210:SER:OG	1:A:211:ASN:N	2.55	0.40
1:B:170:TRP:C	1:B:170:TRP:CD1	2.93	0.40
1:B:192:TYR:CG	1:B:193:GLY:N	2.88	0.40
1:B:197:PRO:O	1:B:199:ARG:HG2	2.20	0.40
1:B:84:VAL:O	1:B:85:TYR:C	2.59	0.40
1:C:55:VAL:HG21	1:C:231:VAL:CG2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:O	1:B:60:VAL:O[6_556]	2.06	0.14

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	389/391 (100%)	315 (81%)	50 (13%)	24 (6%)	1	11
1	B	389/391 (100%)	320 (82%)	46 (12%)	23 (6%)	1	12
1	C	389/391 (100%)	319 (82%)	50 (13%)	20 (5%)	2	15
All	All	1167/1173 (100%)	954 (82%)	146 (12%)	67 (6%)	1	14

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	96	CYS
1	A	97	ASP
1	A	192	TYR

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Mol	Chain	Res	Type
1	A	308	HIS
1	B	69	SER
1	B	89	TRP
1	B	192	TYR
1	B	308	HIS
1	C	87	PHE
1	C	192	TYR
1	C	308	HIS
1	A	65	ALA
1	A	69	SER
1	A	94	CYS
1	A	95	PHE
1	A	117	ASP
1	A	248	GLY
1	A	252	ASN
1	B	65	ALA
1	B	117	ASP
1	B	248	GLY
1	C	24	TYR
1	C	88	MET
1	C	89	TRP
1	C	117	ASP
1	C	248	GLY
1	A	24	TYR
1	B	24	TYR
1	B	101	THR
1	B	252	ASN
1	C	62	CYS
1	C	252	ASN
1	A	23	GLY
1	A	247	LYS
1	A	311	ASP
1	A	390	TYR
1	B	87	PHE
1	B	97	ASP
1	B	247	LYS
1	B	311	ASP
1	B	390	TYR
1	C	23	GLY
1	C	247	LYS
1	C	311	ASP
1	C	390	TYR

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Mol	Chain	Res	Type
1	A	99	GLU
1	A	164	GLY
1	A	270	ASN
1	A	304	ALA
1	B	23	GLY
1	B	270	ASN
1	B	304	ALA
1	C	304	ALA
1	A	22	PRO
1	A	266	VAL
1	B	22	PRO
1	B	91	GLY
1	B	164	GLY
1	B	266	VAL
1	C	85	TYR
1	C	266	VAL
1	B	191	PRO
1	C	22	PRO
1	C	164	GLY
1	A	191	PRO
1	C	191	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	336/336 (100%)	299 (89%)	37 (11%)	6 26
1	B	336/336 (100%)	294 (88%)	42 (12%)	4 21
1	C	336/336 (100%)	296 (88%)	40 (12%)	5 22
All	All	1008/1008 (100%)	889 (88%)	119 (12%)	5 23

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR

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Mol	Chain	Res	Type
1	A	28	THR
1	A	31	MET
1	A	36	THR
1	A	47	ILE
1	A	61	LYS
1	A	62	CYS
1	A	70	THR
1	A	75	ASP
1	A	88	MET
1	A	89	TRP
1	A	93	TYR
1	A	102	GLN
1	A	103	LEU
1	A	139	ASN
1	A	148	VAL
1	A	196	GLN
1	A	230	HIS
1	A	251	LEU
1	A	263	THR
1	A	267	ARG
1	A	271	CYS
1	A	280	MET
1	A	284	ASP
1	A	287	PHE
1	A	305	THR
1	A	308	HIS
1	A	322	THR
1	A	338	THR
1	A	365	PHE
1	A	370	CYS
1	A	377	SER
1	A	381	GLU
1	A	384	LYS
1	A	386	HIS
1	A	388	VAL
1	A	390	TYR
1	B	24	TYR
1	B	28	THR
1	B	31	MET
1	B	36	THR
1	B	47	ILE
1	B	61	LYS

