Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 12:36 AM EST

PDB ID	:	3OBV
Title	:	Autoinhibited Formin mDia1 Structure
Authors	:	Tomchick, D.R.; Rosen, M.K.; Otomo, T.
Deposited on	:	2010-08-09
Resolution	:	2.75 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

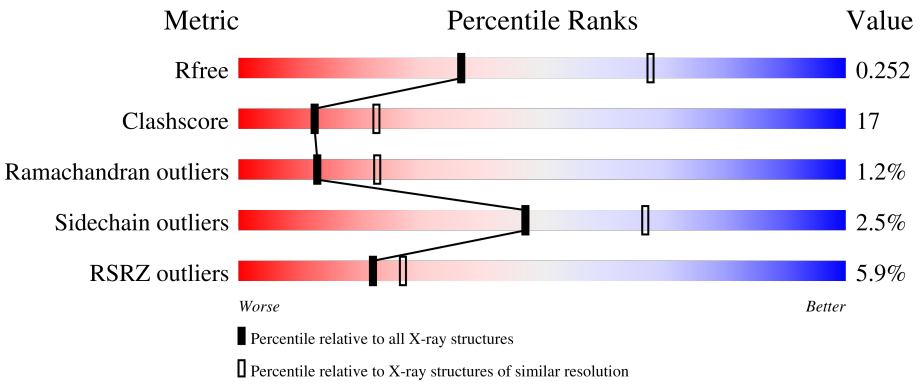
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	327	2%, 77%, 21%
1	B	327	5%, 70%, 26%
1	C	327	2%, 77%, 20%
1	D	327	%, 71%, 27%
2	E	457	7%, 63%, 27%, 8%

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Mol	Chain	Length	Quality of chain
2	F	457	16% 60% 30% • 8%
2	G	457	5% 63% 27% • 8%
2	H	457	4% 61% 28% • 8%
3	I	2	100%
3	J	2	50% 50%
3	K	2	100%
3	L	2	100%
3	M	2	50% 50%
3	N	2	100%
3	O	2	50% 50%
3	P	2	50% 50%

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
3	GLC	I	1	X	-	-	-
3	FRU	I	2	X	-	-	-
3	GLC	J	1	X	-	-	-
3	FRU	J	2	X	-	-	-
3	GLC	K	1	X	-	-	-
3	FRU	K	2	X	-	-	-
3	GLC	L	1	X	-	-	-
3	FRU	L	2	X	-	-	-
3	GLC	M	1	X	-	-	-
3	FRU	M	2	X	-	-	-
3	GLC	N	1	X	-	-	-
3	FRU	N	2	X	-	-	-
3	GLC	O	1	X	-	-	-
3	FRU	O	2	X	-	-	-
3	GLC	P	1	X	-	-	-
3	FRU	P	2	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24400 atoms, of which 176 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.

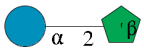
- Molecule 1 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2589	1625	445	497	22	0	0	0
1	B	319	2571	1617	443	489	22	0	0	0
1	C	322	2589	1625	445	497	22	0	0	0
1	D	327	2632	1651	453	506	22	0	0	0

- Molecule 2 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	419	3410	2154	579	656	21	0	0	0
2	F	419	3414	2155	582	656	21	0	0	0
2	G	420	3421	2160	583	657	21	0	0	0
2	H	419	3414	2156	582	655	21	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
3	I	2	45	12	22	11	0	0	0
3	J	2	45	12	22	11	0	0	0

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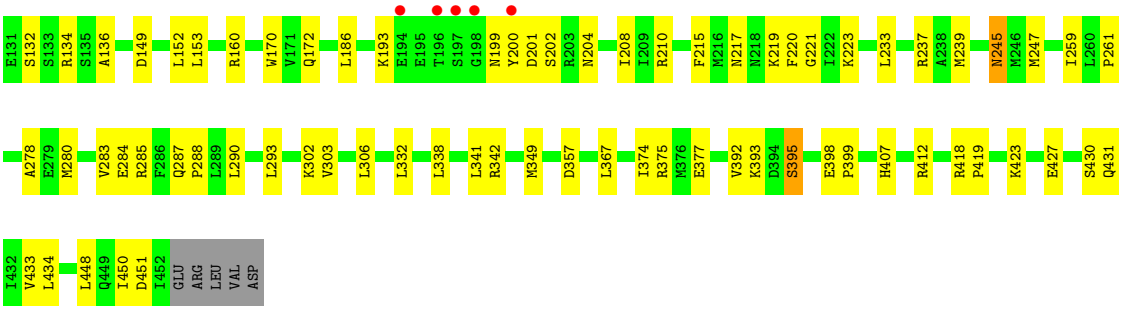
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
3	K	2	45	12	22	11	0	0	0
			Total	C	H	O			
3	L	2	45	12	22	11	0	0	0
			Total	C	H	O			
3	M	2	45	12	22	11	0	0	0
			Total	C	H	O			
3	N	2	45	12	22	11	0	0	0
			Total	C	H	O			
3	O	2	45	12	22	11	0	0	0
			Total	C	H	O			
3	P	2	45	12	22	11	0	0	0

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.

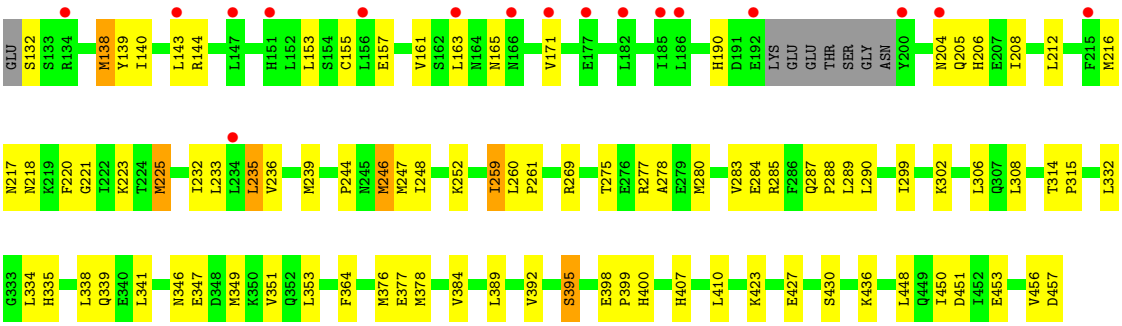
• Molecule 1: Protein diaphanous homolog 1

Chain A:



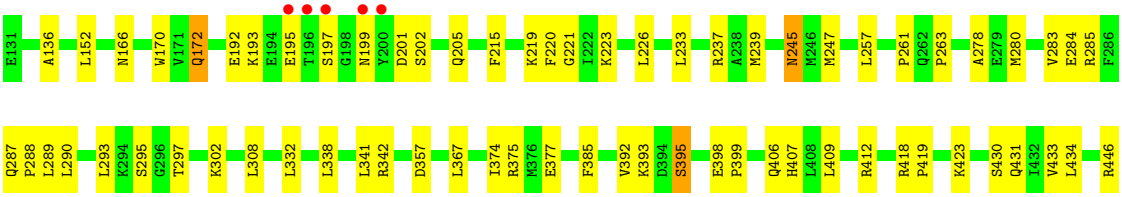
• Molecule 1: Protein diaphanous homolog 1

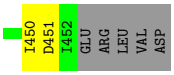
Chain B:



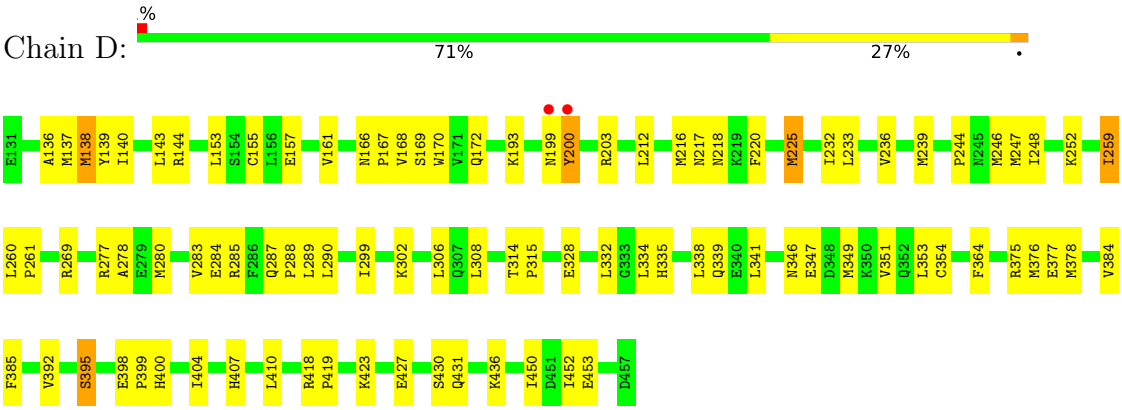
• Molecule 1: Protein diaphanous homolog 1

Chain C:

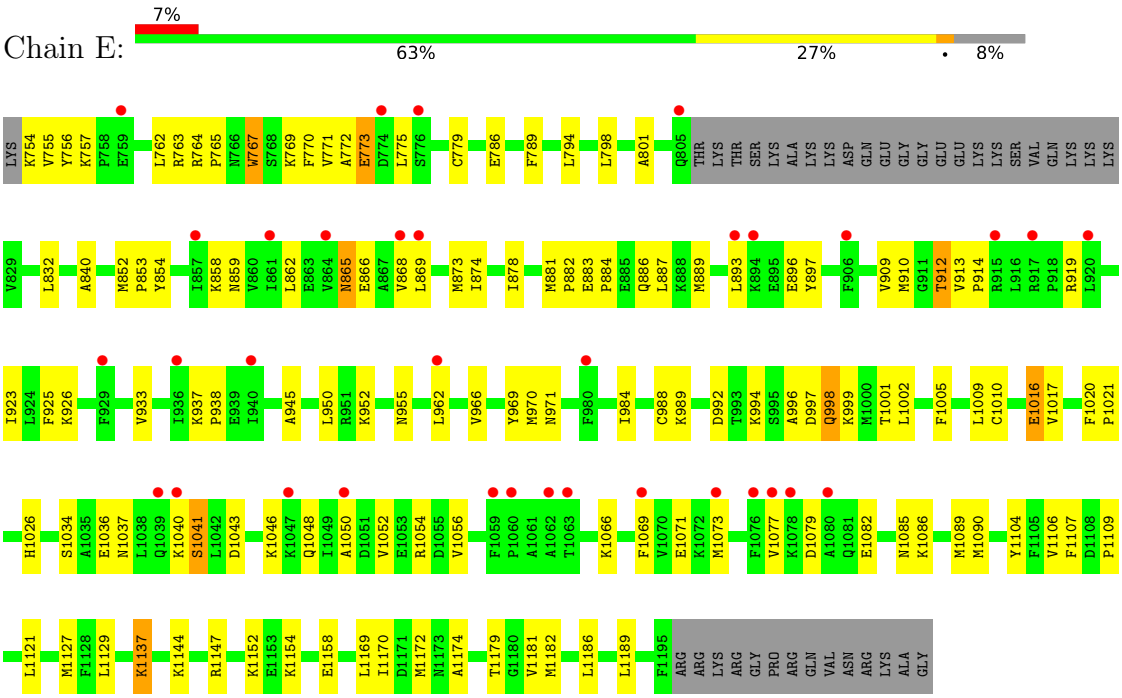




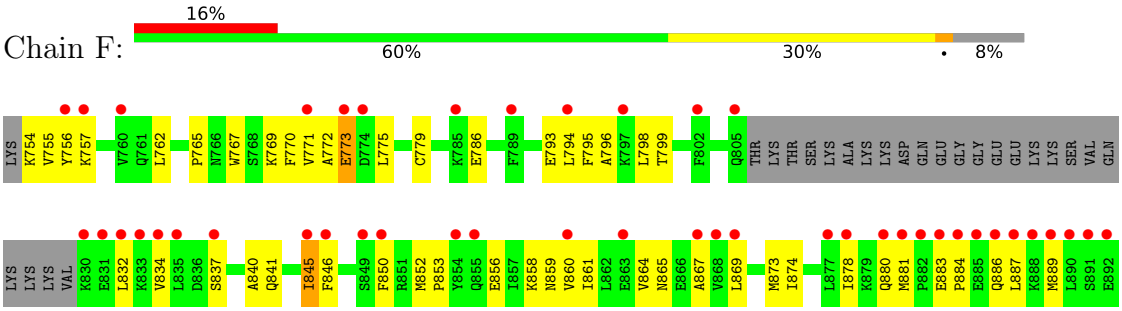
• Molecule 1: Protein diaphanous homolog 1

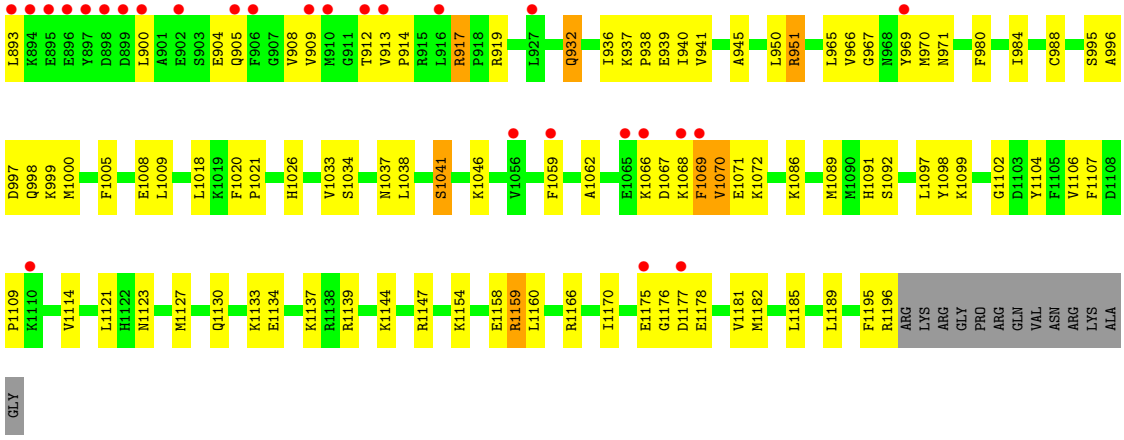


• Molecule 2: Protein diaphanous homolog 1



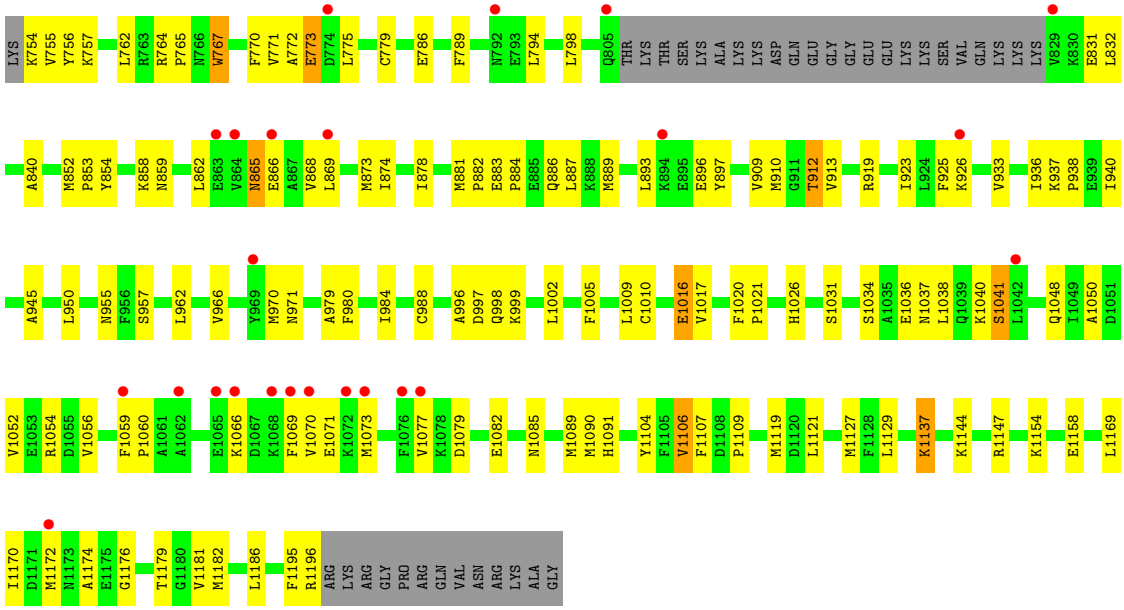
• Molecule 2: Protein diaphanous homolog 1





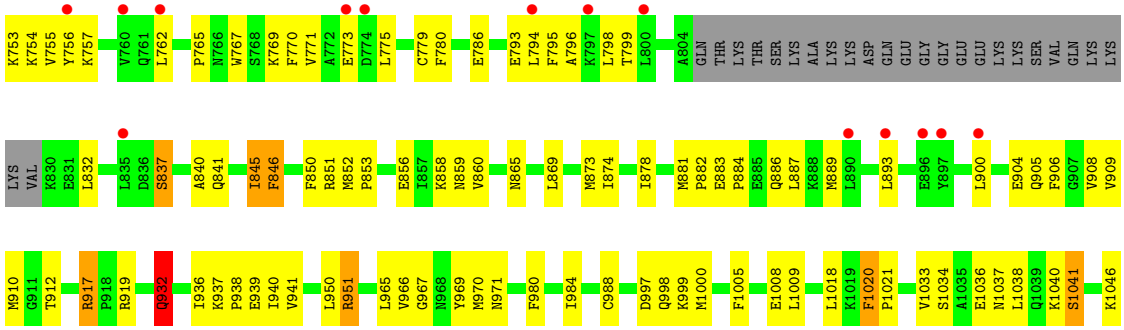
• Molecule 2: Protein diaphanous homolog 1

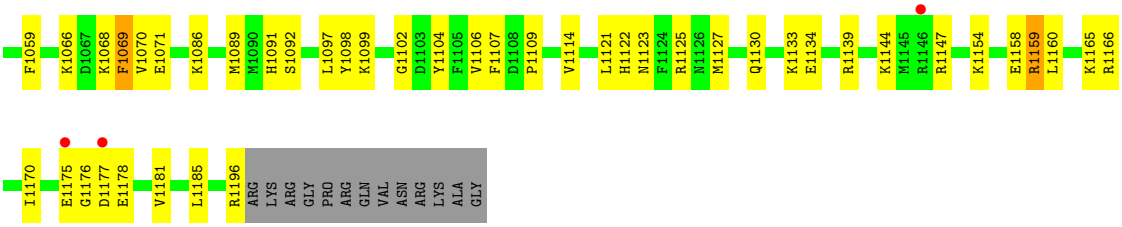
Chain G:



• Molecule 2: Protein diaphanous homolog 1

Chain H:





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain I:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain J:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain K:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

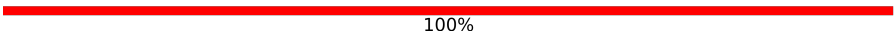
Chain L:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.93Å 208.52Å 131.52Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	29.95 – 2.75 48.54 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.95-2.75) 95.8 (48.54-2.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.199 , 0.261 0.189 , 0.252	Depositor DCC
R_{free} test set	1800 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å^2)	74.7	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FRU

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	0.50	0/2626	0.68	1/3536 (0.0%)
1	B	0.46	0/2607	0.62	0/3510
1	C	0.55	0/2626	0.73	0/3536
1	D	0.50	0/2669	0.65	0/3594
2	E	0.39	0/3462	0.55	0/4641
2	F	0.44	2/3466 (0.1%)	0.56	0/4645
2	G	0.39	0/3473	0.55	0/4655
2	H	0.45	2/3466 (0.1%)	0.58	0/4644
All	All	0.46	4/24395 (0.0%)	0.61	1/32761 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	932	GLN	CD-NE2	-7.82	1.13	1.32
2	F	932	GLN	CD-NE2	-7.53	1.14	1.32
2	F	932	GLN	CD-OE1	-6.13	1.10	1.24
2	H	932	GLN	CD-OE1	-6.08	1.10	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	448	LEU	CB-CG-CD1	-5.92	100.94	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	0	2594	73	0
1	B	2571	0	2584	93	0
1	C	2589	0	2594	75	0
1	D	2632	0	2637	92	0
2	E	3410	0	3416	134	0
2	F	3414	0	3420	163	0
2	G	3421	0	3429	133	0
2	H	3414	0	3425	153	0
3	I	23	22	16	0	0
3	J	23	22	14	3	0
3	K	23	22	15	0	0
3	L	23	22	15	0	0
3	M	23	22	15	2	0
3	N	23	22	15	5	0
3	O	23	22	16	1	0
3	P	23	22	16	4	0
All	All	24224	176	24221	814	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 17.

All (814) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:771:VAL:H	2:G:775:LEU:HD12	1.13	1.10
2:F:771:VAL:H	2:F:775:LEU:HD12	1.14	1.07
1:D:375:ARG:HH22	3:P:1:GLC:H61	1.12	1.07
2:H:771:VAL:H	2:H:775:LEU:HD12	1.12	1.06
2:E:771:VAL:H	2:E:775:LEU:HD12	1.19	1.05
1:C:375:ARG:HH22	3:N:1:GLC:H61	1.23	1.04
2:G:754:LYS:HG3	2:G:755:VAL:H	1.25	1.00
2:E:919:ARG:O	2:E:923:ILE:HG13	1.61	0.99
2:E:754:LYS:HG3	2:E:755:VAL:H	1.23	0.99
2:F:832:LEU:HD21	2:F:840:ALA:CB	1.94	0.98
2:E:1147:ARG:NH1	1:B:376:MET:HG3	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:771:VAL:H	2:H:775:LEU:CD1	1.77	0.97
2:F:771:VAL:H	2:F:775:LEU:CD1	1.78	0.96
2:G:919:ARG:O	2:G:923:ILE:HG13	1.65	0.94
2:H:881:MET:HE1	2:H:887:LEU:HD11	1.50	0.93
2:G:1147:ARG:NH1	1:D:376:MET:HG3	1.83	0.92
2:F:869:LEU:HD23	2:F:873:MET:CE	1.99	0.92
2:H:869:LEU:HD23	2:H:873:MET:CE	2.00	0.91
1:D:375:ARG:HH22	3:P:1:GLC:C6	1.84	0.90
1:A:290:LEU:HD13	1:A:332:LEU:HB3	1.54	0.90
2:F:881:MET:HE1	2:F:887:LEU:HD11	1.51	0.90
1:C:290:LEU:HD13	1:C:332:LEU:HB3	1.53	0.90
2:H:771:VAL:N	2:H:775:LEU:HD12	1.88	0.89
2:E:858:LYS:NZ	2:E:912:THR:HG21	1.89	0.87
2:F:771:VAL:N	2:F:775:LEU:HD12	1.88	0.87
2:G:1154:LYS:O	2:G:1158:GLU:HG2	1.75	0.86
2:H:883:GLU:HG3	2:H:884:PRO:HD2	1.56	0.86
2:F:883:GLU:HG3	2:F:884:PRO:HD2	1.55	0.86
2:E:881:MET:CE	2:E:887:LEU:HD11	2.07	0.85
1:C:418:ARG:HB3	1:C:419:PRO:HD3	1.56	0.85
1:C:430:SER:HA	1:D:407:HIS:CD2	2.12	0.85
2:F:1170:ILE:HD12	2:F:1181:VAL:HG13	1.58	0.84
1:C:431:GLN:HE22	1:C:451:ASP:H	1.25	0.84
2:E:754:LYS:HG3	2:E:755:VAL:N	1.90	0.84
1:A:418:ARG:HB3	1:A:419:PRO:HD3	1.58	0.84
2:F:859:ASN:ND2	2:F:1066:LYS:HD3	1.93	0.83
2:G:881:MET:CE	2:G:887:LEU:HD11	2.08	0.83
2:E:1154:LYS:O	2:E:1158:GLU:HG2	1.76	0.83
1:B:392:VAL:O	1:B:395:SER:HB3	1.78	0.83
2:G:858:LYS:NZ	2:G:912:THR:HG21	1.93	0.83
2:H:859:ASN:ND2	2:H:1066:LYS:HD3	1.93	0.82
1:C:377:GLU:OE1	2:H:1144:LYS:HE2	1.79	0.82
2:E:881:MET:HE3	2:E:882:PRO:HD2	1.62	0.82
1:B:290:LEU:CD1	1:B:332:LEU:HB3	2.09	0.82
2:G:754:LYS:HG3	2:G:755:VAL:N	1.94	0.81
1:D:375:ARG:NH2	3:P:1:GLC:H61	1.94	0.81
1:D:290:LEU:CD1	1:D:332:LEU:HB3	2.11	0.81
1:C:375:ARG:HH22	3:N:1:GLC:C6	1.95	0.80
1:A:398:GLU:HB3	1:A:399:PRO:HD3	1.61	0.80
2:H:1165:LYS:HD3	2:H:1196:ARG:HD2	1.63	0.80
2:H:1020:PHE:CD2	2:H:1021:PRO:HD3	2.17	0.80
2:H:853:PRO:HG2	2:H:856:GLU:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:MET:CE	1:B:225:MET:HG2	2.12	0.79
2:F:832:LEU:HD21	2:F:840:ALA:HB2	1.64	0.79
2:G:1169:LEU:HD13	1:D:259:ILE:CG2	2.12	0.79
2:G:909:VAL:O	2:G:912:THR:HB	1.84	0.78
1:C:398:GLU:HB3	1:C:399:PRO:HD3	1.64	0.78
1:C:430:SER:HA	1:D:407:HIS:HD2	1.48	0.78
2:G:1176:GLY:O	1:D:168:VAL:HG21	1.84	0.78
2:F:853:PRO:HG2	2:F:856:GLU:HG3	1.64	0.78
2:H:937:LYS:O	2:H:941:VAL:HG23	1.82	0.78
2:H:1170:ILE:HD12	2:H:1181:VAL:HG13	1.66	0.77
1:D:216:MET:CE	1:D:225:MET:HG2	2.14	0.77
2:F:937:LYS:O	2:F:941:VAL:HG23	1.84	0.77
1:D:244:PRO:O	1:D:248:ILE:HG13	1.85	0.77
1:A:377:GLU:OE1	2:F:1144:LYS:HE2	1.85	0.77
2:E:909:VAL:O	2:E:912:THR:HB	1.84	0.77
1:D:216:MET:HE1	1:D:225:MET:HG2	1.67	0.77
1:A:430:SER:HA	1:B:407:HIS:CD2	2.20	0.76
2:F:770:PHE:HA	2:F:775:LEU:HD13	1.68	0.76
2:H:967:GLY:HA2	2:H:970:MET:HE2	1.67	0.76
2:F:881:MET:CE	2:F:887:LEU:HD11	2.15	0.76
2:E:865:ASN:OD1	2:E:868:VAL:HG23	1.85	0.76
2:G:1037:ASN:O	2:G:1041:SER:HB3	1.86	0.76
2:H:770:PHE:HA	2:H:775:LEU:HD13	1.66	0.75
2:E:1037:ASN:O	2:E:1041:SER:HB3	1.87	0.75
2:G:771:VAL:N	2:G:775:LEU:HD12	1.98	0.75
2:F:883:GLU:HG3	2:F:884:PRO:CD	2.16	0.75
2:H:883:GLU:HG3	2:H:884:PRO:CD	2.16	0.75
2:E:1169:LEU:HD13	1:B:259:ILE:CG2	2.17	0.75
1:D:166:ASN:HB3	1:D:167:PRO:HD2	1.69	0.75
2:E:1182:MET:HB3	1:B:217:ASN:HA	1.67	0.74
2:G:883:GLU:H	2:G:886:GLN:HE21	1.35	0.74
2:G:865:ASN:OD1	2:G:868:VAL:HG23	1.86	0.74
1:A:431:GLN:HE22	1:A:451:ASP:H	1.33	0.74
2:E:1147:ARG:HH12	1:B:376:MET:HG3	1.51	0.73
2:F:1020:PHE:CD2	2:F:1021:PRO:HD3	2.22	0.73
1:C:375:ARG:NH2	3:N:1:GLC:H61	2.03	0.73
2:E:883:GLU:H	2:E:886:GLN:HE21	1.36	0.72
2:H:951:ARG:HG3	2:H:951:ARG:HH11	1.54	0.72
2:G:771:VAL:O	2:G:775:LEU:HB2	1.89	0.72
2:G:858:LYS:HE3	2:G:912:THR:CG2	2.18	0.72
2:H:832:LEU:HD21	2:H:840:ALA:CB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:881:MET:CE	2:H:887:LEU:HD11	2.19	0.72
2:G:1016:GLU:H	2:G:1016:GLU:CD	1.93	0.72
1:A:199:ASN:CG	1:A:201:ASP:HB2	2.10	0.71
2:F:951:ARG:HG3	2:F:951:ARG:HH11	1.54	0.71
1:D:392:VAL:O	1:D:395:SER:HB3	1.89	0.71
1:A:199:ASN:OD1	1:A:201:ASP:HB2	1.91	0.71
2:F:869:LEU:HD23	2:F:873:MET:HE1	1.72	0.71
2:H:845:ILE:HG22	2:H:846:PHE:N	2.07	0.70
2:G:881:MET:HE3	2:G:882:PRO:HD2	1.73	0.69
2:H:856:GLU:O	2:H:860:VAL:HG23	1.92	0.69
2:F:997:ASP:O	2:F:999:LYS:N	2.24	0.69
2:H:869:LEU:HD23	2:H:873:MET:HE1	1.74	0.69
1:B:216:MET:HE1	1:B:225:MET:HG2	1.75	0.69
1:B:212:LEU:O	1:B:216:MET:HG2	1.92	0.69
2:G:858:LYS:CE	2:G:912:THR:HG21	2.22	0.69
1:D:212:LEU:O	1:D:216:MET:HG2	1.92	0.69
2:E:858:LYS:HE3	2:E:912:THR:CG2	2.23	0.69
2:E:966:VAL:HG12	2:E:970:MET:CE	2.22	0.69
1:C:283:VAL:HG12	1:C:284:GLU:N	2.07	0.69
1:C:392:VAL:O	1:C:395:SER:HB3	1.93	0.69
2:H:859:ASN:HD21	2:H:1066:LYS:HD3	1.58	0.69
2:E:1016:GLU:CD	2:E:1016:GLU:H	1.97	0.68
2:E:771:VAL:O	2:E:775:LEU:HB2	1.92	0.68
2:F:859:ASN:HD21	2:F:1066:LYS:HD3	1.57	0.68
1:B:244:PRO:O	1:B:248:ILE:HG13	1.93	0.68
2:F:771:VAL:O	2:F:775:LEU:HB2	1.93	0.68
2:F:856:GLU:O	2:F:860:VAL:HG23	1.93	0.68
1:A:367:LEU:HD23	1:A:434:LEU:HD23	1.74	0.68
1:B:248:ILE:O	1:B:252:LYS:HG3	1.94	0.68
1:B:306:LEU:HD21	1:B:353:LEU:HD23	1.76	0.68
2:G:1147:ARG:HH12	1:D:376:MET:HG3	1.57	0.67
2:E:852:MET:HG2	2:E:853:PRO:HD2	1.76	0.67
1:A:367:LEU:CD2	1:A:434:LEU:HD23	2.25	0.67
2:H:988:CYS:SG	2:H:1127:MET:HE3	2.34	0.67
2:G:1050:ALA:O	2:G:1054:ARG:HG2	1.94	0.67
2:G:1182:MET:HB3	1:D:217:ASN:HA	1.77	0.67
1:A:430:SER:HA	1:B:407:HIS:HD2	1.59	0.67
1:D:302:LYS:HB3	1:D:349:MET:HE1	1.75	0.66
1:B:278:ALA:HB2	1:B:285:ARG:HA	1.77	0.66
2:G:859:ASN:ND2	2:G:1066:LYS:HD3	2.11	0.66
2:E:1050:ALA:O	2:E:1054:ARG:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:966:VAL:HG12	2:G:970:MET:CE	2.25	0.66
2:G:858:LYS:HE3	2:G:912:THR:HG21	1.77	0.66
2:G:1020:PHE:CD2	2:G:1021:PRO:HD3	2.30	0.66
2:G:764:ARG:HD2	2:H:971:ASN:OD1	1.96	0.66
2:G:771:VAL:H	2:G:775:LEU:CD1	2.00	0.66
2:H:771:VAL:O	2:H:775:LEU:HB2	1.96	0.66
2:E:859:ASN:ND2	2:E:1066:LYS:HD3	2.11	0.65
1:B:299:ILE:HG21	1:B:346:ASN:ND2	2.10	0.65
1:D:278:ALA:HB2	1:D:285:ARG:HA	1.78	0.65
2:H:853:PRO:CG	2:H:856:GLU:HG3	2.27	0.65
1:A:392:VAL:O	1:A:395:SER:HB3	1.97	0.65
2:F:869:LEU:HD22	2:F:874:ILE:HD11	1.78	0.65
1:B:163:LEU:HD23	1:B:171:VAL:HG22	1.78	0.65
2:F:853:PRO:CG	2:F:856:GLU:HG3	2.26	0.65
2:E:858:LYS:HZ2	2:E:912:THR:HG21	1.62	0.65
1:B:190:HIS:CD2	1:B:205:GLN:NE2	2.64	0.65
2:F:869:LEU:HA	2:F:873:MET:CE	2.27	0.65
2:E:858:LYS:CE	2:E:912:THR:HG21	2.26	0.64
2:E:832:LEU:HD21	2:E:840:ALA:CB	2.26	0.64
2:F:845:ILE:HG22	2:F:846:PHE:N	2.12	0.64
2:E:1020:PHE:CD2	2:E:1021:PRO:HD3	2.32	0.64
2:G:881:MET:HE2	2:G:887:LEU:HD11	1.78	0.64
2:H:997:ASP:O	2:H:999:LYS:N	2.23	0.64
1:D:299:ILE:HG21	1:D:346:ASN:ND2	2.11	0.64
2:H:1000:MET:HE3	2:H:1005:PHE:HB2	1.80	0.64
2:G:852:MET:HG2	2:G:853:PRO:HD2	1.78	0.64
1:D:302:LYS:HB3	1:D:349:MET:CE	2.28	0.63
1:B:302:LYS:HD3	1:B:341:LEU:CD2	2.27	0.63
1:B:456:VAL:HG12	1:B:457:ASP:N	2.12	0.63
1:D:169:SER:HA	1:D:172:GLN:HG3	1.78	0.63
2:H:869:LEU:HA	2:H:873:MET:CE	2.28	0.63
2:H:869:LEU:HD22	2:H:874:ILE:HD11	1.80	0.63
2:E:771:VAL:N	2:E:775:LEU:HD12	2.04	0.63
2:E:966:VAL:HG12	2:E:970:MET:HE2	1.80	0.63
2:E:771:VAL:H	2:E:775:LEU:CD1	2.06	0.63
2:G:762:LEU:HD11	2:H:969:TYR:HE2	1.64	0.63
2:G:770:PHE:HA	2:G:775:LEU:HD13	1.79	0.63
1:A:283:VAL:HG12	1:A:284:GLU:N	2.14	0.63
1:B:233:LEU:HD12	1:B:233:LEU:O	1.99	0.63
2:H:1037:ASN:O	2:H:1041:SER:HB2	1.99	0.63
2:F:988:CYS:SG	2:F:1127:MET:HE3	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1000:MET:HE3	2:F:1005:PHE:HB2	1.81	0.62
1:A:431:GLN:HE22	1:A:451:ASP:N	1.98	0.62
1:C:290:LEU:CD1	1:C:332:LEU:HB3	2.28	0.62
1:B:378:MET:HB3	1:B:384:VAL:HG22	1.81	0.62
2:H:869:LEU:HA	2:H:873:MET:HE1	1.80	0.62
1:D:248:ILE:O	1:D:252:LYS:HG3	1.99	0.62
1:C:199:ASN:ND2	1:C:201:ASP:HB2	2.14	0.62
2:G:858:LYS:HZ1	2:G:912:THR:HG21	1.64	0.62
1:A:375:ARG:HH22	3:J:1:GLC:H61	1.65	0.62
1:A:287:GLN:HB3	1:A:288:PRO:HD3	1.81	0.62
1:D:378:MET:HB3	1:D:384:VAL:HG22	1.81	0.61
1:B:335:HIS:HE1	1:B:339:GLN:HE21	1.48	0.61
2:G:881:MET:CE	2:G:882:PRO:HD2	2.31	0.61
1:D:335:HIS:CE1	1:D:339:GLN:HE21	2.18	0.61
1:C:367:LEU:HD23	1:C:434:LEU:HD23	1.83	0.61
2:F:967:GLY:HA2	2:F:970:MET:HE2	1.82	0.61
1:A:427:GLU:HG3	3:J:1:GLC:O3	2.01	0.61
1:B:335:HIS:CE1	1:B:339:GLN:HE21	2.18	0.61
1:D:200:TYR:CD2	1:D:203:ARG:NH2	2.69	0.61
2:E:881:MET:HE1	2:E:887:LEU:HD11	1.81	0.60
1:D:306:LEU:HD21	1:D:353:LEU:HD23	1.81	0.60
1:D:398:GLU:HB3	1:D:399:PRO:HD3	1.81	0.60
1:D:335:HIS:HE1	1:D:339:GLN:HE21	1.48	0.60
1:A:290:LEU:CD1	1:A:332:LEU:HB3	2.30	0.60
2:E:881:MET:HE2	2:E:887:LEU:HD11	1.80	0.60
1:D:364:PHE:CD1	1:D:436:LYS:HA	2.36	0.60
2:E:1147:ARG:NH1	1:B:376:MET:CG	2.59	0.60
2:G:1169:LEU:HD13	1:D:259:ILE:HG23	1.82	0.60
2:E:874:ILE:O	2:E:878:ILE:HG13	2.02	0.60
2:F:1170:ILE:HG13	2:F:1185:LEU:HD21	1.84	0.60
2:F:904:GLU:O	2:F:908:VAL:HG23	2.02	0.60
2:H:1170:ILE:HG13	2:H:1185:LEU:HD21	1.83	0.60
2:H:1033:VAL:CG1	2:H:1034:SER:N	2.65	0.59
2:F:917:ARG:HH11	2:F:917:ARG:HB2	1.67	0.59
1:B:302:LYS:HD3	1:B:341:LEU:HD22	1.83	0.59
2:G:762:LEU:HD11	2:H:969:TYR:CE2	2.36	0.59
2:G:912:THR:HG22	2:G:913:VAL:N	2.17	0.59
1:A:374:ILE:HD12	1:B:410:LEU:HD13	1.84	0.59
1:B:216:MET:HE1	1:B:225:MET:CE	2.33	0.59
2:H:883:GLU:H	2:H:886:GLN:NE2	2.01	0.59
1:D:153:LEU:O	1:D:157:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1123:ASN:O	2:H:1127:MET:HG3	2.02	0.59
2:E:754:LYS:CG	2:E:755:VAL:N	2.65	0.59
2:E:883:GLU:HG3	2:E:884:PRO:HD2	1.84	0.59
1:C:431:GLN:NE2	1:C:451:ASP:H	1.97	0.59
2:E:858:LYS:HE3	2:E:912:THR:HG21	1.85	0.58
1:B:364:PHE:CD1	1:B:436:LYS:HA	2.38	0.58
1:D:302:LYS:HD3	1:D:341:LEU:HD22	1.84	0.58
1:B:216:MET:HE2	1:B:225:MET:HG2	1.83	0.58
1:A:219:LYS:HE3	2:F:1178:GLU:OE1	2.03	0.58
2:G:874:ILE:O	2:G:878:ILE:HG13	2.04	0.58
2:E:881:MET:CE	2:E:882:PRO:HD2	2.32	0.58
2:F:883:GLU:H	2:F:886:GLN:NE2	2.01	0.58
2:F:1008:GLU:HG3	2:F:1139:ARG:NH1	2.18	0.58
1:D:302:LYS:HD3	1:D:341:LEU:CD2	2.32	0.58
2:H:832:LEU:HD21	2:H:840:ALA:HB2	1.85	0.58
1:B:302:LYS:HB3	1:B:349:MET:CE	2.34	0.58
2:F:1037:ASN:O	2:F:1041:SER:HB2	2.04	0.58
2:F:1033:VAL:CG1	2:F:1034:SER:N	2.67	0.58
1:A:239:MET:HA	1:A:247:MET:HG3	1.86	0.57
1:C:367:LEU:CD2	1:C:434:LEU:HD23	2.34	0.57
2:E:988:CYS:SG	2:E:1127:MET:HE3	2.44	0.57
1:B:290:LEU:CD1	1:B:332:LEU:CB	2.82	0.57
1:B:314:THR:HB	1:B:315:PRO:HD3	1.86	0.57
2:E:1144:LYS:HE2	1:B:377:GLU:OE1	2.05	0.57
2:G:779:CYS:HB2	2:H:1104:TYR:O	2.05	0.57
2:G:866:GLU:OE2	2:G:926:LYS:HE3	2.05	0.57
1:D:314:THR:HB	1:D:315:PRO:HD3	1.87	0.57
2:H:917:ARG:HH11	2:H:917:ARG:HB2	1.68	0.57
1:A:393:LYS:HA	1:A:398:GLU:OE1	2.04	0.57
2:E:779:CYS:HB2	2:F:1104:TYR:O	2.04	0.57
2:E:854:TYR:O	2:E:909:VAL:HG11	2.04	0.57
1:D:172:GLN:HA	1:D:220:PHE:CE2	2.39	0.57
1:B:190:HIS:CD2	1:B:205:GLN:HE21	2.22	0.57
1:B:153:LEU:O	1:B:157:GLU:HG3	2.04	0.57
2:G:1147:ARG:NH1	1:D:376:MET:CG	2.65	0.57
2:G:1147:ARG:HH11	1:D:376:MET:HG3	1.65	0.57
2:H:1154:LYS:O	2:H:1158:GLU:HG2	2.04	0.57
1:D:450:ILE:HG22	1:D:452:ILE:HG23	1.87	0.57
2:H:937:LYS:N	2:H:938:PRO:CD	2.67	0.57
2:G:980:PHE:HZ	2:H:753:LYS:HB3	1.70	0.57
1:D:290:LEU:CD1	1:D:332:LEU:CB	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:789:PHE:HB2	2:F:965:LEU:HD22	1.87	0.56
2:G:754:LYS:CG	2:G:755:VAL:N	2.67	0.56
2:H:1008:GLU:HG3	2:H:1139:ARG:NH1	2.19	0.56
2:E:1169:LEU:HD13	1:B:259:ILE:HG23	1.85	0.56
1:B:239:MET:HA	1:B:247:MET:HG3	1.86	0.56
2:H:1020:PHE:CG	2:H:1021:PRO:HD3	2.39	0.56
1:A:431:GLN:NE2	1:A:451:ASP:H	2.01	0.56
2:G:858:LYS:HE3	2:G:912:THR:HG22	1.87	0.56
2:E:997:ASP:O	2:E:999:LYS:N	2.34	0.56
1:D:233:LEU:HD12	1:D:233:LEU:O	2.05	0.56
2:H:1159:ARG:CG	2:H:1160:LEU:N	2.68	0.56
1:C:287:GLN:HB3	1:C:288:PRO:HD3	1.86	0.56
2:E:770:PHE:HA	2:E:775:LEU:HD13	1.87	0.56
2:E:1170:ILE:HD11	2:E:1181:VAL:HG13	1.87	0.56
2:F:1123:ASN:O	2:F:1127:MET:HG3	2.06	0.56
1:B:140:ILE:O	1:B:144:ARG:HG3	2.06	0.56
2:F:1159:ARG:CG	2:F:1160:LEU:N	2.68	0.56
2:G:971:ASN:ND2	2:H:765:PRO:HD2	2.21	0.56