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Mol	Chain	Res	Type
1	B	62	CYS
1	B	70	THR
1	B	75	ASP
1	B	85	TYR
1	B	87	PHE
1	B	88	MET
1	B	95	PHE
1	B	96	CYS
1	B	99	GLU
1	B	100	ASN
1	B	102	GLN
1	B	103	LEU
1	B	148	VAL
1	B	159	THR
1	B	196	GLN
1	B	230	HIS
1	B	251	LEU
1	B	263	THR
1	B	267	ARG
1	B	271	CYS
1	B	280	MET
1	B	284	ASP
1	B	287	PHE
1	B	305	THR
1	B	308	HIS
1	B	322	THR
1	B	338	THR
1	B	363	PRO
1	B	365	PHE
1	B	370	CYS
1	B	377	SER
1	B	381	GLU
1	B	384	LYS
1	B	386	HIS
1	B	388	VAL
1	B	390	TYR
1	C	24	TYR
1	C	28	THR
1	C	31	MET
1	C	36	THR
1	C	47	ILE
1	C	54	VAL

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Mol	Chain	Res	Type
1	C	62	CYS
1	C	70	THR
1	C	78	CYS
1	C	82	THR
1	C	85	TYR
1	C	93	TYR
1	C	95	PHE
1	C	96	CYS
1	C	148	VAL
1	C	155	THR
1	C	159	THR
1	C	196	GLN
1	C	230	HIS
1	C	251	LEU
1	C	263	THR
1	C	267	ARG
1	C	271	CYS
1	C	280	MET
1	C	284	ASP
1	C	287	PHE
1	C	305	THR
1	C	308	HIS
1	C	322	THR
1	C	338	THR
1	C	363	PRO
1	C	365	PHE
1	C	370	CYS
1	C	377	SER
1	C	381	GLU
1	C	384	LYS
1	C	385	ASP
1	C	386	HIS
1	C	388	VAL
1	C	390	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	43	ASN
1	A	102	GLN
1	A	125	HIS

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	152	HIS
1	A	187	GLN
1	A	196	GLN
1	A	211	ASN
1	A	216	ASN
1	A	230	HIS
1	A	235	GLN
1	A	281	ASN
1	A	308	HIS
1	A	340	GLN
1	A	386	HIS
1	B	30	GLN
1	B	43	ASN
1	B	100	ASN
1	B	102	GLN
1	B	142	GLN
1	B	187	GLN
1	B	196	GLN
1	B	211	ASN
1	B	216	ASN
1	B	230	HIS
1	B	235	GLN
1	B	281	ASN
1	B	308	HIS
1	B	340	GLN
1	B	386	HIS
1	C	30	GLN
1	C	43	ASN
1	C	77	GLN
1	C	100	ASN
1	C	125	HIS
1	C	142	GLN
1	C	187	GLN
1	C	196	GLN
1	C	211	ASN
1	C	216	ASN
1	C	230	HIS
1	C	281	ASN
1	C	308	HIS
1	C	340	GLN
1	C	386	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

15 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	D	1	1,2	14,14,15	0.68	0	17,19,21	1.19	1 (5%)
2	NAG	D	2	2	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
2	BMA	D	3	2	11,11,12	1.38	2 (18%)	15,15,17	0.69	1 (6%)
2	BMA	D	4	2	11,11,12	1.39	3 (27%)	15,15,17	1.16	2 (13%)
2	NAG	D	5	2	14,14,15	1.20	0	17,19,21	0.76	0
2	FUL	D	6	2	10,10,11	0.92	1 (10%)	14,14,16	0.66	0
3	NAG	E	1	1,3	14,14,15	0.94	0	17,19,21	1.28	2 (11%)
3	NAG	E	2	3	14,14,15	0.84	0	17,19,21	0.90	1 (5%)
3	BMA	E	3	3	11,11,12	1.38	1 (9%)	15,15,17	1.64	3 (20%)
3	MAN	E	4	3	11,11,12	1.66	2 (18%)	15,15,17	1.50	3 (20%)
3	NAG	E	5	3	14,14,15	1.52	3 (21%)	17,19,21	0.98	1 (5%)
3	MAN	E	6	3	11,11,12	1.40	2 (18%)	15,15,17	1.30	3 (20%)
3	FUC	E	7	3	10,10,11	1.37	2 (20%)	14,14,16	0.99	1 (7%)
4	NAG	F	1	1,4	14,14,15	1.19	2 (14%)	17,19,21	0.66	0
4	NAG	F	2	4	14,14,15	1.35	3 (21%)	17,19,21	0.99	1 (5%)