1:A:199:ASN:ND2	1:A:201:ASP:HB2	2.21	0.56
1:A:261:PRO:HG3	2:F:1166:ARG:O	2.05	0.56
2:E:866:GLU:OE2	2:E:926:LYS:HE3	2.05	0.56
1:A:136:ALA:HB2	1:A:170:TRP:CE2	2.41	0.55
2:F:852:MET:CE	2:F:856:GLU:HB3	2.36	0.55
2:G:966:VAL:HG12	2:G:970:MET:HE2	1.87	0.55
1:B:453:GLU:OE1	1:C:295:SER:O	2.24	0.55
2:H:1107:PHE:O	2:H:1109:PRO:HD3	2.06	0.55
2:E:858:LYS:HE3	2:E:912:THR:HG22	1.88	0.55
2:E:1085:ASN:O	2:E:1089:MET:HG2	2.06	0.55
2:G:883:GLU:HG3	2:G:884:PRO:HD2	1.88	0.55
2:G:1085:ASN:O	2:G:1089:MET:HG2	2.05	0.55
2:H:883:GLU:HB2	2:H:886:GLN:HE21	1.71	0.55
2:F:988:CYS:HB3	2:F:1127:MET:HE1	1.88	0.55
1:C:374:ILE:HD12	1:D:410:LEU:HD13	1.88	0.55
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.71	0.55
1:B:457:ASP:HB3	1:C:245:ASN:HD21	1.72	0.55
1:C:136:ALA:HB2	1:C:170:TRP:CE2	2.41	0.55
1:C:239:MET:HA	1:C:247:MET:HG3	1.89	0.55
2:H:858:LYS:HE3	2:H:912:THR:HB	1.89	0.55
2:H:950:LEU:HD13	2:H:1121:LEU:HD21	1.89	0.55
2:F:756:TYR:O	2:F:757:LYS:HG3	2.06	0.55
2:F:771:VAL:N	2:F:775:LEU:CD1	2.57	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:869:LEU:HA	2:F:873:MET:HE2	1.89	0.55
2:E:852:MET:HG2	2:E:853:PRO:CD	2.36	0.55
2:E:970:MET:HE1	2:E:1002:LEU:CD1	2.36	0.55
2:F:869:LEU:HA	2:F:873:MET:HE1	1.89	0.55
2:F:1154:LYS:O	2:F:1158:GLU:HG2	2.07	0.55
2:G:1170:ILE:HD11	2:G:1181:VAL:HG13	1.89	0.55
2:H:852:MET:CE	2:H:856:GLU:HB3	2.36	0.55
1:B:334:LEU:HD11	1:B:338:LEU:HD21	1.88	0.55
2:H:859:ASN:HD21	2:H:1066:LYS:CE	2.20	0.55
1:B:398:GLU:HB3	1:B:399:PRO:HD3	1.89	0.55
2:F:883:GLU:HB2	2:F:886:GLN:HE21	1.72	0.55
2:H:756:TYR:O	2:H:757:LYS:HG3	2.07	0.55
2:F:859:ASN:HD21	2:F:1066:LYS:CE	2.21	0.54
2:G:988:CYS:SG	2:G:1127:MET:HE3	2.47	0.54
2:G:854:TYR:O	2:G:909:VAL:HG11	2.06	0.54
1:C:237:ARG:CZ	1:C:280:MET:HE1	2.38	0.54
2:G:859:ASN:HD22	2:G:1066:LYS:HD3	1.72	0.54
2:E:1147:ARG:HH11	1:B:376:MET:CG	2.17	0.54
1:D:140:ILE:O	1:D:144:ARG:HG3	2.07	0.54
2:H:859:ASN:HD21	2:H:1066:LYS:CD	2.20	0.54
2:F:988:CYS:HA	2:F:1127:MET:HE3	1.90	0.54
2:G:1005:PHE:CE1	2:H:798:LEU:HD13	2.43	0.54
2:H:966:VAL:O	2:H:970:MET:HG3	2.08	0.54
2:E:1052:VAL:HG12	2:E:1077:VAL:CG2	2.38	0.53
2:G:980:PHE:CZ	2:H:753:LYS:HB3	2.43	0.53
2:F:859:ASN:HD21	2:F:1066:LYS:CD	2.20	0.53
2:G:852:MET:HG2	2:G:853:PRO:CD	2.38	0.53
2:E:962:LEU:HD11	2:E:1009:LEU:HD13	1.91	0.53
2:G:881:MET:HE1	2:G:887:LEU:HD11	1.87	0.53
2:G:955:ASN:OD1	2:G:1016:GLU:HB2	2.09	0.53
2:G:1104:TYR:O	2:H:779:CYS:HB2	2.08	0.53
2:E:859:ASN:HD22	2:E:1066:LYS:HD3	1.74	0.53
2:E:910:MET:C	2:E:912:THR:H	2.12	0.53
2:F:937:LYS:N	2:F:938:PRO:CD	2.71	0.53
2:H:858:LYS:HE3	2:H:912:THR:CB	2.39	0.53
2:E:994:LYS:HB2	2:E:998:GLN:OE1	2.09	0.53
2:F:860:VAL:HG13	2:F:865:ASN:HB3	1.91	0.53
2:F:966:VAL:O	2:F:970:MET:HG3	2.09	0.53
1:D:423:LYS:O	1:D:427:GLU:HG3	2.08	0.53
2:H:860:VAL:HG13	2:H:865:ASN:HB3	1.91	0.53
2:H:869:LEU:HD23	2:H:873:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:MET:CE	1:B:138:MET:HA	2.39	0.53
1:C:283:VAL:CG1	1:C:284:GLU:N	2.72	0.53
2:G:754:LYS:HB2	2:G:786:GLU:OE2	2.09	0.53
2:G:925:PHE:CE1	2:G:1048:GLN:HB3	2.43	0.53
2:G:937:LYS:HE3	2:G:1090:MET:CE	2.39	0.53
1:B:161:VAL:O	1:B:165:ASN:HB2	2.09	0.52
2:H:937:LYS:N	2:H:938:PRO:HD2	2.24	0.52
2:F:793:GLU:O	2:F:796:ALA:HB3	2.10	0.52
2:H:793:GLU:O	2:H:796:ALA:HB3	2.08	0.52
2:E:925:PHE:CE1	2:E:1048:GLN:HB3	2.44	0.52
1:C:431:GLN:HE22	1:C:451:ASP:N	2.01	0.52
2:G:1147:ARG:HH11	1:D:376:MET:CG	2.20	0.52
1:D:216:MET:HE1	1:D:225:MET:CE	2.40	0.52
2:H:905:GLN:O	2:H:909:VAL:HG23	2.10	0.52
2:F:905:GLN:O	2:F:909:VAL:HG23	2.09	0.52
1:C:245:ASN:N	1:C:245:ASN:HD22	2.07	0.52
2:E:762:LEU:HD11	2:F:969:TYR:HE2	1.75	0.52
2:F:1008:GLU:HG3	2:F:1139:ARG:HH12	1.73	0.52
1:C:166:ASN:ND2	1:C:170:TRP:CE2	2.78	0.52
2:G:1021:PRO:HG2	2:G:1129:LEU:HD21	1.91	0.52
2:H:997:ASP:C	2:H:999:LYS:H	2.11	0.52
2:E:966:VAL:HG12	2:E:970:MET:HE1	1.91	0.52
2:G:937:LYS:HB3	2:G:938:PRO:HD3	1.92	0.52
2:G:970:MET:HE3	2:H:765:PRO:HG3	1.92	0.52
2:G:979:ALA:HA	2:H:769:LYS:HD2	1.90	0.52
2:H:1008:GLU:HG3	2:H:1139:ARG:HH12	1.73	0.52
2:F:1175:GLU:HB3	2:F:1178:GLU:HG3	1.92	0.52
2:E:754:LYS:HB2	2:E:786:GLU:OE2	2.10	0.52
2:E:937:LYS:HE3	2:E:1090:MET:CE	2.40	0.52
1:B:289:LEU:HD21	1:B:308:LEU:HD23	1.92	0.52
2:G:798:LEU:HD21	2:H:966:VAL:HG13	1.91	0.52
2:G:962:LEU:HD11	2:G:1009:LEU:HD13	1.90	0.52
1:D:138:MET:HA	1:D:138:MET:CE	2.39	0.52
1:A:293:LEU:HD22	1:A:341:LEU:HD11	1.92	0.52
1:C:393:LYS:HA	1:C:398:GLU:OE1	2.09	0.52
2:H:889:MET:O	2:H:893:LEU:HD13	2.10	0.52
2:E:754:LYS:HB2	2:E:786:GLU:CD	2.31	0.52
2:F:858:LYS:HE3	2:F:912:THR:HB	1.91	0.52
1:A:302:LYS:HD3	1:A:341:LEU:CD2	2.40	0.51
2:F:988:CYS:CB	2:F:1127:MET:CE	2.88	0.51
2:F:1107:PHE:O	2:F:1109:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:754:LYS:HB2	2:G:786:GLU:CD	2.31	0.51
1:A:433:VAL:CG1	1:B:410:LEU:HB3	2.40	0.51
1:C:199:ASN:CG	1:C:201:ASP:HB2	2.30	0.51
1:C:302:LYS:HD3	1:C:341:LEU:CD2	2.40	0.51
2:E:881:MET:HE3	2:E:882:PRO:CD	2.37	0.51
1:C:293:LEU:HD22	1:C:341:LEU:HD11	1.92	0.51
1:D:375:ARG:NH2	3:P:1:GLC:C6	2.62	0.51
2:H:1175:GLU:HB3	2:H:1178:GLU:HG3	1.93	0.51
2:E:955:ASN:OD1	2:E:1016:GLU:HB2	2.10	0.51
2:F:754:LYS:CG	2:F:755:VAL:H	2.24	0.51
2:F:762:LEU:HD21	2:F:799:THR:HG23	1.93	0.51
2:F:837:SER:O	2:F:841:GLN:HG3	2.11	0.51
2:E:970:MET:HE1	2:E:1002:LEU:HD13	1.92	0.51
2:H:859:ASN:HD21	2:H:1066:LYS:HE2	1.76	0.51
2:H:883:GLU:H	2:H:886:GLN:HE21	1.59	0.51
1:A:237:ARG:CZ	1:A:280:MET:HE1	2.40	0.50
1:B:456:VAL:CG1	1:B:457:ASP:N	2.74	0.50
2:G:889:MET:O	2:G:893:LEU:HD13	2.11	0.50
1:D:136:ALA:HB2	1:D:170:TRP:CE2	2.46	0.50
1:D:239:MET:HA	1:D:247:MET:HG3	1.93	0.50
2:G:910:MET:C	2:G:912:THR:H	2.13	0.50
2:G:966:VAL:HG12	2:G:970:MET:HE1	1.91	0.50
2:E:764:ARG:HD2	2:F:971:ASN:OD1	2.12	0.50
2:E:772:ALA:N	2:F:980:PHE:CD2	2.80	0.50
2:E:969:TYR:CD1	2:F:795:PHE:CD2	2.98	0.50
2:E:937:LYS:HB3	2:E:938:PRO:HD3	1.93	0.50
1:D:290:LEU:HD11	1:D:332:LEU:CB	2.42	0.50
2:F:1130:GLN:O	2:F:1134:GLU:HG3	2.12	0.50
1:D:283:VAL:HG12	1:D:284:GLU:H	1.76	0.50
2:F:937:LYS:N	2:F:938:PRO:HD2	2.27	0.50
1:C:192:GLU:HA	1:C:195:GLU:OE1	2.11	0.50
1:C:418:ARG:HB3	1:C:419:PRO:CD	2.36	0.50
2:G:756:TYR:O	2:G:757:LYS:HG3	2.12	0.50
2:G:1052:VAL:HG12	2:G:1077:VAL:CG2	2.42	0.50
1:A:201:ASP:O	1:A:202:SER:C	2.49	0.49
1:A:245:ASN:N	1:A:245:ASN:HD22	2.10	0.49
2:E:1104:TYR:O	2:F:779:CYS:HB2	2.12	0.49
1:B:290:LEU:HD11	1:B:332:LEU:CB	2.42	0.49
2:F:1020:PHE:CG	2:F:1021:PRO:HD3	2.46	0.49
2:G:925:PHE:CZ	2:G:1048:GLN:HB3	2.47	0.49
2:H:951:ARG:HG3	2:H:951:ARG:NH1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:852:MET:CG	2:E:853:PRO:HD2	2.41	0.49
2:E:912:THR:HG22	2:E:913:VAL:N	2.27	0.49
2:F:859:ASN:HD21	2:F:1066:LYS:HE2	1.77	0.49
1:C:201:ASP:O	1:C:202:SER:C	2.50	0.49
2:G:970:MET:HE1	2:G:1002:LEU:CD1	2.42	0.49
2:G:997:ASP:O	2:G:999:LYS:N	2.36	0.49
1:D:290:LEU:HD13	1:D:332:LEU:HB3	1.93	0.49
2:H:881:MET:HE3	2:H:882:PRO:HD2	1.94	0.49
2:E:1021:PRO:HG2	2:E:1129:LEU:HD21	1.94	0.49
1:C:433:VAL:CG1	1:D:410:LEU:HB3	2.42	0.49
2:H:754:LYS:CG	2:H:755:VAL:H	2.25	0.49
2:F:1086:LYS:O	2:F:1089:MET:HB2	2.12	0.49
1:C:193:LYS:HD2	1:C:205:GLN:HE22	1.78	0.49
2:E:765:PRO:CG	2:F:970:MET:HE3	2.42	0.49
2:G:1069:PHE:O	2:G:1071:GLU:N	2.46	0.49
1:D:334:LEU:HD11	1:D:338:LEU:HD21	1.93	0.49
1:D:347:GLU:O	1:D:351:VAL:HG23	2.13	0.49
2:H:837:SER:O	2:H:841:GLN:HG3	2.12	0.49
1:C:433:VAL:HG11	1:D:407:HIS:O	2.13	0.49
2:G:945:ALA:HB3	2:G:1026:HIS:CD2	2.48	0.49
2:H:1086:LYS:O	2:H:1089:MET:HB2	2.13	0.49
1:A:259:ILE:HG13	2:F:1189:LEU:HD21	1.95	0.49
2:H:771:VAL:N	2:H:775:LEU:CD1	2.57	0.49
2:H:904:GLU:O	2:H:908:VAL:HG23	2.13	0.49
2:H:988:CYS:SG	2:H:1127:MET:CE	2.99	0.49
2:F:917:ARG:HB2	2:F:917:ARG:NH1	2.27	0.49
2:E:889:MET:O	2:E:893:LEU:HD13	2.11	0.49
2:F:889:MET:O	2:F:893:LEU:HD13	2.12	0.49
2:G:1010:CYS:SG	2:G:1017:VAL:HG11	2.52	0.49
2:F:950:LEU:HD13	2:F:1121:LEU:HD21	1.94	0.49
1:C:342:ARG:NH2	1:C:357:ASP:OD1	2.46	0.49
2:G:852:MET:CG	2:G:853:PRO:HD2	2.42	0.49
3:N:1:GLC:O6	3:N:2:FRU:H61	2.13	0.48
2:H:1176:GLY:C	2:H:1178:GLU:H	2.16	0.48
2:F:858:LYS:HE3	2:F:912:THR:CB	2.43	0.48
2:F:997:ASP:C	2:F:999:LYS:H	2.11	0.48
1:C:374:ILE:HD12	1:D:410:LEU:CD1	2.43	0.48
1:C:430:SER:HB2	1:D:407:HIS:NE2	2.27	0.48
2:H:1130:GLN:O	2:H:1134:GLU:HG3	2.13	0.48
2:E:858:LYS:CE	2:E:912:THR:CG2	2.88	0.48
2:F:883:GLU:H	2:F:886:GLN:HE21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:754:LYS:CB	2:G:786:GLU:OE1	2.61	0.48
2:E:767:TRP:CH2	2:F:967:GLY:HA3	2.49	0.48
2:F:1176:GLY:C	2:F:1178:GLU:H	2.16	0.48
1:C:375:ARG:NH2	3:N:1:GLC:C6	2.71	0.48
1:D:299:ILE:HG21	1:D:346:ASN:HD21	1.78	0.48
2:E:897:TYR:C	2:E:897:TYR:CD2	2.87	0.48
1:B:218:ASN:ND2	1:B:220:PHE:HB3	2.29	0.48
2:F:1133:LYS:HB2	2:F:1133:LYS:HE3	1.61	0.48
1:C:338:LEU:O	1:C:342:ARG:HG3	2.14	0.48
2:G:1021:PRO:CG	2:G:1129:LEU:HD21	2.43	0.48
1:B:138:MET:HA	1:B:138:MET:HE3	1.94	0.48
2:F:988:CYS:SG	2:F:1127:MET:CE	3.02	0.48
2:G:1144:LYS:HE2	1:D:377:GLU:OE1	2.13	0.48
2:E:969:TYR:CE1	2:F:795:PHE:CD2	3.02	0.48
1:C:199:ASN:HD21	1:C:201:ASP:HB2	1.78	0.48
2:G:957:SER:HB3	2:H:780:PHE:CE1	2.48	0.48
2:E:859:ASN:ND2	2:E:1066:LYS:CD	2.76	0.47
2:F:999:LYS:O	2:F:999:LYS:HG2	2.13	0.47
1:C:233:LEU:O	1:C:237:ARG:HG3	2.13	0.47
2:G:859:ASN:ND2	2:G:1066:LYS:CD	2.75	0.47
2:G:997:ASP:OD2	2:G:999:LYS:HB3	2.14	0.47
2:H:852:MET:HE1	2:H:856:GLU:HB3	1.96	0.47
1:A:259:ILE:CG1	2:F:1189:LEU:HD21	2.44	0.47
2:E:945:ALA:HB3	2:E:1026:HIS:CD2	2.49	0.47
1:B:216:MET:HE1	1:B:225:MET:HE3	1.96	0.47
2:F:881:MET:HE1	2:F:887:LEU:HD21	1.96	0.47
1:C:446:ARG:HA	1:C:446:ARG:HD2	1.67	0.47
2:G:1195:PHE:O	2:G:1196:ARG:C	2.51	0.47
2:H:858:LYS:HE3	2:H:912:THR:HG21	1.95	0.47
2:H:937:LYS:HB3	2:H:938:PRO:HD3	1.96	0.47
2:H:762:LEU:HD21	2:H:799:THR:HG23	1.94	0.47
2:H:917:ARG:HB2	2:H:917:ARG:NH1	2.29	0.47
2:H:1170:ILE:CG1	2:H:1185:LEU:HD21	2.43	0.47
2:E:754:LYS:CB	2:E:786:GLU:OE1	2.62	0.47
1:B:283:VAL:HG12	1:B:284:GLU:H	1.79	0.47
1:D:289:LEU:HD21	1:D:308:LEU:HD23	1.96	0.47
2:F:1170:ILE:CG1	2:F:1185:LEU:HD21	2.43	0.47
2:G:789:PHE:HB2	2:H:965:LEU:HD22	1.96	0.47
2:E:971:ASN:ND2	2:F:765:PRO:HD2	2.29	0.47
2:F:932:GLN:O	2:F:936:ILE:HG13	2.15	0.47
2:H:850:PHE:HE1	2:H:873:MET:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:ASP:O	2:E:1082:GLU:HB3	2.15	0.47
2:G:772:ALA:O	2:G:773:GLU:O	2.32	0.47
1:C:199:ASN:OD1	1:C:201:ASP:HB2	2.15	0.47
2:G:862:LEU:HD21	2:G:913:VAL:HG13	1.96	0.47
1:D:193:LYS:HA	1:D:199:ASN:ND2	2.30	0.47
2:E:1010:CYS:SG	2:E:1017:VAL:HG11	2.54	0.47
2:E:1020:PHE:N	2:E:1021:PRO:CD	2.78	0.47
1:C:261:PRO:HG3	2:H:1166:ARG:O	2.15	0.47
1:C:285:ARG:NH1	3:M:2:FRU:H62	2.30	0.47
1:A:217:ASN:HA	2:F:1182:MET:HB3	1.96	0.47
2:E:772:ALA:O	2:E:773:GLU:O	2.33	0.47
2:G:1107:PHE:O	2:G:1109:PRO:HD3	2.15	0.47
1:D:216:MET:HE2	1:D:225:MET:HG2	1.94	0.47
2:G:765:PRO:HG3	2:H:970:MET:HE3	1.97	0.46
2:G:1020:PHE:CG	2:G:1021:PRO:HD3	2.50	0.46
1:B:232:ILE:HD12	1:B:269:ARG:HD2	1.96	0.46
2:F:852:MET:HE1	2:F:856:GLU:HB3	1.97	0.46
2:G:1036:GLU:CG	2:G:1040:LYS:HE2	2.45	0.46
1:A:233:LEU:O	1:A:237:ARG:HG3	2.15	0.46
2:G:897:TYR:C	2:G:897:TYR:CD2	2.88	0.46
1:D:168:VAL:O	1:D:172:GLN:HG3	2.15	0.46
1:D:218:ASN:ND2	1:D:220:PHE:HB3	2.31	0.46
1:A:430:SER:HB2	1:B:407:HIS:NE2	2.31	0.46
2:E:1107:PHE:O	2:E:1109:PRO:HD3	2.15	0.46
1:C:412:ARG:NH1	1:C:412:ARG:HG2	2.31	0.46
1:A:418:ARG:HB3	1:A:419:PRO:CD	2.38	0.46
2:G:754:LYS:HB3	2:G:786:GLU:OE1	2.16	0.46
2:G:970:MET:HE1	2:G:1002:LEU:HD13	1.97	0.46
2:E:869:LEU:HD23	2:E:873:MET:CE	2.45	0.46
1:C:423:LYS:HB2	1:D:400:HIS:NE2	2.31	0.46
2:G:765:PRO:CG	2:H:970:MET:HE3	2.46	0.46
2:G:869:LEU:HD23	2:G:873:MET:CE	2.46	0.46
2:H:1000:MET:HE1	2:H:1005:PHE:HA	1.98	0.46
1:A:374:ILE:HD12	1:B:410:LEU:CD1	2.45	0.46
2:E:925:PHE:CZ	2:E:1048:GLN:HB3	2.51	0.46
1:B:302:LYS:HD3	1:B:341:LEU:HD21	1.98	0.46
2:F:852:MET:HE2	2:F:856:GLU:HB3	1.98	0.46
2:F:1170:ILE:CD1	2:F:1181:VAL:HG13	2.38	0.46
2:G:957:SER:HB3	2:H:780:PHE:HE1	1.80	0.46
2:G:1034:SER:HB3	2:G:1037:ASN:HB2	1.98	0.46
2:H:754:LYS:CG	2:H:755:VAL:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:932:GLN:O	2:H:936:ILE:HG13	2.14	0.46
1:A:278:ALA:HB2	1:A:285:ARG:HA	1.98	0.46
2:E:756:TYR:O	2:E:757:LYS:HG3	2.15	0.46
2:E:772:ALA:HB2	2:F:980:PHE:CZ	2.51	0.46
1:B:347:GLU:O	1:B:351:VAL:HG23	2.15	0.46
1:C:166:ASN:ND2	1:C:170:TRP:CD2	2.72	0.46
2:H:1133:LYS:HB2	2:H:1133:LYS:HE3	1.66	0.46
1:A:375:ARG:NH2	3:J:1:GLC:H61	2.29	0.46
2:G:1169:LEU:CD1	1:D:259:ILE:HG23	2.45	0.46
1:D:398:GLU:N	1:D:399:PRO:CD	2.79	0.46
1:A:153:LEU:HB2	1:A:204:ASN:OD1	2.15	0.46
1:A:160:ARG:HD3	1:A:210:ARG:HB3	1.98	0.46
2:E:772:ALA:HB2	2:F:980:PHE:CE2	2.50	0.46
1:C:377:GLU:CD	2:H:1147:ARG:HH21	2.18	0.46
2:G:1079:ASP:O	2:G:1082:GLU:HB3	2.16	0.46
2:H:1033:VAL:HG13	2:H:1034:SER:N	2.30	0.46
2:E:862:LEU:HD21	2:E:913:VAL:HG13	1.98	0.45
2:G:1020:PHE:N	2:G:1021:PRO:CD	2.78	0.45
1:A:283:VAL:CG1	1:A:284:GLU:N	2.79	0.45
2:E:1020:PHE:CG	2:E:1021:PRO:HD3	2.51	0.45
2:F:850:PHE:HE1	2:F:873:MET:HG3	1.81	0.45
2:G:950:LEU:HD13	2:G:1121:LEU:HD21	1.98	0.45
1:A:152:LEU:HD12	1:A:152:LEU:O	2.16	0.45
1:A:215:PHE:O	1:A:221:GLY:HA3	2.16	0.45
2:G:869:LEU:HA	2:G:873:MET:CE	2.46	0.45
2:H:940:ILE:HD13	2:H:1091:HIS:HB2	1.97	0.45
2:E:1021:PRO:CG	2:E:1129:LEU:HD21	2.47	0.45
2:F:1154:LYS:HE3	2:F:1154:LYS:HB2	1.86	0.45
2:F:869:LEU:HD23	2:F:873:MET:HE3	1.90	0.45
2:F:997:ASP:OD2	2:F:999:LYS:HB3	2.16	0.45
2:F:1069:PHE:O	2:F:1071:GLU:N	2.49	0.45
1:D:347:GLU:HA	1:D:347:GLU:OE1	2.16	0.45
2:H:858:LYS:HE3	2:H:912:THR:CG2	2.47	0.45
2:H:900:LEU:HD22	2:H:904:GLU:OE2	2.16	0.45
2:E:762:LEU:HD11	2:F:969:TYR:CE2	2.51	0.45
2:E:1147:ARG:HH11	1:B:376:MET:HG3	1.64	0.45
2:F:1020:PHE:N	2:F:1021:PRO:CD	2.79	0.45
2:H:874:ILE:O	2:H:878:ILE:HG13	2.16	0.45
2:H:1020:PHE:N	2:H:1021:PRO:CD	2.80	0.45
2:H:1122:HIS:CE1	2:H:1125:ARG:HH21	2.34	0.45
1:A:278:ALA:HB1	1:A:283:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:754:LYS:CG	2:F:755:VAL:N	2.79	0.45
1:D:138:MET:HA	1:D:138:MET:HE3	1.98	0.45
2:F:1033:VAL:HG13	2:F:1034:SER:N	2.31	0.45
2:G:767:TRP:CH2	2:H:967:GLY:HA3	2.52	0.45
1:D:232:ILE:HD12	1:D:269:ARG:HD2	1.98	0.45
1:B:299:ILE:HG21	1:B:346:ASN:HD21	1.79	0.45
1:B:347:GLU:HA	1:B:347:GLU:OE1	2.17	0.45
2:G:1021:PRO:CB	2:G:1129:LEU:HD21	2.47	0.45
2:H:1175:GLU:CG	2:H:1178:GLU:HG3	2.47	0.45
2:F:832:LEU:HD21	2:F:840:ALA:HB3	1.93	0.44
2:F:846:PHE:CG	2:F:880:GLN:HG3	2.52	0.44
2:G:832:LEU:HD11	2:G:840:ALA:CB	2.47	0.44
1:D:139:TYR:O	1:D:143:LEU:HG	2.17	0.44
2:E:913:VAL:HA	2:E:914:PRO:HD3	1.78	0.44
2:E:997:ASP:OD2	2:E:999:LYS:HB3	2.18	0.44
1:B:302:LYS:HB3	1:B:349:MET:HE3	1.99	0.44
1:B:457:ASP:HB3	1:C:245:ASN:ND2	2.32	0.44
2:F:1175:GLU:CG	2:F:1178:GLU:HG3	2.47	0.44
1:A:450:ILE:HD13	1:A:450:ILE:N	2.33	0.44
2:E:801:ALA:O	2:F:995:SER:HB2	2.18	0.44
2:F:754:LYS:HB2	2:F:786:GLU:OE2	2.18	0.44
2:E:1069:PHE:O	2:E:1071:GLU:N	2.51	0.44
1:B:239:MET:CA	1:B:247:MET:HG3	2.47	0.44
1:C:450:ILE:HG12	1:D:450:ILE:HD12	2.00	0.44
2:G:1052:VAL:HG11	2:G:1073:MET:CE	2.47	0.44
1:A:407:HIS:CD2	1:B:430:SER:HA	2.52	0.44
1:C:215:PHE:O	1:C:221:GLY:HA3	2.17	0.44
1:C:385:PHE:CZ	1:D:385:PHE:HB2	2.53	0.44
1:C:407:HIS:CD2	1:D:430:SER:HA	2.53	0.44
2:H:951:ARG:HH11	2:H:951:ARG:CG	2.28	0.44
1:A:412:ARG:NH1	1:A:412:ARG:HG2	2.32	0.44
2:E:1005:PHE:CE1	2:F:798:LEU:HD13	2.53	0.44
2:G:772:ALA:N	2:H:980:PHE:CD2	2.85	0.44
1:D:277:ARG:O	1:D:280:MET:HG2	2.17	0.44
2:H:852:MET:HE2	2:H:856:GLU:HB3	1.99	0.44
1:A:433:VAL:HG11	1:B:410:LEU:HB3	1.99	0.44
1:B:302:LYS:CD	1:B:341:LEU:HD22	2.48	0.44
2:F:900:LEU:HD22	2:F:904:GLU:OE2	2.17	0.44
2:F:951:ARG:HG3	2:F:951:ARG:NH1	2.25	0.44
1:C:278:ALA:HB2	1:C:285:ARG:HA	1.99	0.44
1:A:433:VAL:HG11	1:B:407:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:798:LEU:HD21	2:F:966:VAL:HG13	2.00	0.44
2:H:966:VAL:HG12	2:H:970:MET:HE1	2.00	0.44
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.33	0.44
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.79	0.44
1:A:204:ASN:O	1:A:208:ILE:HG13	2.18	0.44
2:E:883:GLU:HG3	2:E:884:PRO:CD	2.48	0.44
1:A:219:LYS:O	1:A:223:LYS:HG3	2.17	0.43
2:E:754:LYS:HB3	2:E:786:GLU:OE1	2.18	0.43
2:E:763:ARG:NH2	2:F:996:ALA:HA	2.33	0.43
2:E:794:LEU:HD11	2:F:1009:LEU:HD11	2.00	0.43
2:E:1169:LEU:CD1	1:B:259:ILE:HG23	2.48	0.43
1:B:204:ASN:O	1:B:208:ILE:HG13	2.18	0.43
1:C:278:ALA:HB1	1:C:283:VAL:O	2.18	0.43
1:A:398:GLU:HB3	1:A:399:PRO:CD	2.42	0.43
1:A:450:ILE:HG12	1:B:450:ILE:HD12	2.00	0.43
2:E:1034:SER:HB3	2:E:1037:ASN:HB2	2.00	0.43
2:F:939:GLU:HB3	2:F:1033:VAL:HG22	2.00	0.43
2:F:1000:MET:HE1	2:F:1005:PHE:HA	2.00	0.43
2:F:1102:GLY:HA2	2:F:1107:PHE:CE2	2.53	0.43
1:D:400:HIS:O	1:D:404:ILE:HG13	2.18	0.43
1:A:342:ARG:NH2	1:A:357:ASP:OD1	2.49	0.43
2:E:1056:VAL:O	2:E:1056:VAL:CG1	2.67	0.43
2:H:999:LYS:O	2:H:999:LYS:HG2	2.17	0.43
2:H:858:LYS:NZ	2:H:912:THR:HG21	2.34	0.43
1:C:219:LYS:O	1:C:223:LYS:HG3	2.19	0.43
2:G:1069:PHE:C	2:G:1071:GLU:N	2.70	0.43
2:G:1137:LYS:HD2	2:G:1137:LYS:HA	1.65	0.43
1:D:328:GLU:CD	3:O:1:GLC:H61	2.38	0.43
2:F:795:PHE:N	2:F:795:PHE:CD1	2.87	0.43
2:F:937:LYS:HB3	2:F:938:PRO:HD3	2.01	0.43
2:F:1069:PHE:O	2:F:1070:VAL:C	2.56	0.43
2:E:910:MET:C	2:E:912:THR:N	2.72	0.43
1:B:290:LEU:HD12	1:B:332:LEU:HD13	2.01	0.43
2:H:794:LEU:C	2:H:794:LEU:CD2	2.87	0.43
2:H:1098:TYR:CD2	2:H:1114:VAL:HG22	2.53	0.43
1:B:290:LEU:HD13	1:B:332:LEU:HB3	1.93	0.43
2:F:852:MET:HG2	2:F:853:PRO:HD2	2.01	0.43
2:G:1106:VAL:HB	2:H:770:PHE:CE1	2.52	0.43
1:D:290:LEU:HD11	1:D:332:LEU:HB2	2.01	0.43
2:E:1069:PHE:C	2:E:1071:GLU:N	2.72	0.43
1:A:423:LYS:HB2	1:B:400:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1021:PRO:CB	2:E:1129:LEU:HD21	2.49	0.43
1:B:236:VAL:HG12	1:B:277:ARG:HD2	2.01	0.43
2:F:1099:LYS:O	2:F:1099:LYS:HD3	2.19	0.43
2:H:1046:LYS:HE3	2:H:1046:LYS:HB2	1.86	0.43
2:E:1152:LYS:HE3	2:E:1152:LYS:HB2	1.91	0.42
2:F:864:VAL:HG12	2:F:864:VAL:O	2.18	0.42
2:H:853:PRO:HB2	2:H:856:GLU:HG3	2.01	0.42
2:F:1137:LYS:HD2	2:F:1137:LYS:HA	1.81	0.42
1:A:303:VAL:HG23	1:A:349:MET:HE2	2.00	0.42
2:E:769:LYS:CG	2:E:770:PHE:N	2.82	0.42
2:F:1069:PHE:O	2:F:1072:LYS:N	2.53	0.42
1:C:285:ARG:CZ	3:M:2:FRU:H62	2.49	0.42
1:C:430:SER:CA	1:D:407:HIS:CD2	2.96	0.42
2:G:936:ILE:HG23	2:G:1038:LEU:HD22	2.00	0.42
2:G:937:LYS:HE3	2:G:1090:MET:HE1	2.01	0.42
2:G:1056:VAL:O	2:G:1056:VAL:CG1	2.67	0.42
1:D:431:GLN:HG3	1:D:450:ILE:HG23	2.01	0.42
2:E:1036:GLU:CG	2:E:1040:LYS:HE2	2.49	0.42
2:F:988:CYS:CB	2:F:1127:MET:HE1	2.48	0.42
2:F:1175:GLU:HG2	2:F:1178:GLU:HG3	2.01	0.42
1:C:398:GLU:N	1:C:399:PRO:CD	2.82	0.42
2:H:754:LYS:HB2	2:H:786:GLU:OE2	2.19	0.42
2:H:769:LYS:HG3	2:H:770:PHE:N	2.34	0.42
2:H:869:LEU:HA	2:H:873:MET:HE2	2.00	0.42
2:H:1036:GLU:CG	2:H:1040:LYS:HE2	2.49	0.42
1:A:149:ASP:OD1	1:A:200:TYR:HE1	2.02	0.42
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.74	0.42
1:B:275:THR:O	1:B:278:ALA:HB3	2.19	0.42
1:C:284:GLU:HG3	1:C:332:LEU:HD21	2.02	0.42
2:G:910:MET:C	2:G:912:THR:N	2.72	0.42
2:F:861:ILE:HG22	2:F:919:ARG:HD2	2.02	0.42
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.88	0.42
2:H:939:GLU:HB3	2:H:1033:VAL:HG22	2.01	0.42
2:H:1122:HIS:ND1	2:H:1125:ARG:NH2	2.56	0.42
2:H:1159:ARG:HG3	2:H:1160:LEU:N	2.34	0.42
2:E:1052:VAL:HG11	2:E:1073:MET:CE	2.50	0.42
2:E:1137:LYS:HA	2:E:1137:LYS:HD2	1.65	0.42
1:C:283:VAL:HG12	1:C:284:GLU:H	1.83	0.42
1:C:287:GLN:HB3	1:C:288:PRO:CD	2.50	0.42
2:G:1059:PHE:HA	2:G:1060:PRO:HD3	1.87	0.42
2:H:1033:VAL:HG13	2:H:1034:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1043:ASP:O	2:E:1046:LYS:HB3	2.20	0.42
1:B:206:HIS:HA	1:B:246:MET:HG3	2.01	0.42
1:B:290:LEU:HD11	1:B:332:LEU:HB2	2.02	0.42
2:F:769:LYS:HG3	2:F:770:PHE:N	2.35	0.42
2:F:945:ALA:HB1	2:F:1026:HIS:ND1	2.35	0.42
1:A:172:GLN:HA	1:A:220:PHE:CE2	2.54	0.42
2:E:950:LEU:HD13	2:E:1121:LEU:HD21	2.02	0.42
2:E:1169:LEU:O	2:E:1170:ILE:HG12	2.20	0.42
2:F:852:MET:CG	2:F:853:PRO:HD2	2.49	0.42
2:F:865:ASN:OD1	2:F:867:ALA:HB3	2.20	0.42
2:F:940:ILE:HD13	2:F:1091:HIS:HB2	2.01	0.42
2:F:951:ARG:HG3	2:F:951:ARG:O	2.20	0.42
2:G:794:LEU:HD11	2:H:1009:LEU:HD11	2.02	0.42
2:G:1036:GLU:HG2	2:G:1040:LYS:HE2	2.01	0.42
2:H:769:LYS:CG	2:H:770:PHE:N	2.82	0.42
2:E:988:CYS:HA	2:E:1127:MET:HE3	2.01	0.42
2:E:1186:LEU:HD22	1:B:252:LYS:HB3	2.02	0.42
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.85	0.42
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.86	0.42
1:B:423:LYS:O	1:B:427:GLU:HG3	2.20	0.42
2:F:794:LEU:C	2:F:794:LEU:CD2	2.88	0.42
2:F:794:LEU:C	2:F:794:LEU:HD23	2.40	0.42
2:F:1097:LEU:HA	2:F:1097:LEU:HD23	1.83	0.42
2:F:1159:ARG:HG3	2:F:1160:LEU:N	2.35	0.42
1:D:218:ASN:HD22	1:D:220:PHE:H	1.67	0.42
1:A:287:GLN:CB	1:A:288:PRO:HD3	2.49	0.41
2:E:754:LYS:HB2	2:E:786:GLU:OE1	2.19	0.41
2:F:1062:ALA:HB1	2:F:1067:ASP:HB3	2.02	0.41
1:C:297:THR:OG1	1:C:302:LYS:NZ	2.53	0.41
2:H:794:LEU:C	2:H:794:LEU:HD23	2.40	0.41
2:H:919:ARG:HG3	2:H:1069:PHE:CD1	2.55	0.41
2:F:913:VAL:HA	2:F:914:PRO:HD3	1.88	0.41
1:C:289:LEU:HD21	1:C:308:LEU:HD23	2.02	0.41
1:D:450:ILE:HG22	1:D:452:ILE:CG2	2.51	0.41
2:F:1038:LEU:HD12	2:F:1038:LEU:HA	1.94	0.41
1:D:233:LEU:O	1:D:236:VAL:HB	2.20	0.41
2:H:906:PHE:O	2:H:910:MET:HG2	2.20	0.41
2:H:1154:LYS:HE3	2:H:1154:LYS:HB2	1.88	0.41
1:A:398:GLU:N	1:A:399:PRO:CD	2.84	0.41
1:B:218:ASN:HD22	1:B:220:PHE:H	1.67	0.41
2:F:1046:LYS:HE3	2:F:1046:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1016:GLU:CD	2:G:1016:GLU:N	2.68	0.41
1:D:418:ARG:HB3	1:D:419:PRO:HD3	2.01	0.41
2:H:850:PHE:O	2:H:851:ARG:HB2	2.20	0.41
2:H:1175:GLU:HG2	2:H:1178:GLU:HG3	2.01	0.41
1:A:290:LEU:CD1	1:A:332:LEU:CB	2.98	0.41
2:E:789:PHE:HB2	2:F:965:LEU:CD2	2.51	0.41
2:E:858:LYS:HZ1	2:E:912:THR:HG21	1.81	0.41
2:E:970:MET:HE3	2:F:765:PRO:HG3	2.03	0.41
1:B:218:ASN:ND2	1:B:221:GLY:H	2.18	0.41
2:F:853:PRO:HB2	2:F:856:GLU:HG3	2.02	0.41
1:C:418:ARG:N	1:C:419:PRO:CD	2.82	0.41
1:D:157:GLU:O	1:D:161:VAL:HG23	2.20	0.41
2:E:952:LYS:HG2	2:E:952:LYS:O	2.20	0.41
1:A:338:LEU:O	1:A:342:ARG:HG3	2.21	0.41
2:E:1086:LYS:O	2:E:1089:MET:HB2	2.21	0.41
2:F:769:LYS:CG	2:F:770:PHE:N	2.83	0.41
2:F:772:ALA:O	2:F:773:GLU:C	2.59	0.41
2:F:874:ILE:O	2:F:878:ILE:HG13	2.20	0.41
1:C:172:GLN:HA	1:C:220:PHE:CE2	2.56	0.41
1:C:219:LYS:HE3	2:H:1178:GLU:OE1	2.21	0.41
2:G:754:LYS:HB2	2:G:786:GLU:OE1	2.20	0.41
1:D:260:LEU:HA	1:D:261:PRO:HD3	1.90	0.41
1:A:193:LYS:HD2	1:A:199:ASN:HD22	1.85	0.41
1:B:277:ARG:O	1:B:280:MET:HG2	2.21	0.41
2:F:919:ARG:HG3	2:F:1069:PHE:CD1	2.56	0.41
2:F:1098:TYR:CD2	2:F:1114:VAL:HG22	2.56	0.41
2:G:883:GLU:HG3	2:G:884:PRO:CD	2.50	0.41
1:D:236:VAL:HG12	1:D:277:ARG:HD2	2.02	0.41
1:A:377:GLU:CD	2:F:1147:ARG:HH21	2.23	0.41
2:E:989:LYS:O	2:E:992:ASP:HB2	2.21	0.41
2:E:1189:LEU:HD21	1:B:259:ILE:HG12	2.02	0.41
1:B:233:LEU:O	1:B:236:VAL:HB	2.21	0.41
2:F:858:LYS:HE3	2:F:912:THR:HG21	2.03	0.41
2:H:858:LYS:CE	2:H:912:THR:HG21	2.50	0.41
2:H:881:MET:HE1	2:H:887:LEU:HD21	2.03	0.41
2:H:1069:PHE:O	2:H:1071:GLU:N	2.54	0.41
2:H:1099:LYS:O	2:H:1099:LYS:HD3	2.21	0.41
2:F:1195:PHE:C	2:F:1196:ARG:HG3	2.42	0.41
1:C:406:GLN:O	1:C:409:LEU:HB2	2.21	0.41
2:G:1031:SER:HB2	2:G:1119:MET:HA	2.03	0.41
2:H:988:CYS:HA	2:H:1127:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:O	1:B:143:LEU:HG	2.21	0.40
1:B:302:LYS:HB3	1:B:349:MET:HE1	2.00	0.40
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.81	0.40
2:F:853:PRO:CB	2:F:856:GLU:HG3	2.51	0.40
2:G:764:ARG:HA	2:G:765:PRO:HD3	1.86	0.40
2:H:1038:LEU:HD12	2:H:1038:LEU:HA	1.93	0.40
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.78	0.40
1:B:287:GLN:N	1:B:288:PRO:CD	2.84	0.40
2:F:858:LYS:NZ	2:F:912:THR:HG21	2.37	0.40
2:H:1102:GLY:HA2	2:H:1107:PHE:CE2	2.56	0.40
1:B:190:HIS:HD2	1:B:205:GLN:NE2	2.18	0.40
2:H:852:MET:HG2	2:H:853:PRO:HD2	2.03	0.40
1:C:152:LEU:O	1:C:152:LEU:HD12	2.21	0.40
2:G:1169:LEU:O	2:G:1170:ILE:HG12	2.21	0.40
2:H:795:PHE:N	2:H:795:PHE:CD1	2.88	0.40
1:A:418:ARG:N	1:A:419:PRO:CD	2.85	0.40
1:C:226:LEU:HD21	1:C:257:LEU:HD22	2.04	0.40
2:G:940:ILE:HD13	2:G:1091:HIS:HB2	2.03	0.40
2:G:1069:PHE:C	2:G:1071:GLU:H	2.25	0.40
2:G:1186:LEU:HD22	1:D:252:LYS:HB3	2.02	0.40
1:D:287:GLN:N	1:D:288:PRO:CD	2.85	0.40
2:H:754:LYS:HB2	2:H:786:GLU:CD	2.42	0.40
2:H:852:MET:O	2:H:853:PRO:C	2.59	0.40
2:H:1097:LEU:HA	2:H:1097:LEU:HD23	1.89	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	320/327 (98%)	311 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	315/327 (96%)	300 (95%)	15 (5%)	0	100	100
1	C	320/327 (98%)	309 (97%)	11 (3%)	0	100	100
1	D	325/327 (99%)	313 (96%)	12 (4%)	0	100	100
2	E	415/457 (91%)	375 (90%)	33 (8%)	7 (2%)	9	16
2	F	415/457 (91%)	368 (89%)	37 (9%)	10 (2%)	6	9
2	G	416/457 (91%)	376 (90%)	32 (8%)	8 (2%)	8	14
2	H	415/457 (91%)	366 (88%)	39 (9%)	10 (2%)	6	9
All	All	2941/3136 (94%)	2718 (92%)	188 (6%)	35 (1%)	13	23