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	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	BMA	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	3/6/23/26	0/1/1/1
2	FUL	D	6	2	-	-	0/1/1/1
3	NAG	E	1	1,3	1/1/5/7	6/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	4/6/23/26	0/1/1/1
3	MAN	E	6	3	-	1/2/19/22	0/1/1/1
3	FUC	E	7	3	1/1/4/5	-	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	NAG	C1-C2	3.26	1.57	1.52
3	E	4	MAN	C2-C3	3.11	1.57	1.52
3	E	4	MAN	O2-C2	3.01	1.49	1.43
3	E	3	BMA	C2-C3	2.96	1.56	1.52
4	F	1	NAG	C1-C2	2.92	1.56	1.52
3	E	6	MAN	C2-C3	2.80	1.56	1.52
3	E	5	NAG	C3-C2	2.64	1.58	1.52
2	D	3	BMA	C2-C3	2.50	1.56	1.52
4	F	2	NAG	C4-C5	2.44	1.58	1.53
3	E	7	FUC	C4-C3	2.44	1.58	1.52
2	D	4	BMA	C2-C3	2.43	1.56	1.52
4	F	2	NAG	C3-C2	2.40	1.57	1.52
3	E	5	NAG	C8-C7	2.34	1.55	1.50
2	D	4	BMA	O2-C2	2.33	1.48	1.43
2	D	3	BMA	C4-C5	2.30	1.57	1.53
3	E	7	FUC	C2-C3	2.11	1.55	1.52
2	D	6	FUL	C2-C3	2.09	1.55	1.52
4	F	2	NAG	C4-C3	2.07	1.57	1.52
3	E	6	MAN	C1-C2	2.06	1.56	1.52
2	D	4	BMA	C1-C2	2.04	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	C8-C7	2.04	1.54	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C2-N2-C7	-3.98	117.23	122.90
3	E	3	BMA	C3-C4-C5	3.90	117.19	110.24
3	E	3	BMA	C2-C3-C4	3.68	117.26	110.89
3	E	4	MAN	O2-C2-C1	3.54	116.40	109.15
3	E	6	MAN	C1-C2-C3	3.07	113.44	109.67
3	E	1	NAG	C3-C4-C5	-3.01	104.87	110.24
3	E	4	MAN	C2-C3-C4	2.76	115.67	110.89
3	E	3	BMA	C1-C2-C3	2.63	112.90	109.67
3	E	6	MAN	C1-O5-C5	2.44	115.49	112.19
3	E	7	FUC	C1-C2-C3	2.44	112.66	109.67
3	E	2	NAG	C2-N2-C7	-2.36	119.54	122.90
2	D	4	BMA	C6-C5-C4	2.31	118.42	113.00
2	D	4	BMA	C3-C4-C5	-2.29	106.15	110.24
2	D	2	NAG	C3-C4-C5	2.27	114.28	110.24
4	F	2	NAG	C2-N2-C7	-2.24	119.72	122.90
3	E	6	MAN	C3-C4-C5	2.14	114.05	110.24
3	E	5	NAG	C4-C3-C2	2.11	114.11	111.02
3	E	1	NAG	O5-C5-C6	2.06	110.44	107.20
2	D	3	BMA	C6-C5-C4	2.04	117.78	113.00
3	E	4	MAN	O2-C2-C3	2.01	114.17	110.14

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1
3	E	7	FUC	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	5	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	5	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	E	5	NAG	O5-C5-C6-O6
2	D	4	BMA	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	4	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
2	D	4	BMA	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	NAG	2	0
2	D	1	NAG	2	0
4	F	1	NAG	5	0