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	773	GLU
2	E	996	ALA
2	F	773	GLU
2	G	773	GLU
2	H	773	GLU
2	E	1174	ALA
2	F	998	GLN
2	F	1070	VAL
2	G	996	ALA
2	G	1174	ALA
2	H	998	GLN
2	E	865	ASN
2	F	845	ILE
2	G	865	ASN
2	H	845	ILE
2	H	1070	VAL
2	H	1177	ASP
2	E	998	GLN
2	E	1172	MET
2	F	1177	ASP
2	G	998	GLN
2	G	1172	MET
2	H	1018	LEU
2	F	1018	LEU
2	F	1069	PHE
2	H	846	PHE
2	F	984	ILE
2	H	1069	PHE

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Mol	Chain	Res	Type
2	G	1070	VAL
2	E	1106	VAL
2	F	834	VAL
2	F	1106	VAL
2	G	1106	VAL
2	H	984	ILE
2	H	1106	VAL

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	292/297 (98%)	289 (99%)	3 (1%)	76	85
1	B	290/297 (98%)	279 (96%)	11 (4%)	33	53
1	C	292/297 (98%)	287 (98%)	5 (2%)	60	76
1	D	297/297 (100%)	287 (97%)	10 (3%)	37	58
2	E	378/410 (92%)	368 (97%)	10 (3%)	46	66
2	F	378/410 (92%)	370 (98%)	8 (2%)	53	71
2	G	379/410 (92%)	369 (97%)	10 (3%)	46	66
2	H	378/410 (92%)	367 (97%)	11 (3%)	42	62
All	All	2684/2828 (95%)	2616 (98%)	68 (2%)	47	67

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	245	ASN
1	A	395	SER
2	E	767	TRP
2	E	896	GLU
2	E	912	THR
2	E	933	VAL
2	E	984	ILE

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Mol	Chain	Res	Type
2	E	1001	THR
2	E	1016	GLU
2	E	1041	SER
2	E	1137	LYS
2	E	1179	THR
1	B	132	SER
1	B	138	MET
1	B	155	CYS
1	B	223	LYS
1	B	225	MET
1	B	235	LEU
1	B	246	MET
1	B	259	ILE
1	B	395	SER
1	B	448	LEU
1	B	451	ASP
2	F	767	TRP
2	F	917	ARG
2	F	951	ARG
2	F	1041	SER
2	F	1059	PHE
2	F	1068	LYS
2	F	1092	SER
2	F	1159	ARG
1	C	172	GLN
1	C	197	SER
1	C	245	ASN
1	C	263	PRO
1	C	395	SER
2	G	767	TRP
2	G	831	GLU
2	G	896	GLU
2	G	912	THR
2	G	933	VAL
2	G	984	ILE
2	G	1016	GLU
2	G	1041	SER
2	G	1137	LYS
2	G	1179	THR
1	D	137	MET
1	D	138	MET
1	D	155	CYS

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Mol	Chain	Res	Type
1	D	200	TYR
1	D	225	MET
1	D	246	MET
1	D	259	ILE
1	D	354	CYS
1	D	395	SER
1	D	453	GLU
2	H	767	TRP
2	H	837	SER
2	H	917	ARG
2	H	932	GLN
2	H	951	ARG
2	H	1020	PHE
2	H	1041	SER
2	H	1059	PHE
2	H	1068	LYS
2	H	1092	SER
2	H	1159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	262	GLN
1	A	431	GLN
2	E	761	GLN
2	E	859	ASN
2	E	876	ASN
2	E	886	GLN
2	E	1026	HIS
1	B	190	HIS
1	B	205	GLN
1	B	218	ASN
1	B	262	GLN
1	B	335	HIS
1	B	435	HIS
1	B	437	ASN
2	F	842	ASN
2	F	859	ASN
2	F	880	GLN
2	F	886	GLN
2	F	932	GLN

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Mol	Chain	Res	Type
1	C	165	ASN
1	C	172	GLN
1	C	245	ASN
1	C	262	GLN
1	C	431	GLN
2	G	761	GLN
2	G	859	ASN
2	G	876	ASN
2	G	886	GLN
2	G	1026	HIS
1	D	165	ASN
1	D	172	GLN
1	D	205	GLN
1	D	218	ASN
1	D	262	GLN
1	D	335	HIS
1	D	435	HIS
1	D	437	ASN
2	H	859	ASN
2	H	886	GLN
2	H	932	GLN
2	H	1014	HIS
2	H	1173	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

16 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	$\#\|Z\| > 2$
3	GLC	I	1	3	11,11,12	1.17	1 (9%)	15,15,17	3.67	9 (60%)
3	FRU	I	2	3	11,12,12	1.17	1 (9%)	10,18,18	3.25	4 (40%)
3	GLC	J	1	3	11,11,12	1.25	1 (9%)	15,15,17	4.21	11 (73%)
3	FRU	J	2	3	11,12,12	1.13	1 (9%)	10,18,18	3.24	4 (40%)
3	GLC	K	1	3	11,11,12	1.39	1 (9%)	15,15,17	3.44	7 (46%)
3	FRU	K	2	3	11,12,12	1.05	1 (9%)	10,18,18	3.56	5 (50%)
3	GLC	L	1	3	11,11,12	1.47	2 (18%)	15,15,17	3.49	7 (46%)
3	FRU	L	2	3	11,12,12	1.15	1 (9%)	10,18,18	3.25	4 (40%)
3	GLC	M	1	3	11,11,12	1.28	1 (9%)	15,15,17	3.94	8 (53%)
3	FRU	M	2	3	11,12,12	1.31	1 (9%)	10,18,18	3.31	4 (40%)
3	GLC	N	1	3	11,11,12	1.53	1 (9%)	15,15,17	3.87	9 (60%)
3	FRU	N	2	3	11,12,12	1.13	1 (9%)	10,18,18	3.30	4 (40%)
3	GLC	O	1	3	11,11,12	1.36	1 (9%)	15,15,17	2.86	4 (26%)
3	FRU	O	2	3	11,12,12	1.23	1 (9%)	10,18,18	3.25	4 (40%)
3	GLC	P	1	3	11,11,12	1.64	2 (18%)	15,15,17	3.12	8 (53%)
3	FRU	P	2	3	11,12,12	1.22	1 (9%)	10,18,18	3.30	4 (40%)

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
3	GLC	I	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	I	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	J	1	3	3/3/5/5	1/2/19/22	0/1/1/1
3	FRU	J	2	3	2/2/4/4	2/5/24/24	0/1/1/1
3	GLC	K	1	3	2/2/5/5	1/2/19/22	0/1/1/1
3	FRU	K	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	L	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	L	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	M	1	3	2/2/5/5	1/2/19/22	0/1/1/1
3	FRU	M	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	N	1	3	3/3/5/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	N	2	3	2/2/4/4	2/5/24/24	0/1/1/1
3	GLC	O	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	O	2	3	2/2/4/4	5/5/24/24	0/1/1/1
3	GLC	P	1	3	3/3/5/5	0/2/19/22	0/1/1/1
3	FRU	P	2	3	2/2/4/4	2/5/24/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	GLC	O3-C3	-2.99	1.35	1.43
3	P	1	GLC	O3-C3	-2.98	1.36	1.43
3	M	1	GLC	O3-C3	-2.87	1.36	1.43
3	L	1	GLC	O3-C3	-2.82	1.36	1.43
3	K	1	GLC	O3-C3	-2.82	1.36	1.43
3	O	1	GLC	O3-C3	-2.82	1.36	1.43
3	J	1	GLC	O3-C3	-2.63	1.36	1.43
3	M	2	FRU	O3-C3	-2.61	1.37	1.42
3	L	2	FRU	O3-C3	-2.55	1.37	1.42
3	I	1	GLC	O3-C3	-2.54	1.37	1.43
3	O	2	FRU	O3-C3	-2.54	1.37	1.42
3	P	2	FRU	O3-C3	-2.53	1.37	1.42
3	N	2	FRU	O3-C3	-2.51	1.37	1.42
3	I	2	FRU	O3-C3	-2.45	1.37	1.42
3	J	2	FRU	O3-C3	-2.39	1.38	1.42
3	P	1	GLC	O4-C4	-2.30	1.37	1.43
3	L	1	GLC	O4-C4	-2.29	1.37	1.43
3	K	2	FRU	O3-C3	-2.12	1.38	1.42

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1	GLC	C1-C2-C3	9.62	121.50	109.67
3	O	1	GLC	C1-C2-C3	7.69	119.12	109.67
3	I	1	GLC	O2-C2-C3	7.31	124.79	110.14
3	J	1	GLC	O2-C2-C3	7.05	124.25	110.14
3	M	1	GLC	O5-C5-C6	6.74	117.78	107.20
3	L	1	GLC	O2-C2-C3	6.62	123.41	110.14
3	J	1	GLC	O5-C5-C6	6.62	117.58	107.20
3	N	2	FRU	O5-C5-C6	6.53	127.03	108.85
3	N	1	GLC	O2-C2-C3	6.51	123.18	110.14
3	L	2	FRU	O5-C5-C6	6.47	126.85	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	FRU	O5-C5-C6	6.43	126.76	108.85
3	K	2	FRU	O5-C5-C6	6.29	126.36	108.85
3	I	1	GLC	O2-C2-C1	6.21	121.86	109.15
3	J	1	GLC	O2-C2-C1	6.18	121.80	109.15
3	J	2	FRU	O5-C5-C6	6.11	125.86	108.85
3	L	1	GLC	C2-C3-C4	6.07	121.40	110.89
3	I	1	GLC	C2-C3-C4	6.02	121.31	110.89
3	K	1	GLC	O2-C2-C3	5.97	122.10	110.14
3	K	1	GLC	C1-C2-C3	5.96	117.00	109.67
3	K	1	GLC	C2-C3-C4	5.89	121.08	110.89
3	K	2	FRU	O4-C4-C5	5.87	128.01	111.05
3	N	1	GLC	O3-C3-C2	5.67	120.86	109.99
3	M	2	FRU	O4-C4-C5	5.64	127.35	111.05
3	N	1	GLC	O2-C2-C1	5.47	120.34	109.15
3	J	1	GLC	C2-C3-C4	5.47	120.36	110.89
3	I	2	FRU	O4-C4-C5	5.41	126.70	111.05
3	I	2	FRU	O5-C5-C6	5.41	123.92	108.85
3	K	2	FRU	O4-C4-C3	5.34	128.13	112.15
3	O	1	GLC	O2-C2-C3	5.28	120.72	110.14
3	O	2	FRU	O4-C4-C5	5.26	126.27	111.05
3	O	2	FRU	O5-C5-C6	5.25	123.46	108.85
3	N	1	GLC	O4-C4-C5	5.24	122.31	109.30
3	P	1	GLC	C2-C3-C4	5.23	119.95	110.89
3	N	2	FRU	O4-C4-C5	5.15	125.95	111.05
3	J	1	GLC	O3-C3-C2	5.14	119.83	109.99
3	L	1	GLC	O2-C2-C1	5.12	119.63	109.15
3	M	1	GLC	O5-C5-C4	5.10	123.25	110.83
3	L	1	GLC	C1-C2-C3	5.05	115.88	109.67
3	M	2	FRU	O5-C5-C6	5.02	122.83	108.85
3	K	1	GLC	O2-C2-C1	5.00	119.37	109.15
3	J	2	FRU	O4-C4-C5	4.95	125.37	111.05
3	P	2	FRU	O4-C4-C5	4.94	125.32	111.05
3	M	2	FRU	O4-C4-C3	4.92	126.89	112.15
3	O	2	FRU	O4-C4-C3	4.89	126.80	112.15
3	P	1	GLC	O4-C4-C5	4.86	121.35	109.30
3	J	2	FRU	O4-C4-C3	4.84	126.66	112.15
3	L	2	FRU	O4-C4-C3	4.84	126.65	112.15
3	L	2	FRU	O4-C4-C5	4.83	125.02	111.05
3	P	1	GLC	O3-C3-C2	4.83	119.24	109.99
3	K	1	GLC	O3-C3-C2	4.82	119.22	109.99
3	L	1	GLC	O3-C3-C2	4.77	119.13	109.99
3	P	2	FRU	O4-C4-C3	4.74	126.35	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	GLC	C1-O5-C5	-4.71	105.81	112.19
3	N	2	FRU	O4-C4-C3	4.65	126.07	112.15
3	M	1	GLC	O2-C2-C3	4.65	119.45	110.14
3	M	2	FRU	C6-C5-C4	4.64	126.28	115.09
3	P	1	GLC	O4-C4-C3	4.60	120.99	110.35
3	N	1	GLC	O4-C4-C3	4.55	120.86	110.35
3	J	1	GLC	O5-C5-C4	4.52	121.82	110.83
3	I	2	FRU	O4-C4-C3	4.51	125.65	112.15
3	N	1	GLC	C2-C3-C4	4.42	118.54	110.89
3	N	1	GLC	C1-C2-C3	4.41	115.08	109.67
3	I	2	FRU	C6-C5-C4	4.36	125.59	115.09
3	O	2	FRU	C6-C5-C4	4.30	125.45	115.09
3	O	1	GLC	O2-C2-C1	4.28	117.91	109.15
3	I	1	GLC	O3-C3-C2	4.18	118.00	109.99
3	N	1	GLC	O3-C3-C4	4.08	119.79	110.35
3	I	1	GLC	O3-C3-C4	4.03	119.67	110.35
3	P	1	GLC	O3-C3-C4	3.88	119.32	110.35
3	M	1	GLC	O2-C2-C1	3.78	116.90	109.15
3	K	1	GLC	O3-C3-C4	3.68	118.85	110.35
3	J	1	GLC	O3-C3-C4	3.60	118.68	110.35
3	P	2	FRU	C6-C5-C4	3.60	123.76	115.09
3	N	2	FRU	C6-C5-C4	3.55	123.65	115.09
3	J	2	FRU	C6-C5-C4	3.55	123.63	115.09
3	P	1	GLC	C3-C4-C5	3.43	116.36	110.24
3	L	1	GLC	O3-C3-C4	3.37	118.13	110.35
3	P	1	GLC	O5-C5-C6	3.35	112.46	107.20
3	K	2	FRU	C6-C5-C4	3.34	123.14	115.09
3	L	2	FRU	C6-C5-C4	3.28	123.00	115.09
3	I	1	GLC	O5-C1-C2	3.18	115.68	110.77
3	M	1	GLC	C1-O5-C5	3.14	116.45	112.19
3	N	1	GLC	C3-C4-C5	3.05	115.68	110.24
3	I	1	GLC	C1-O5-C5	-2.94	108.21	112.19
3	L	1	GLC	O5-C5-C6	2.84	111.66	107.20
3	J	1	GLC	C6-C5-C4	2.65	119.20	113.00
3	I	1	GLC	O5-C5-C6	2.64	111.34	107.20
3	M	1	GLC	C2-C3-C4	2.62	115.43	110.89
3	K	2	FRU	O3-C3-C4	2.49	121.93	113.32
3	J	1	GLC	O5-C1-C2	2.42	114.50	110.77
3	P	1	GLC	O5-C1-C2	2.21	114.18	110.77
3	K	1	GLC	O5-C5-C6	2.15	110.57	107.20
3	O	1	GLC	C1-O5-C5	-2.10	109.34	112.19
3	I	1	GLC	C3-C4-C5	2.09	113.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1	GLC	O5-C1-C2	2.03	113.90	110.77
3	J	1	GLC	C1-C2-C3	2.03	112.16	109.67

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	1	GLC	C2
3	I	1	GLC	C3
3	I	2	FRU	C5
3	I	2	FRU	C4
3	J	1	GLC	C5
3	J	1	GLC	C2
3	J	1	GLC	C3
3	J	2	FRU	C5
3	J	2	FRU	C4
3	K	1	GLC	C2
3	K	1	GLC	C3
3	K	2	FRU	C5
3	K	2	FRU	C4
3	L	1	GLC	C2
3	L	1	GLC	C3
3	L	2	FRU	C5
3	L	2	FRU	C4
3	M	1	GLC	C2
3	M	1	GLC	C3
3	M	2	FRU	C5
3	M	2	FRU	C4
3	N	1	GLC	C2
3	N	1	GLC	C4
3	N	1	GLC	C3
3	N	2	FRU	C5
3	N	2	FRU	C4
3	O	1	GLC	C2
3	O	1	GLC	C3
3	O	2	FRU	C5
3	O	2	FRU	C4
3	P	1	GLC	C2
3	P	1	GLC	C4
3	P	1	GLC	C3
3	P	2	FRU	C5
3	P	2	FRU	C4

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	2	FRU	O1-C1-C2-C3
3	O	2	FRU	O1-C1-C2-O2
3	L	2	FRU	O5-C5-C6-O6
3	I	2	FRU	C4-C5-C6-O6
3	K	2	FRU	C4-C5-C6-O6
3	M	2	FRU	C4-C5-C6-O6
3	N	2	FRU	C4-C5-C6-O6
3	O	2	FRU	C4-C5-C6-O6
3	M	1	GLC	O5-C5-C6-O6
3	J	2	FRU	O5-C5-C6-O6
3	N	2	FRU	O5-C5-C6-O6
3	O	2	FRU	O5-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
3	I	2	FRU	O5-C5-C6-O6
3	P	2	FRU	O5-C5-C6-O6
3	M	2	FRU	O5-C5-C6-O6
3	O	2	FRU	O1-C1-C2-O5
3	J	2	FRU	C4-C5-C6-O6
3	K	2	FRU	O5-C5-C6-O6
3	K	1	GLC	O5-C5-C6-O6
3	L	2	FRU	C4-C5-C6-O6
3	M	2	FRU	O1-C1-C2-C3
3	I	2	FRU	O1-C1-C2-C3
3	K	2	FRU	O1-C1-C2-C3
3	L	2	FRU	O1-C1-C2-C3
3	P	2	FRU	O1-C1-C2-C3

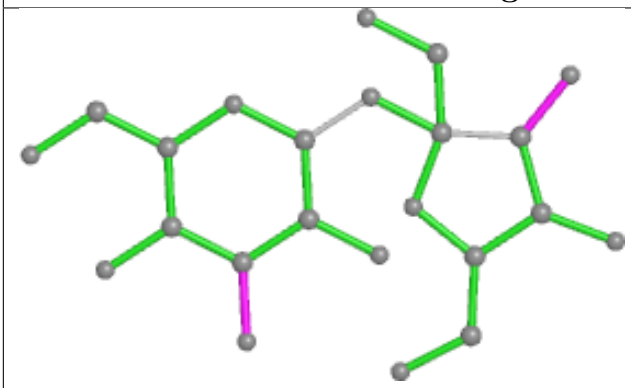
There are no ring outliers.

6 monomers are involved in 15 short contacts:

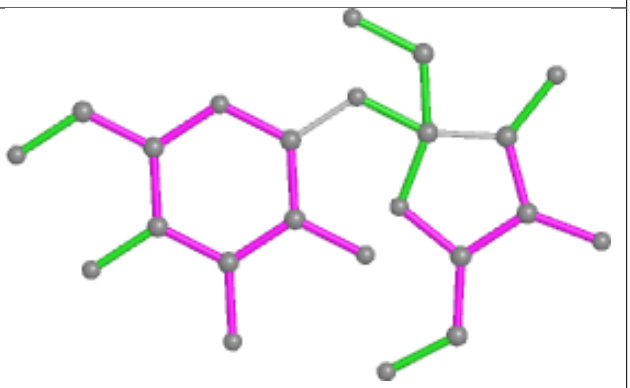
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	GLC	1	0
3	N	1	GLC	5	0
3	M	2	FRU	2	0
3	J	1	GLC	3	0
3	N	2	FRU	1	0
3	P	1	GLC	4	0