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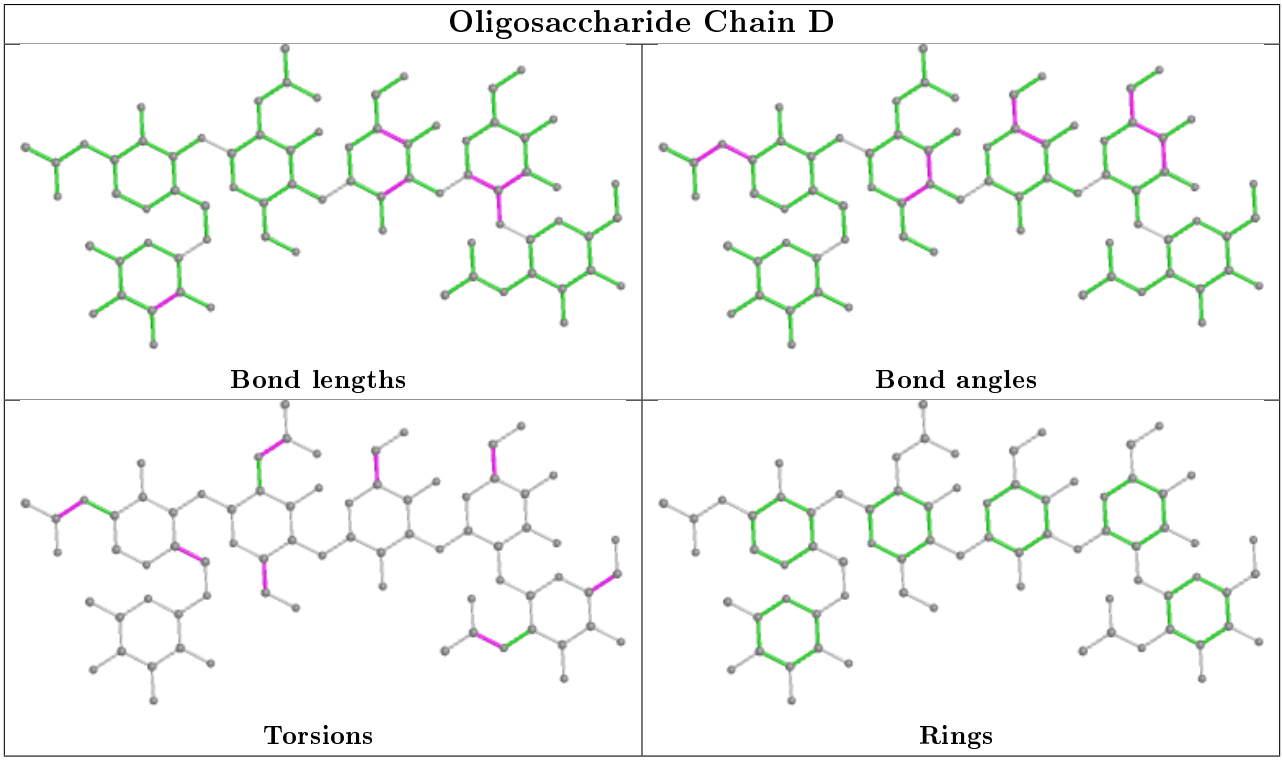
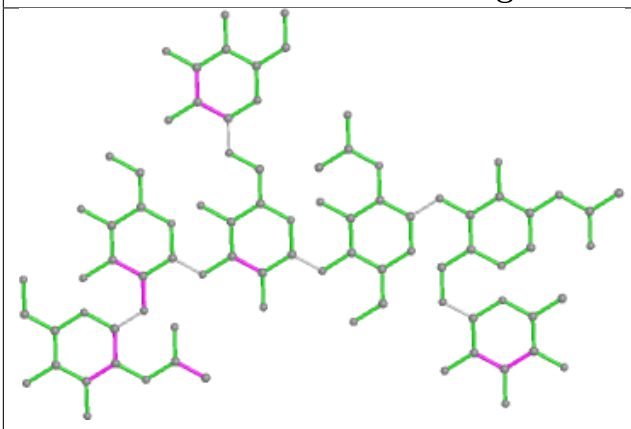
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	2	0
3	E	7	FUC	2	0
3	E	2	NAG	2	0
3	E	4	MAN	2	0
2	D	3	BMA	3	0
2	D	2	NAG	2	0
4	F	2	NAG	3	0
2	D	5	NAG	3	0

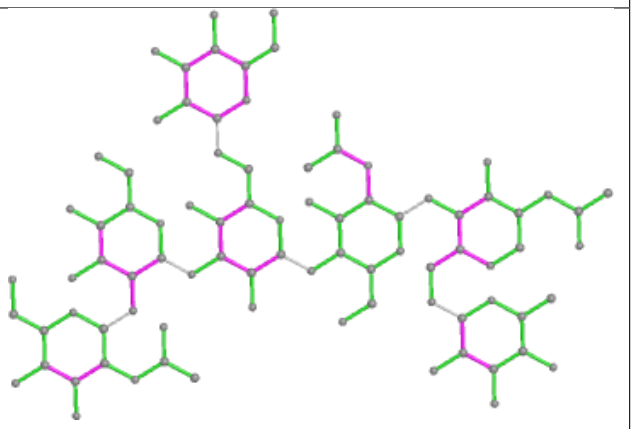
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



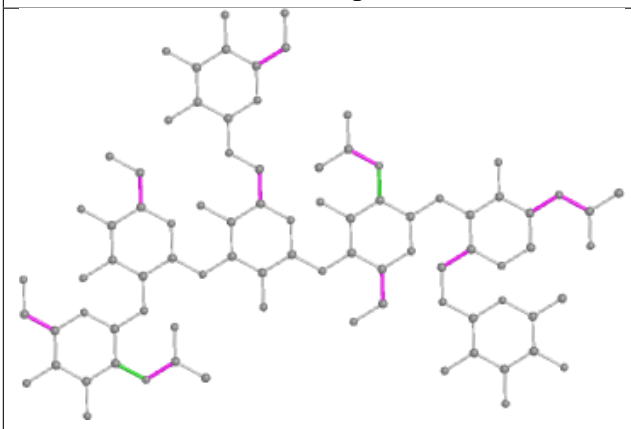
Oligosaccharide Chain E



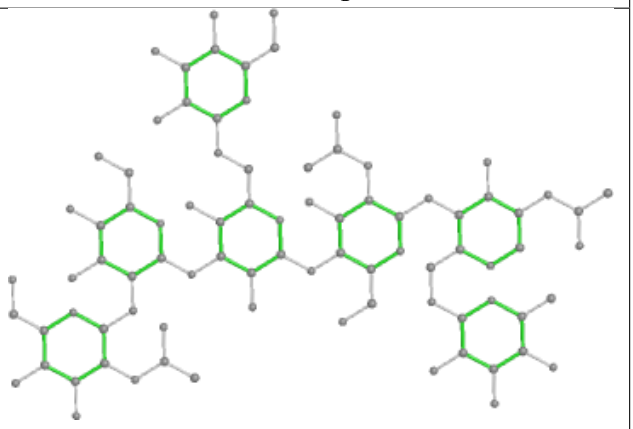
Bond lengths



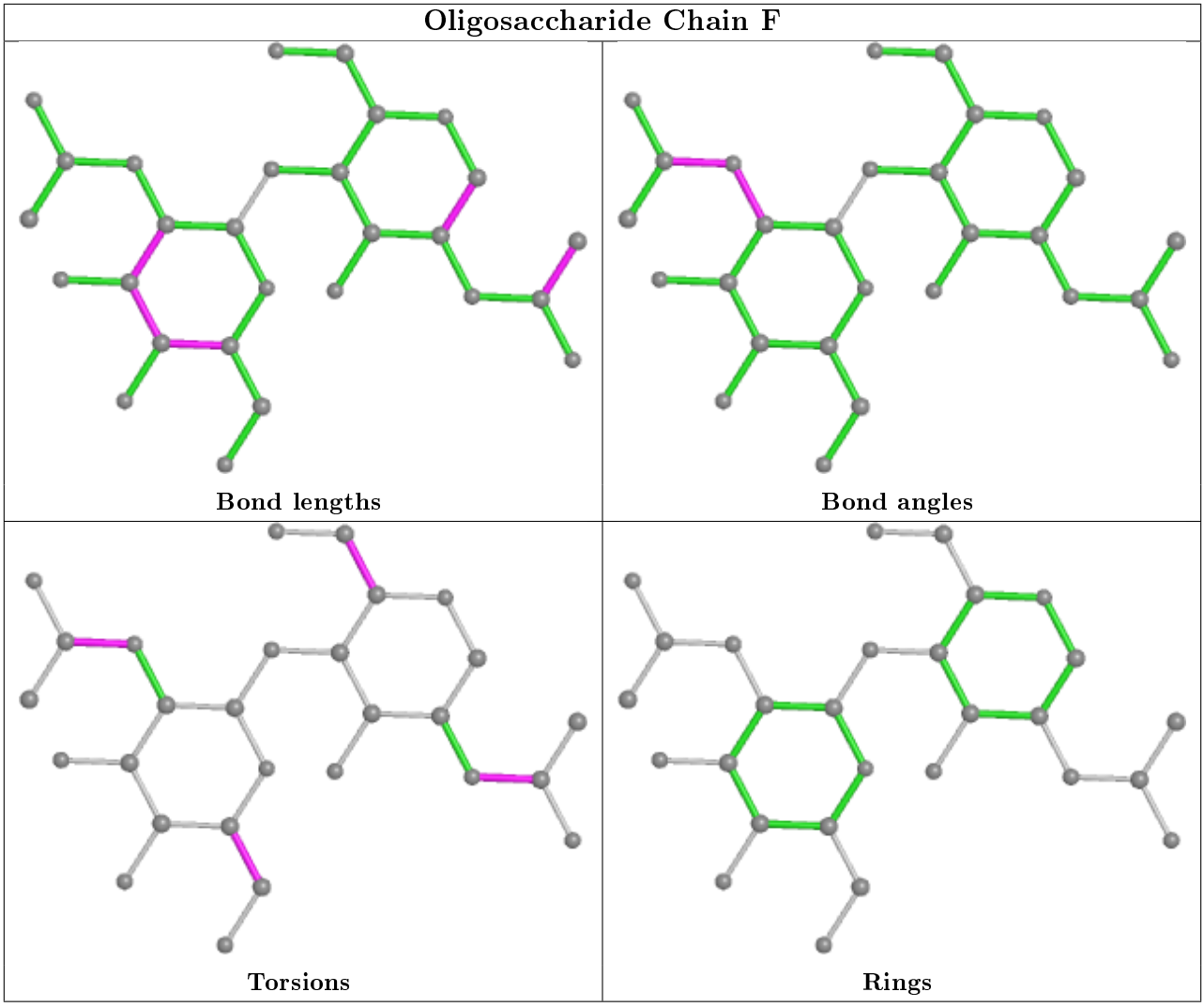
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
7	PO4	B	415	-	4,4,4	0.56	0	6,6,6	0.50	0