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

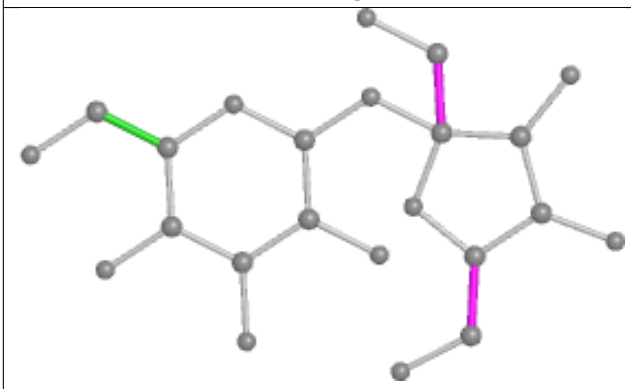
Oligosaccharide Chain I



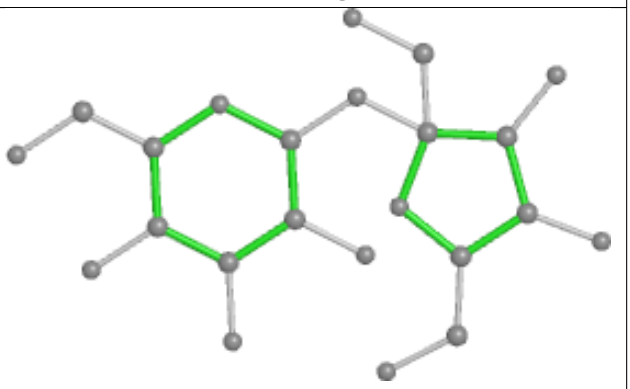
Bond lengths



Bond angles

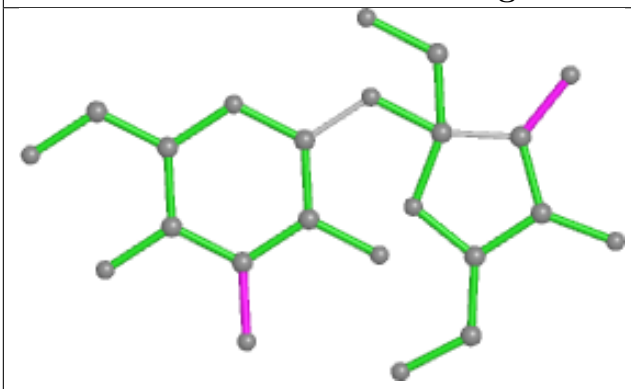


Torsions

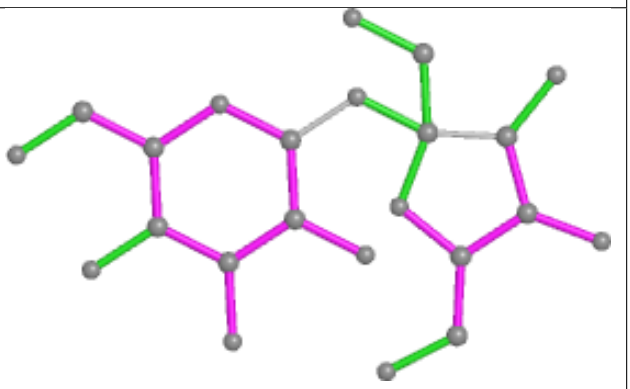


Rings

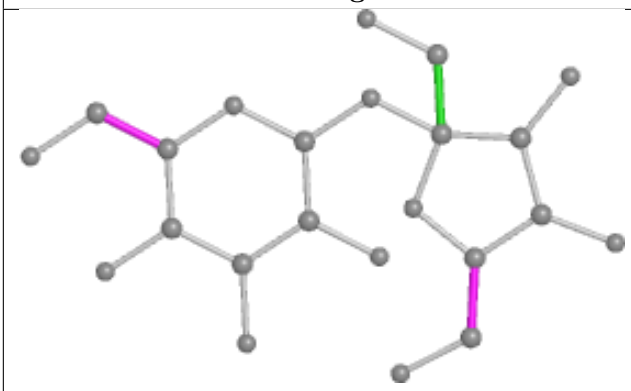
Oligosaccharide Chain J



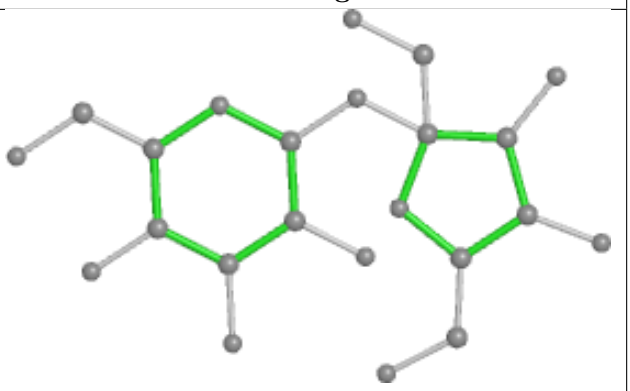
Bond lengths



Bond angles

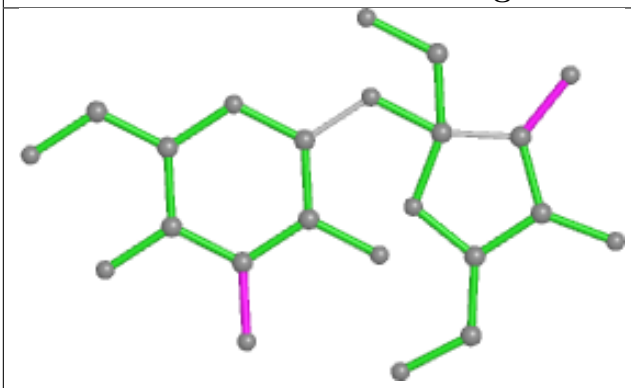


Torsions

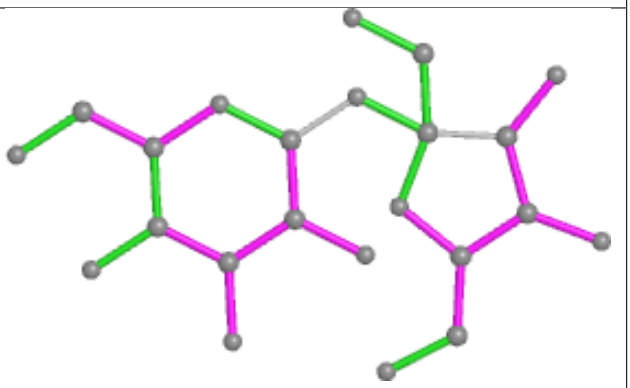


Rings

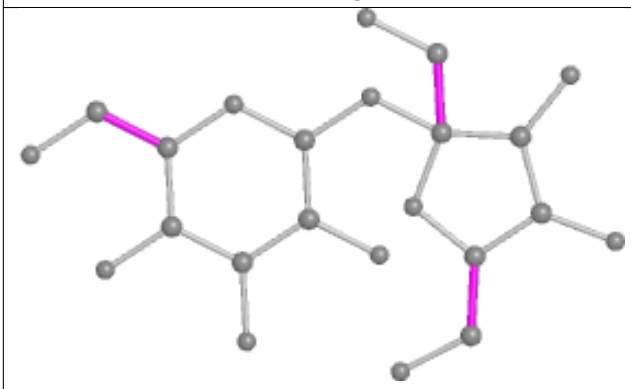
Oligosaccharide Chain K



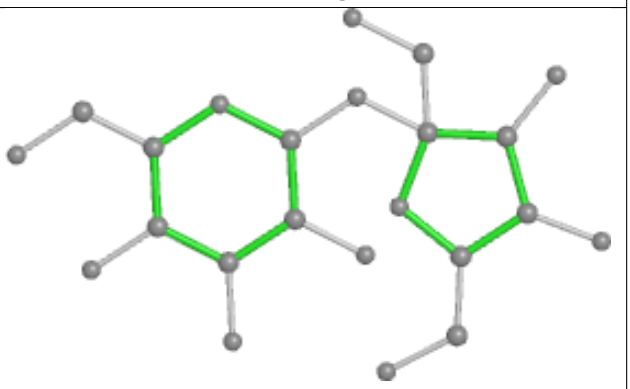
Bond lengths



Bond angles

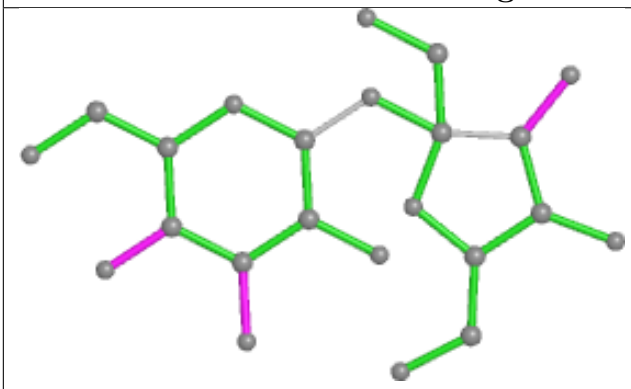


Torsions

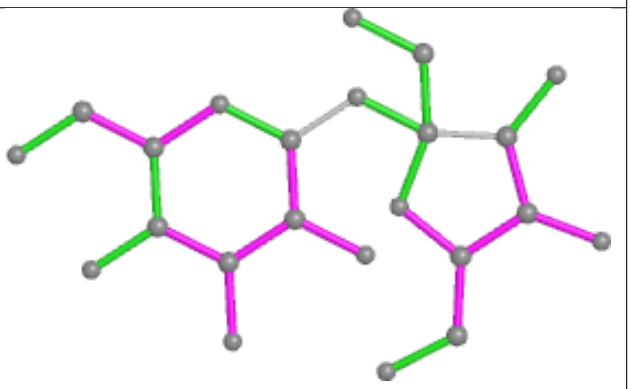


Rings

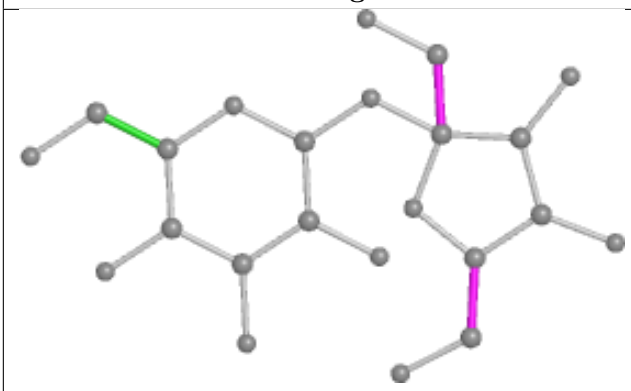
Oligosaccharide Chain L



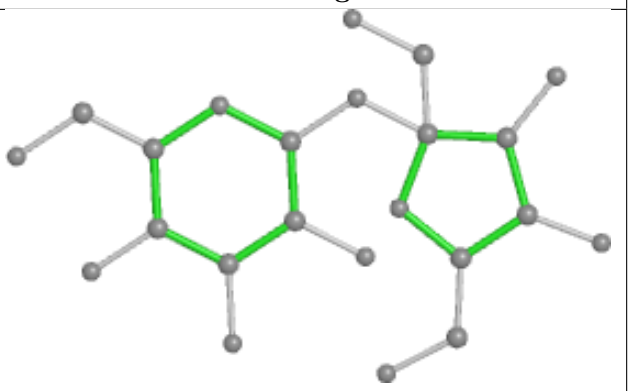
Bond lengths



Bond angles

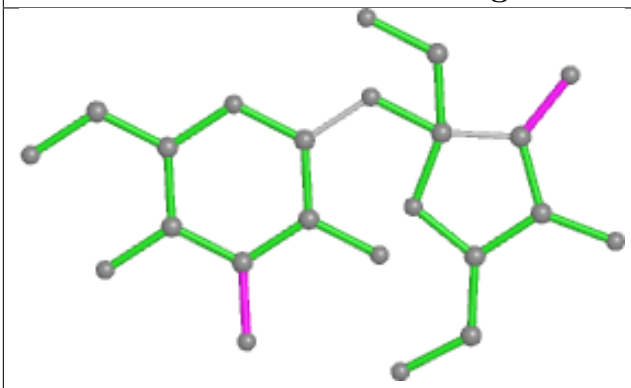


Torsions

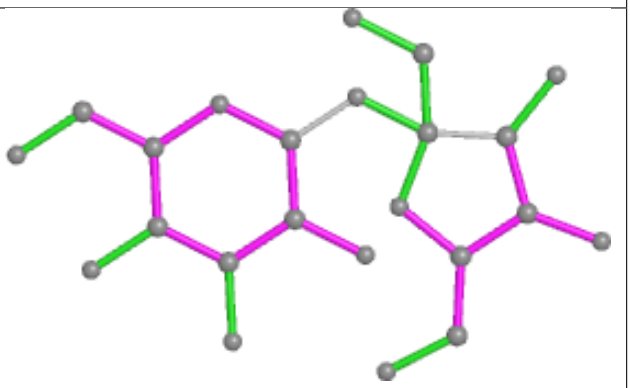


Rings

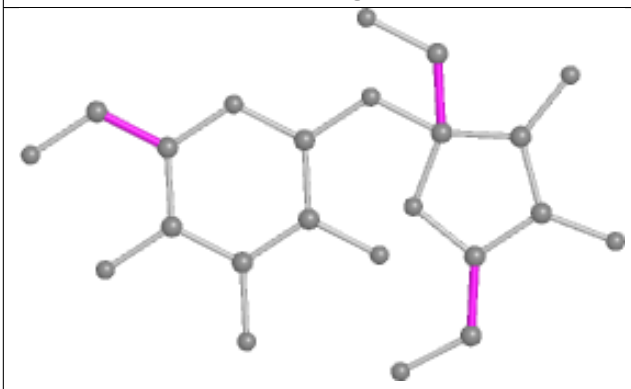
Oligosaccharide Chain M



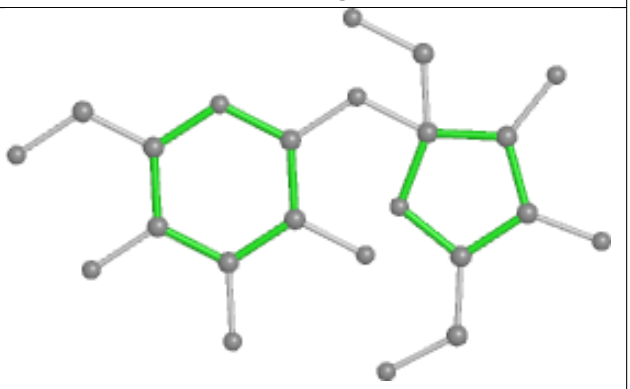
Bond lengths



Bond angles

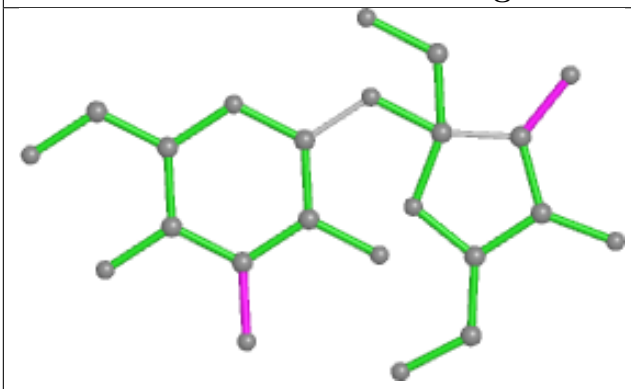


Torsions

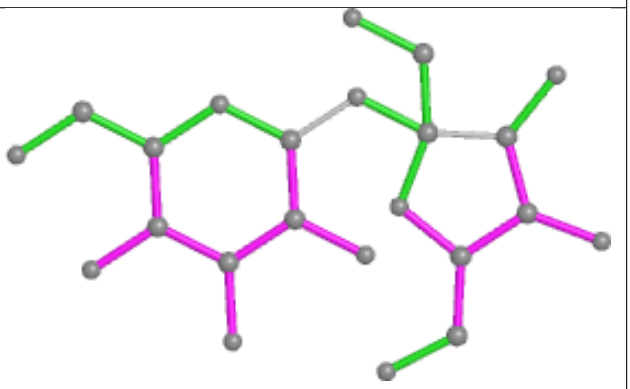


Rings

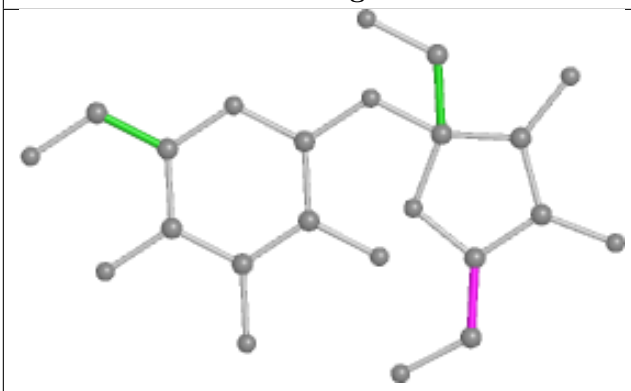
Oligosaccharide Chain N



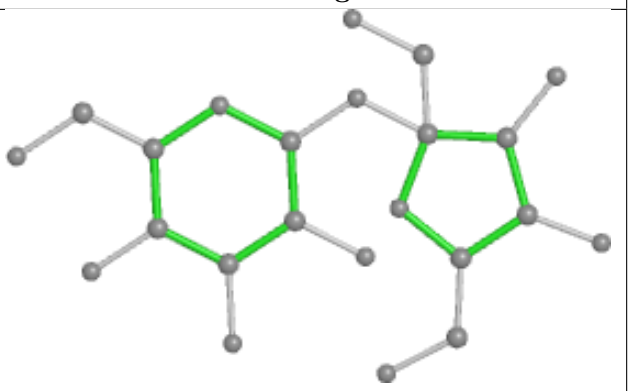
Bond lengths



Bond angles

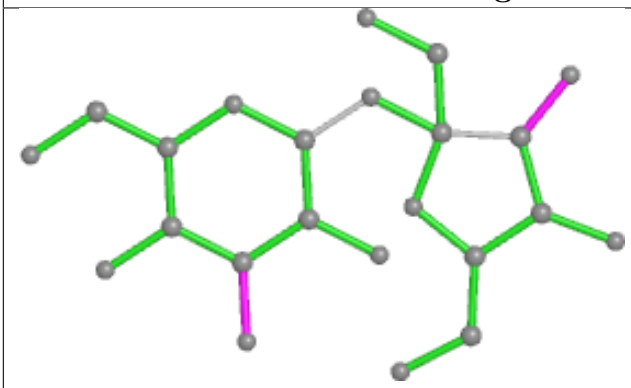


Torsions

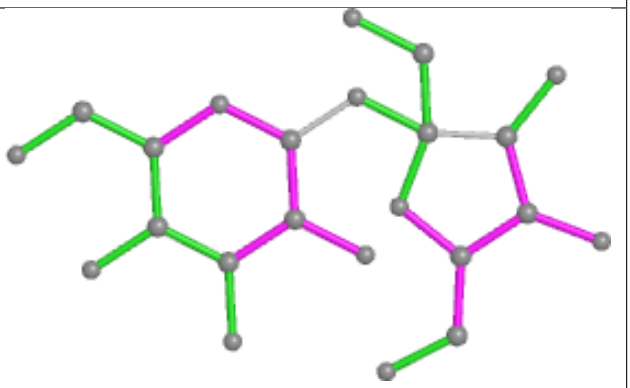


Rings

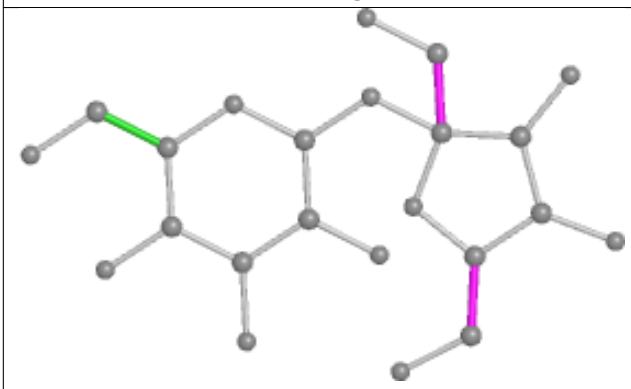
Oligosaccharide Chain O



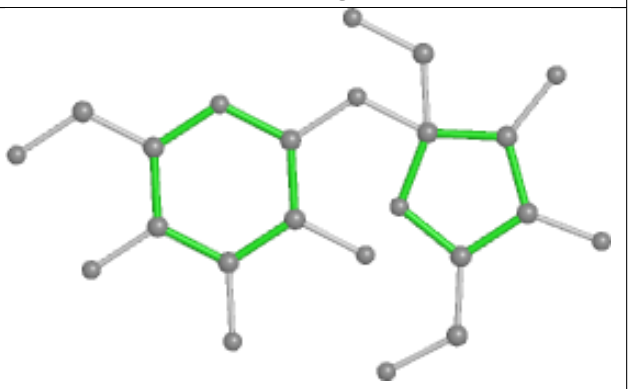
Bond lengths



Bond angles

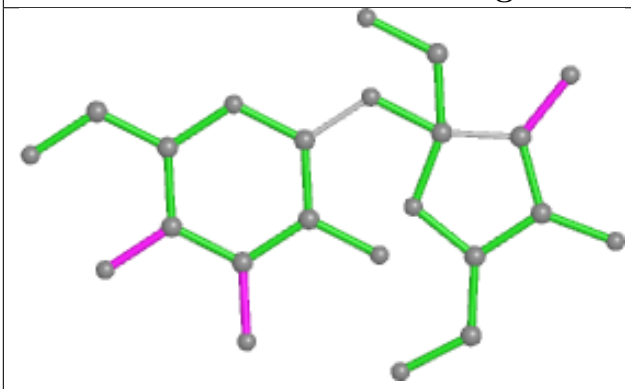


Torsions

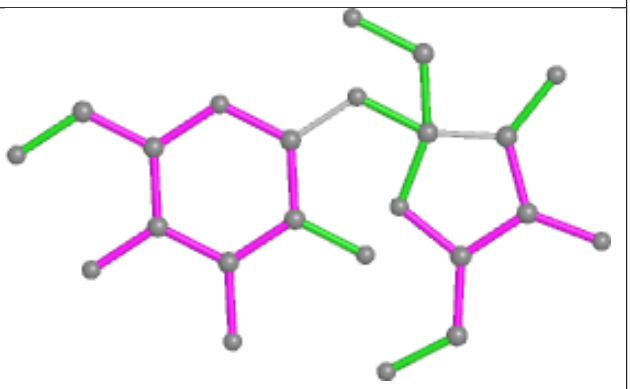


Rings

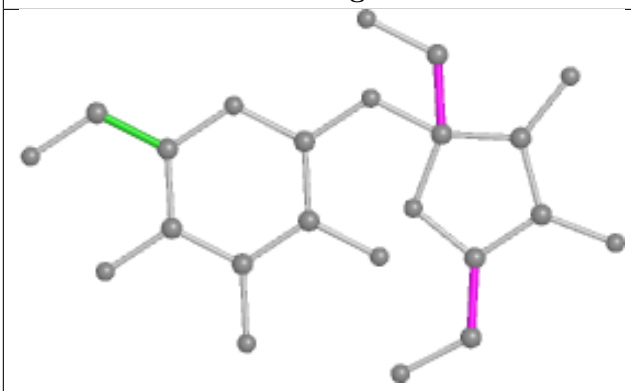
Oligosaccharide Chain P



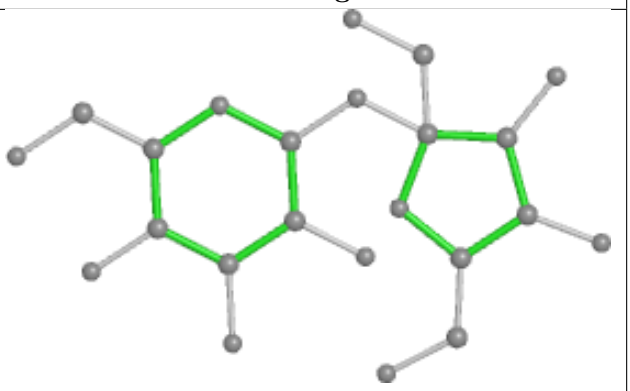
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	322/327 (98%)	0.16	5 (1%)	72	79	53, 74, 117, 180	0
1	B	319/327 (97%)	0.33	17 (5%)	26	31	54, 88, 139, 197	0
1	C	322/327 (98%)	0.17	5 (1%)	72	79	48, 70, 108, 191	0
1	D	327/327 (100%)	0.17	2 (0%)	89	92	52, 81, 127, 185	0
2	E	419/457 (91%)	0.47	34 (8%)	12	14	62, 110, 160, 200	0
2	F	419/457 (91%)	0.86	72 (17%)	1	1	59, 107, 173, 214	0
2	G	420/457 (91%)	0.47	24 (5%)	23	28	68, 111, 159, 201	0
2	H	419/457 (91%)	0.41	17 (4%)	37	44	62, 105, 166, 205	0
All	All	2967/3136 (94%)	0.40	176 (5%)	22	27	48, 96, 157, 214	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	900	LEU	10.4
2	F	906	PHE	9.7
2	F	835	LEU	7.5
2	F	897	TYR	7.1
2	F	868	VAL	6.6
2	F	899	ASP	6.2
2	F	834	VAL	5.8
2	F	757	LYS	5.8
2	F	893	LEU	5.5
2	F	886	GLN	5.2
2	F	832	LEU	5.2
2	F	887	LEU	5.0
2	E	1062	ALA	4.9
2	G	1065	GLU	4.9
2	F	909	VAL	4.8
2	F	1065	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	890	LEU	4.6
2	F	880	GLN	4.5
2	E	868	VAL	4.4
2	F	1059	PHE	4.3
2	F	913	VAL	4.3
2	F	760	VAL	4.2
2	F	889	MET	4.2
2	G	864	VAL	4.2
2	E	1073	MET	4.1
2	F	891	SER	4.1
1	B	200	TYR	4.0
2	F	910	MET	4.0
1	C	200	TYR	4.0
2	F	833	LYS	3.9
2	F	794	LEU	3.9
2	H	1177	ASP	3.9
2	F	895	GLU	3.9
2	E	869	LEU	3.8
2	F	805	GLN	3.8
2	H	897	TYR	3.8
2	E	917	ARG	3.8
2	F	905	GLN	3.8
2	F	896	GLU	3.7
2	F	773	GLU	3.7
2	F	888	LYS	3.7
2	F	830	LYS	3.7
2	F	1068	LYS	3.7
2	F	881	MET	3.6
2	F	882	PRO	3.6
2	F	831	GLU	3.6
2	E	1069	PHE	3.6
2	E	1077	VAL	3.6
2	H	1175	GLU	3.6
2	F	902	GLU	3.5
2	F	774	ASP	3.4
2	G	866	GLU	3.4
2	F	1175	GLU	3.4
2	G	1073	MET	3.3
1	C	195	GLU	3.3
2	H	893	LEU	3.3
2	H	794	LEU	3.3
2	G	1076	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	773	GLU	3.2
2	E	980	PHE	3.2
2	F	1056	VAL	3.2
2	F	892	GLU	3.2
2	E	1076	PHE	3.1
2	E	774	ASP	3.1
2	G	774	ASP	3.1
2	F	894	LYS	3.0
2	E	1080	ALA	3.0
2	E	759	GLU	3.0
2	G	1059	PHE	3.0
2	E	1063	THR	3.0
1	A	197	SER	3.0
2	G	792	ASN	3.0
2	E	936	ILE	3.0
2	E	861	ILE	2.9
2	F	1066	LYS	2.9
2	G	869	LEU	2.8
2	E	940	ILE	2.8
2	E	805	GLN	2.8
2	H	762	LEU	2.8
2	E	1040	LYS	2.8
2	G	1062	ALA	2.8
1	A	200	TYR	2.8
2	F	837	SER	2.8
2	G	1077	VAL	2.8
2	F	854	TYR	2.7
2	F	884	PRO	2.7
1	B	151	HIS	2.7
2	F	789	PHE	2.7
2	H	900	LEU	2.7
1	B	143	LEU	2.7
2	F	850	PHE	2.7
2	G	805	GLN	2.7
2	E	1047	LYS	2.7
2	G	1172	MET	2.7
2	F	756	TYR	2.7
2	H	896	GLU	2.7
2	H	1146	ARG	2.7
1	B	171	VAL	2.7
2	H	835	LEU	2.7
2	H	797	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	204	ASN	2.6
2	H	890	LEU	2.6
1	C	197	SER	2.6
2	F	867	ALA	2.6
2	E	893	LEU	2.6
1	B	192	GLU	2.6
1	B	147	LEU	2.6
2	F	898	ASP	2.5
2	H	800	LEU	2.5
1	B	134	ARG	2.5
2	F	916	LEU	2.5
2	G	926	LYS	2.5
2	F	869	LEU	2.5
2	G	969	TYR	2.5
2	E	1039	GLN	2.5
2	G	829	VAL	2.5
1	B	166	ASN	2.4
2	E	857	ILE	2.4
2	F	878	ILE	2.4
2	F	885	GLU	2.4
2	E	864	VAL	2.4
2	H	760	VAL	2.4
2	F	785	LYS	2.4
1	B	234	LEU	2.4
2	G	863	GLU	2.4
2	F	927	LEU	2.3
1	B	186	LEU	2.3
2	F	877	LEU	2.3
2	G	1070	VAL	2.3
2	E	894	LYS	2.3
2	G	894	LYS	2.3
2	F	863	GLU	2.3
1	B	163	LEU	2.3
1	B	156	LEU	2.3
2	E	915	ARG	2.3
2	H	774	ASP	2.3
2	G	1068	LYS	2.3
1	D	199	ASN	2.3
1	C	196	THR	2.3
1	B	215	PHE	2.3
2	F	1177	ASP	2.3
2	E	920	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	849	SER	2.3
2	H	756	TYR	2.3
1	D	200	TYR	2.2
2	F	969	TYR	2.2
2	F	912	THR	2.2
2	F	860	VAL	2.2
2	F	883	GLU	2.2
2	G	1042	LEU	2.2
2	G	1072	LYS	2.2
2	F	771	VAL	2.2
2	E	1050	ALA	2.2
1	A	196	THR	2.2
2	F	846	PHE	2.2
2	E	906	PHE	2.2
1	B	185	ILE	2.1
2	E	1059	PHE	2.1
2	G	1069	PHE	2.1
2	F	845	ILE	2.1
2	F	1110	LYS	2.1
2	F	1069	PHE	2.1
1	B	177	GLU	2.1
1	B	182	LEU	2.1
2	E	1060	PRO	2.1
1	C	199	ASN	2.1
2	E	776	SER	2.1
1	A	198	GLY	2.1
2	E	929	PHE	2.1
1	A	194	GLU	2.0
2	F	797	LYS	2.0
2	F	802	PHE	2.0
2	G	1066	LYS	2.0
2	E	962	LEU	2.0
2	E	1078	LYS	2.0
2	F	855	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

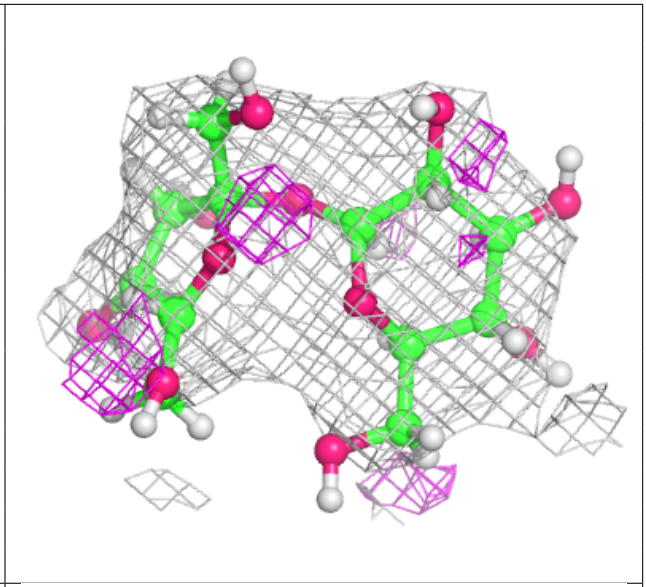
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

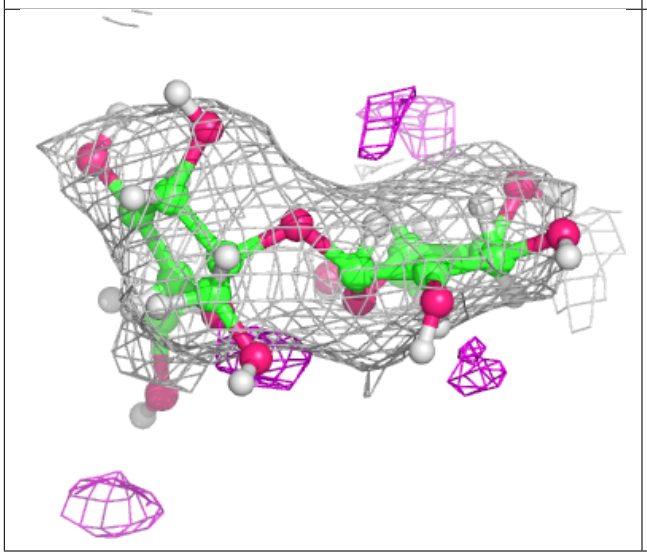
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FRU	N	2	12/12	0.78	0.30	186,223,266,269	0
3	FRU	M	2	12/12	0.82	0.24	173,193,232,251	0
3	GLC	P	1	11/12	0.86	0.27	173,199,226,239	0
3	GLC	L	1	11/12	0.87	0.24	179,215,252,273	0
3	FRU	K	2	12/12	0.87	0.22	147,171,192,198	0
3	GLC	I	1	11/12	0.88	0.20	162,181,212,217	0
3	GLC	N	1	11/12	0.89	0.30	185,217,256,261	0
3	GLC	M	1	11/12	0.89	0.18	173,194,218,225	0
3	GLC	O	1	11/12	0.89	0.20	153,178,205,214	0
3	FRU	O	2	12/12	0.89	0.21	153,176,208,211	0
3	FRU	J	2	12/12	0.89	0.24	181,204,244,254	0
3	FRU	P	2	12/12	0.90	0.24	173,208,265,286	0
3	FRU	I	2	12/12	0.91	0.19	162,187,204,207	0
3	FRU	L	2	12/12	0.91	0.21	179,215,269,298	0
3	GLC	J	1	11/12	0.92	0.30	181,197,229,237	0
3	GLC	K	1	11/12	0.93	0.15	147,167,190,200	0