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	391/391 (100%)	0.21	8 (2%) 65 51	15, 63, 132, 186	0
1	B	391/391 (100%)	0.35	18 (4%) 32 20	19, 61, 133, 189	0
1	C	391/391 (100%)	0.26	7 (1%) 68 55	19, 64, 129, 171	0
All	All	1173/1173 (100%)	0.28	33 (2%) 53 37	15, 63, 132, 189	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	TYR	6.4
1	B	59	TYR	4.6
1	B	84	VAL	4.2
1	B	90	GLY	4.0
1	B	64	GLY	3.9
1	B	94	CYS	3.7
1	B	58	PRO	3.6
1	A	90	GLY	3.6
1	C	282	LEU	3.5
1	B	60	VAL	3.3
1	A	285	SER	3.2
1	B	85	TYR	3.2
1	B	101	THR	3.2
1	B	22	PRO	3.0
1	B	65	ALA	2.9
1	B	89	TRP	2.7
1	A	91	GLY	2.6
1	C	92	ALA	2.6
1	A	89	TRP	2.6
1	B	103	LEU	2.6
1	C	316	LEU	2.5
1	C	367	VAL	2.4
1	A	101	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	365	PHE	2.4
1	C	296	ILE	2.4
1	B	61	LYS	2.4
1	C	102	GLN	2.4
1	B	316	LEU	2.2
1	A	96	CYS	2.2
1	B	86	PRO	2.2
1	C	1	TYR	2.1
1	B	225	SER	2.1
1	A	316	LEU	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)

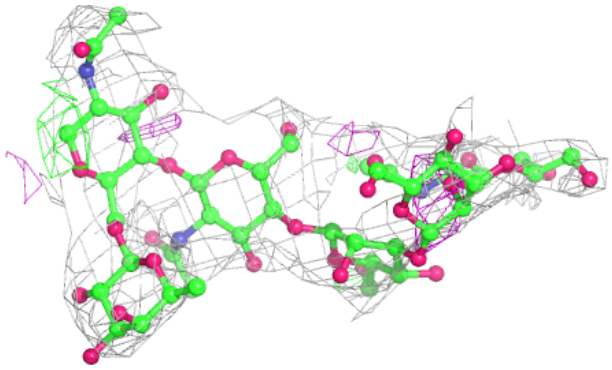
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