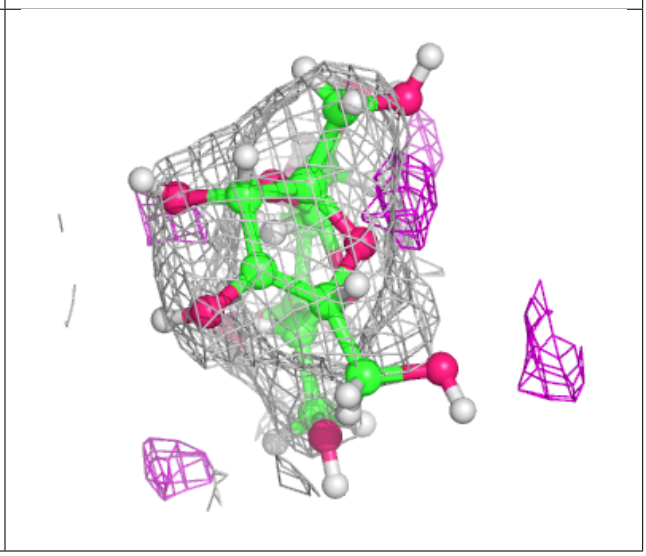
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

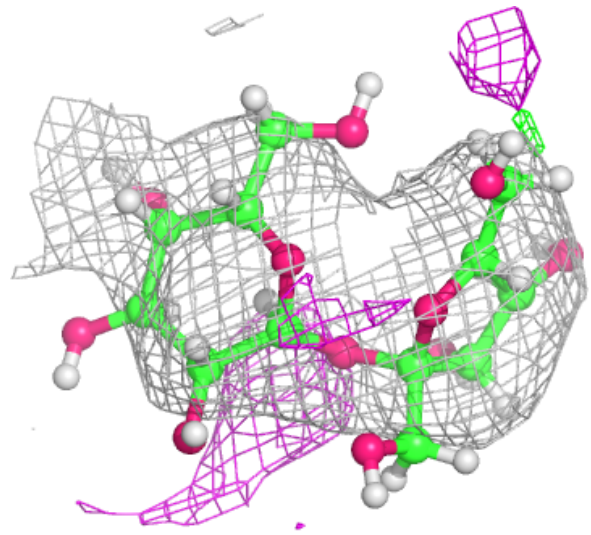


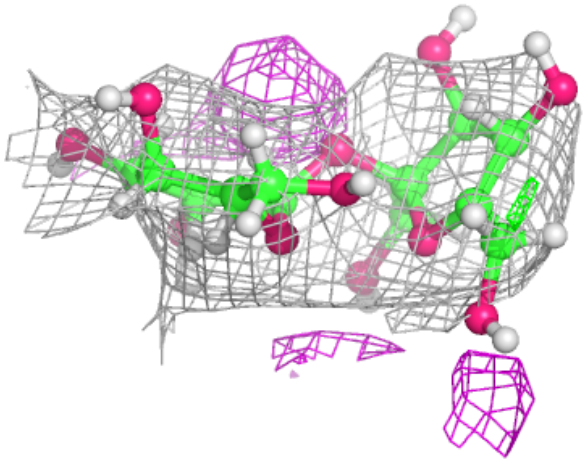


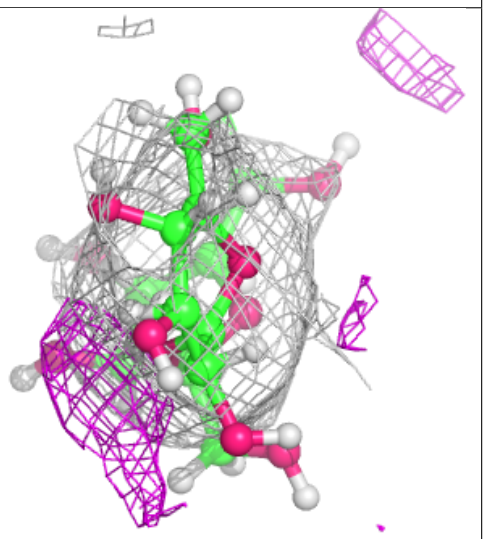


Electron density around Chain J:

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

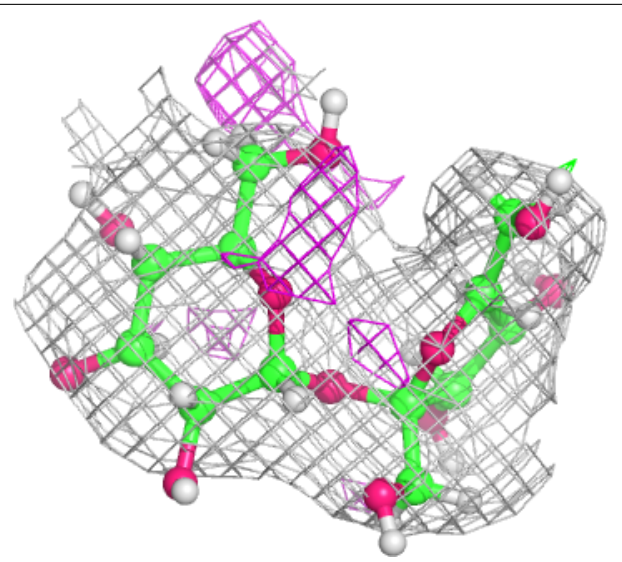


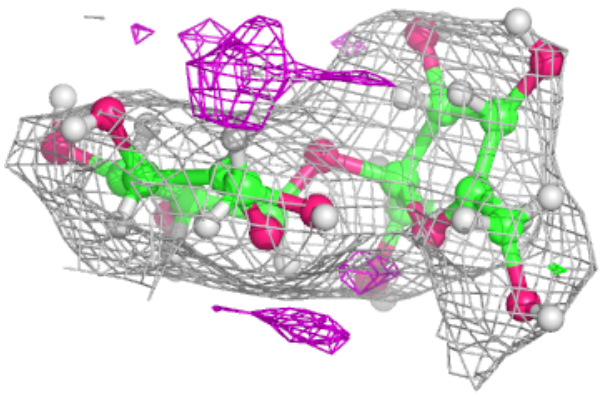


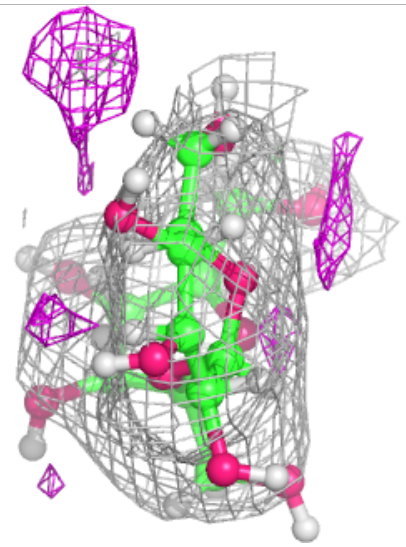


Electron density around Chain K:

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

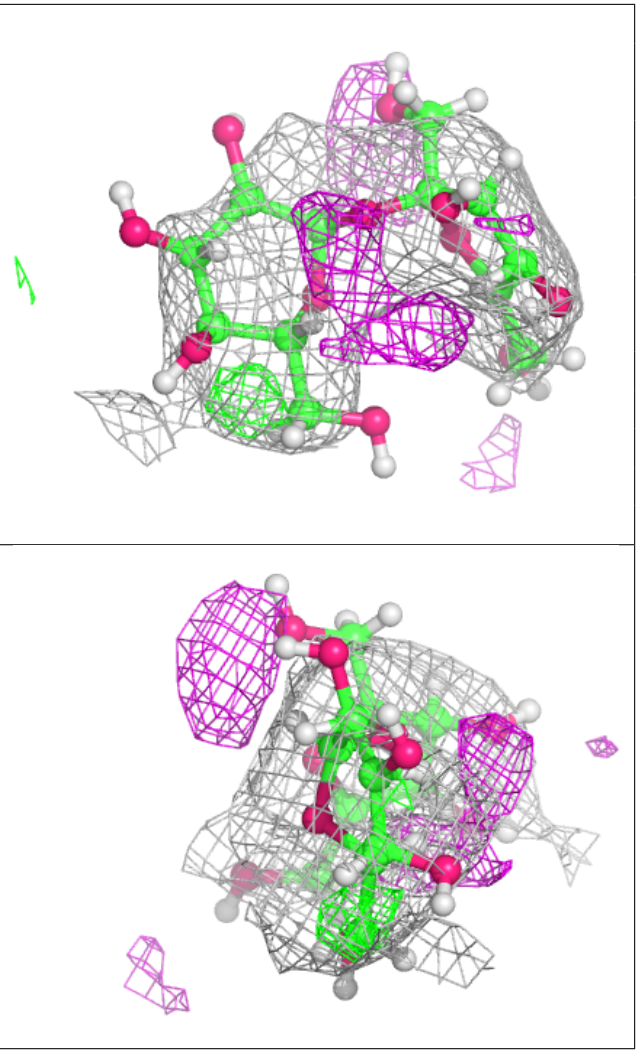






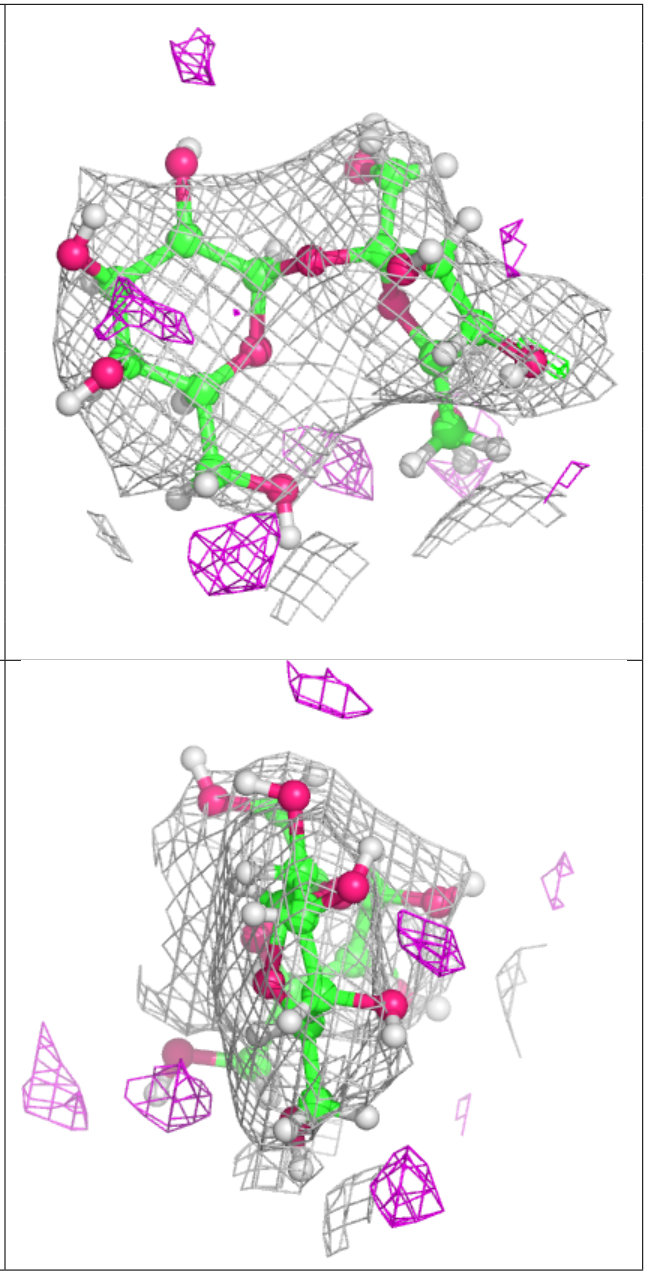
Electron density around Chain L:

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



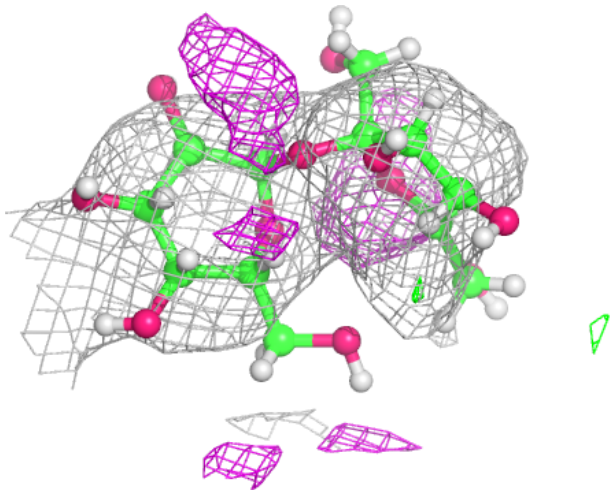
Electron density around Chain M:

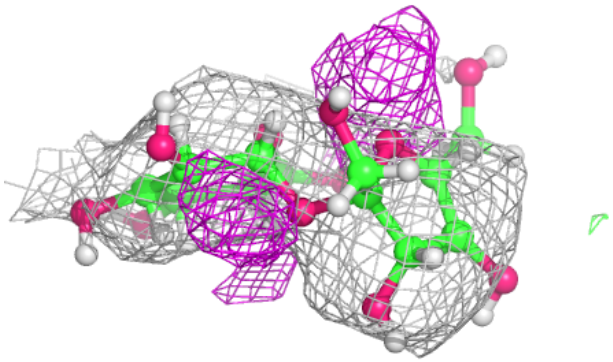
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

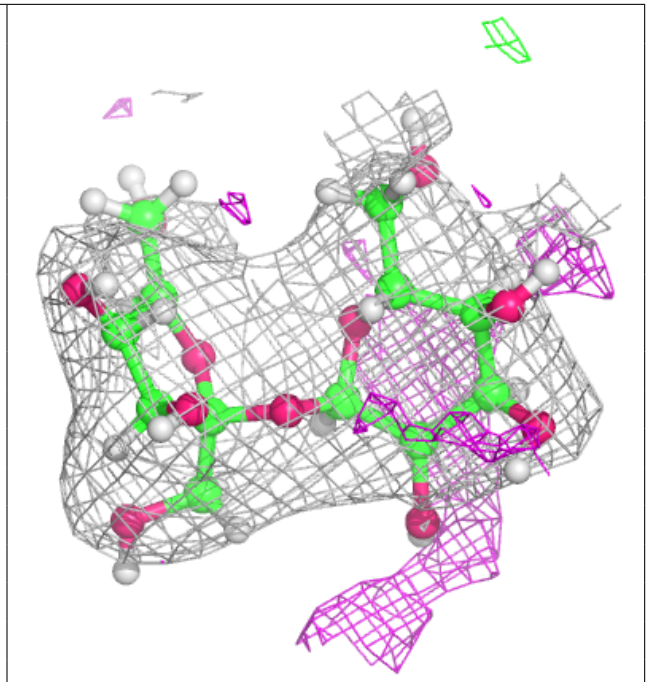
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

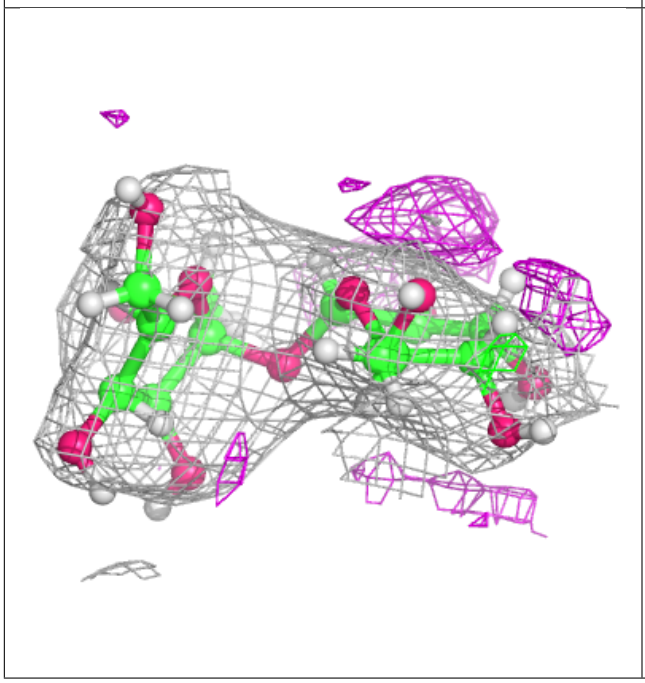


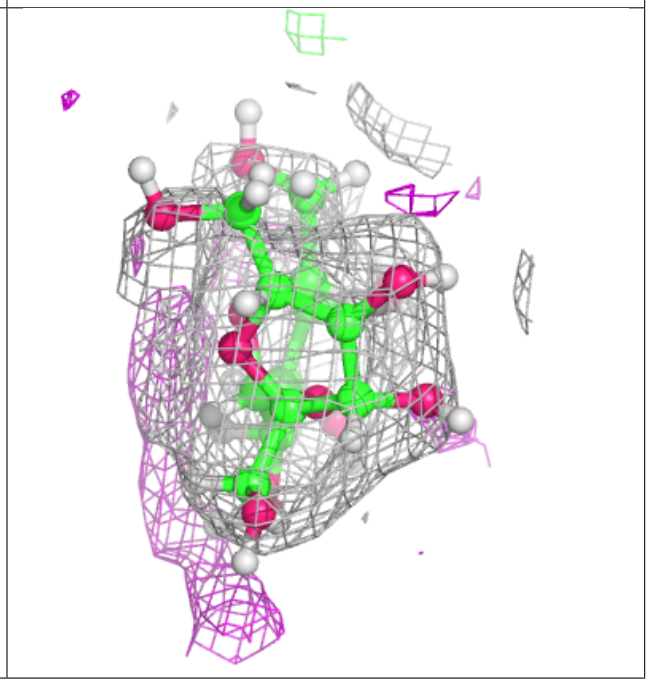


Electron density around Chain O:

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

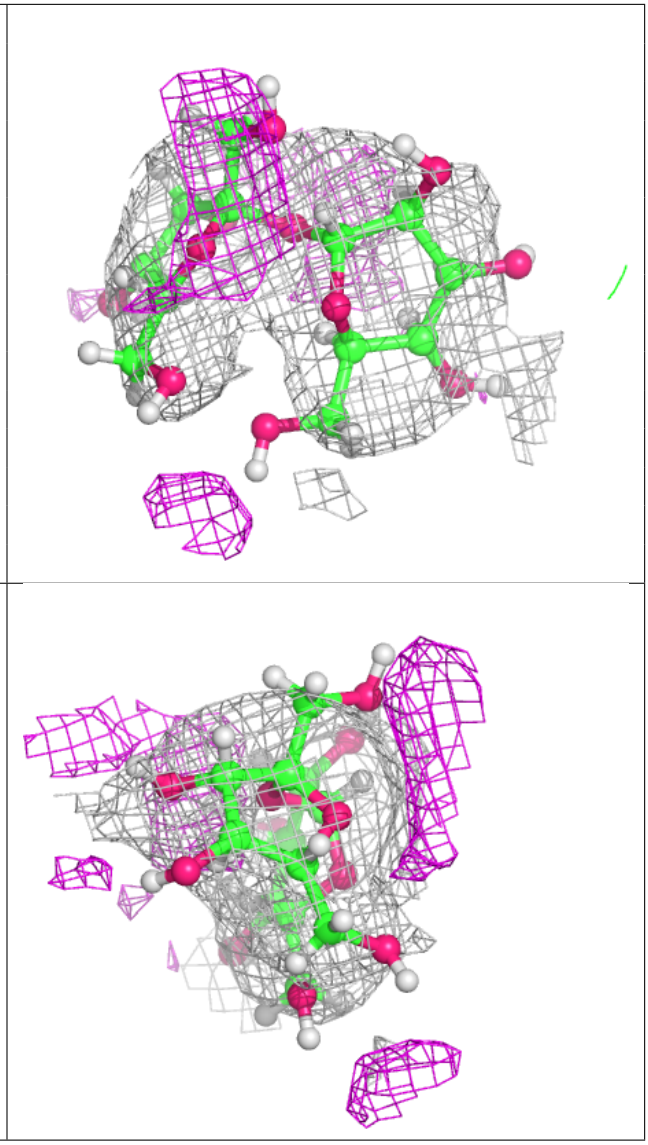






Electron density around Chain P:

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



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.