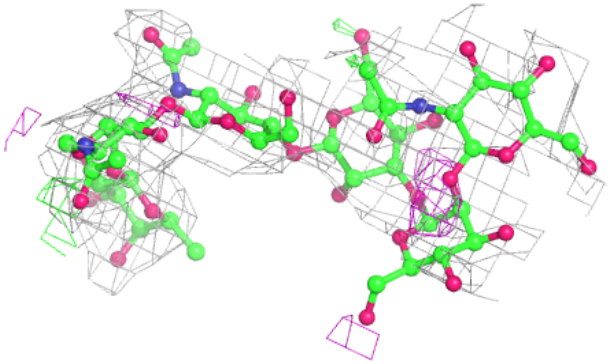
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.44	0.36	177,178,179,179	0
3	FUC	E	7	10/11	0.51	0.35	112,113,114,114	0
3	MAN	E	6	11/12	0.58	0.56	138,139,140,141	0
3	NAG	E	5	14/15	0.65	0.41	175,176,178,178	0
4	NAG	F	1	14/15	0.66	0.34	152,155,158,158	0
2	BMA	D	4	11/12	0.67	0.50	164,164,165,166	0
4	NAG	F	2	14/15	0.67	0.47	195,198,199,200	0
2	NAG	D	5	14/15	0.67	0.19	191,195,197,198	0
3	MAN	E	4	11/12	0.78	0.46	177,178,178,179	0
2	NAG	D	2	14/15	0.85	0.19	135,137,139,139	0
3	NAG	E	1	14/15	0.86	0.24	66,68,70,71	0
3	BMA	E	3	11/12	0.90	0.29	182,183,184,185	0
3	NAG	E	2	14/15	0.92	0.24	95,97,98,99	0
2	FUL	D	6	10/11	0.92	0.38	86,87,88,88	0
2	NAG	D	1	14/15	0.92	0.20	46,52,56,56	0

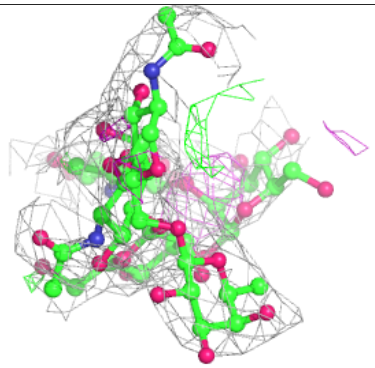
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

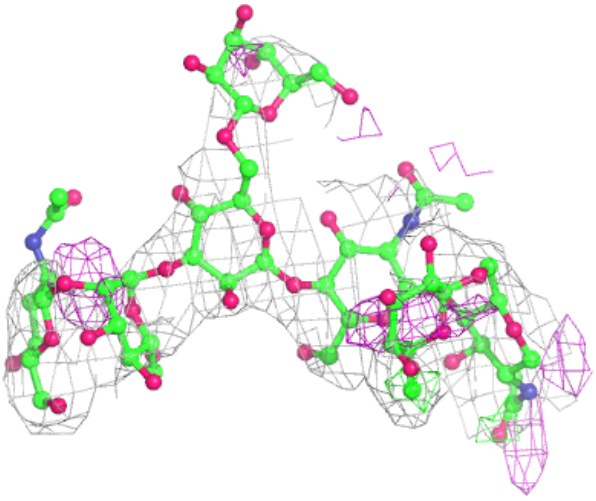


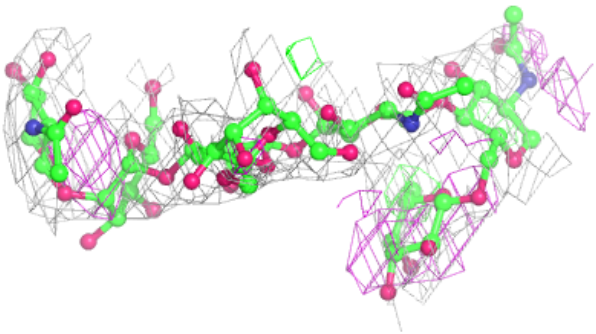


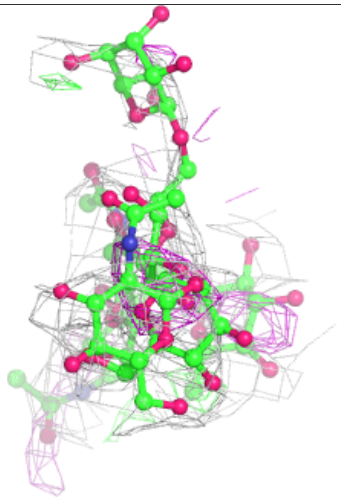


Electron density around Chain E:

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

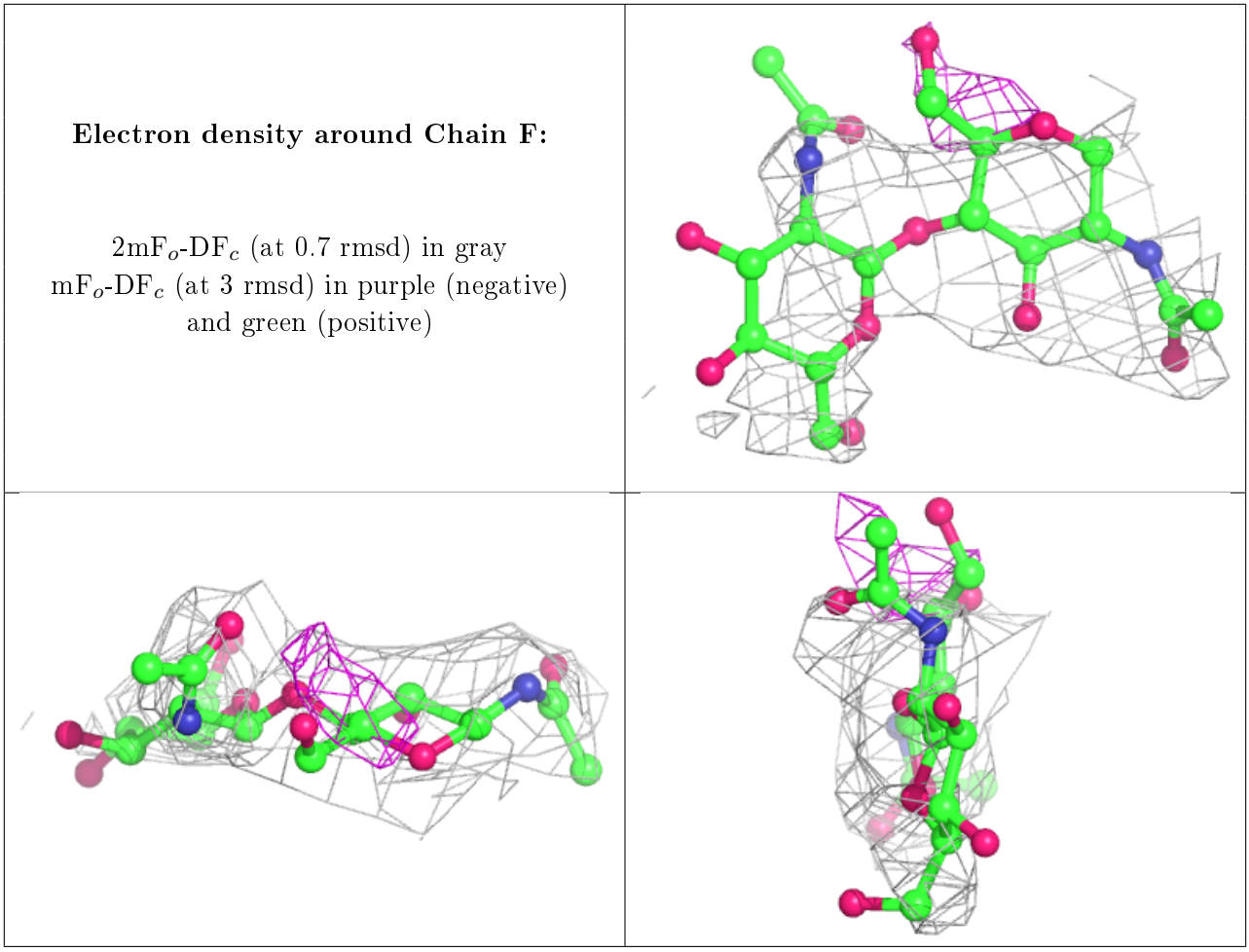






Electron density around Chain F:

$2mF_o$-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
7	PO4	B	415	5/5	0.85	0.22	78,79,81,82	0
5	BR	A	417	1/1	0.87	0.18	95,95,95,95	0
5	BR	B	418	1/1	0.93	0.11	77,77,77,77	0
6	HO	C	414	1/1	0.97	0.13	69,69,69,69	0
5	BR	C	416	1/1	0.98	0.15	83,83,83,83	0
6	HO	B	413	1/1	0.99	0.14	77,77,77,77	0
6	HO	A	412	1/1	0.99	0.15	67,67,67,67	0
6	HO	A	411	1/1	1.00	0.20	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.