Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:15 AM JST

PDB ID	:	7EKX
Title	:	Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (W470A E564Q) in complex with maltononaose
Authors	:	Shen, M.; Xiang, S.
Deposited on	:	2021-04-07
Resolution	:	3.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

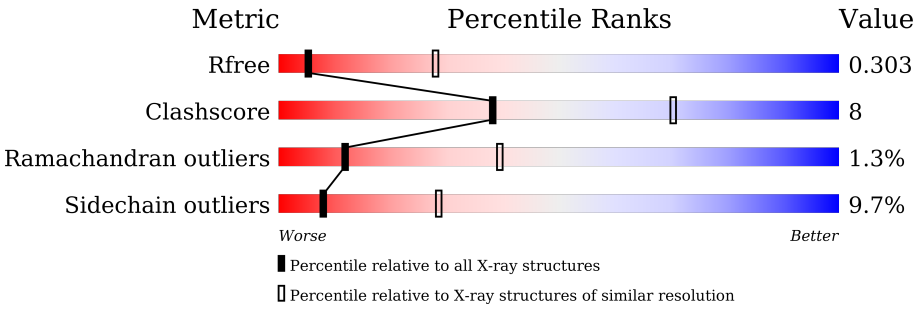
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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%

Mol	Chain	Length	Quality of chain
1	A	1536	74% 23%
1	B	1536	73% 23%
2	C	3	100%
3	D	2	50% 50%
4	E	5	60% 40%
5	F	7	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24729 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.

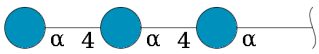
- Molecule 1 is a protein called 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12269	7822	2065	2330	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12269	7822	2065	2330	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ALA	TRP	engineered mutation	UNP Q6FSK0
A	564	GLN	GLU	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-	expression tag	UNP Q6FSK0
A	1535	HIS	-	expression tag	UNP Q6FSK0
A	1536	HIS	-	expression tag	UNP Q6FSK0
B	470	ALA	TRP	engineered mutation	UNP Q6FSK0
B	564	GLN	GLU	engineered mutation	UNP Q6FSK0
B	1529	LEU	-	expression tag	UNP Q6FSK0
B	1530	GLU	-	expression tag	UNP Q6FSK0
B	1531	HIS	-	expression tag	UNP Q6FSK0
B	1532	HIS	-	expression tag	UNP Q6FSK0
B	1533	HIS	-	expression tag	UNP Q6FSK0
B	1534	HIS	-	expression tag	UNP Q6FSK0
B	1535	HIS	-	expression tag	UNP Q6FSK0
B	1536	HIS	-	expression tag	UNP Q6FSK0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

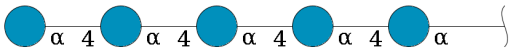


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	3	Total C O 34 18 16	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

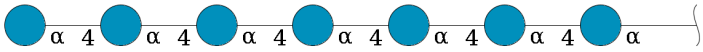
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C O 23 12 11	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	5	Total C O 56 30 26	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



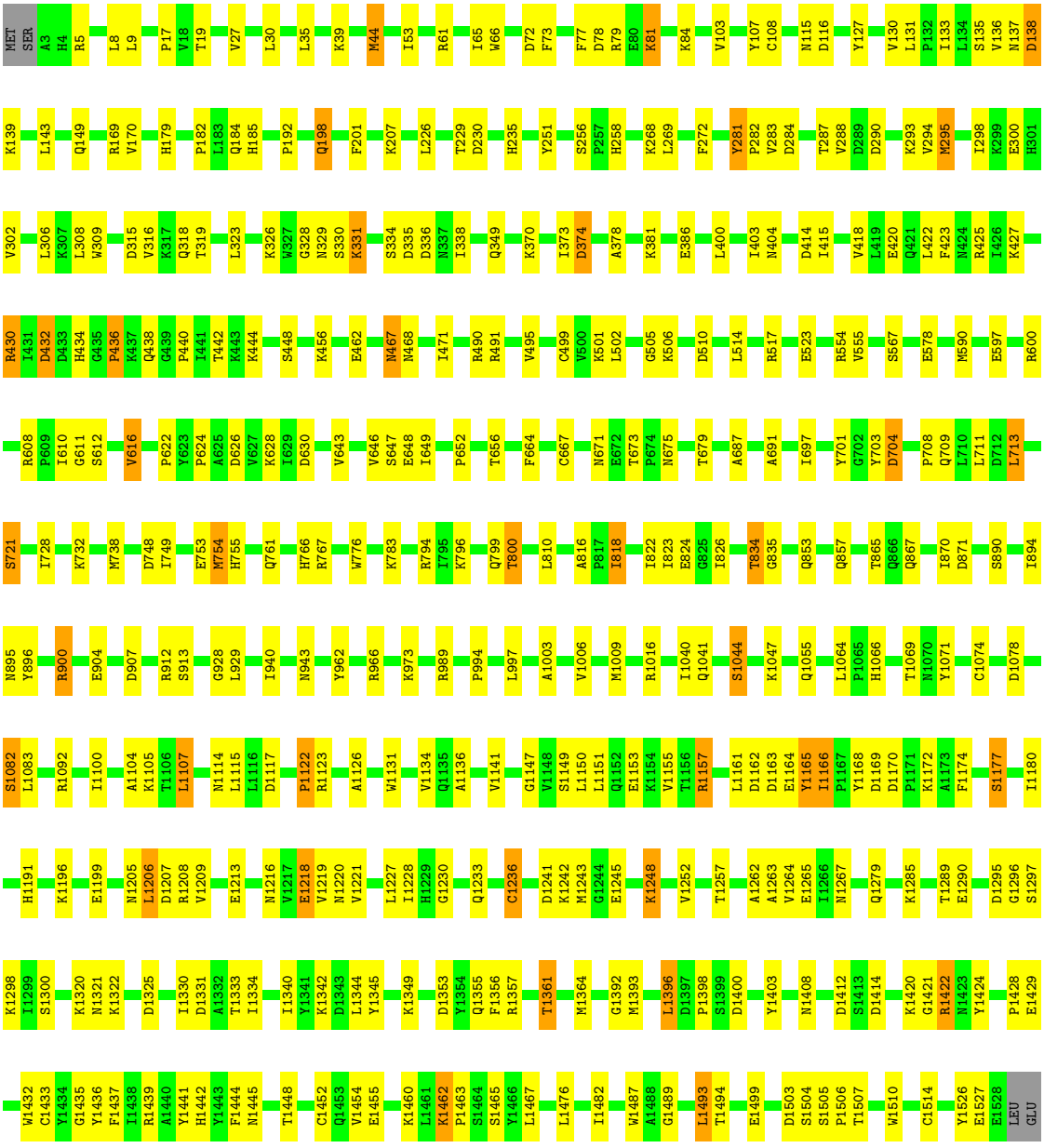
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	7	Total C O 78 42 36	0	0	0

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. 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. 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.

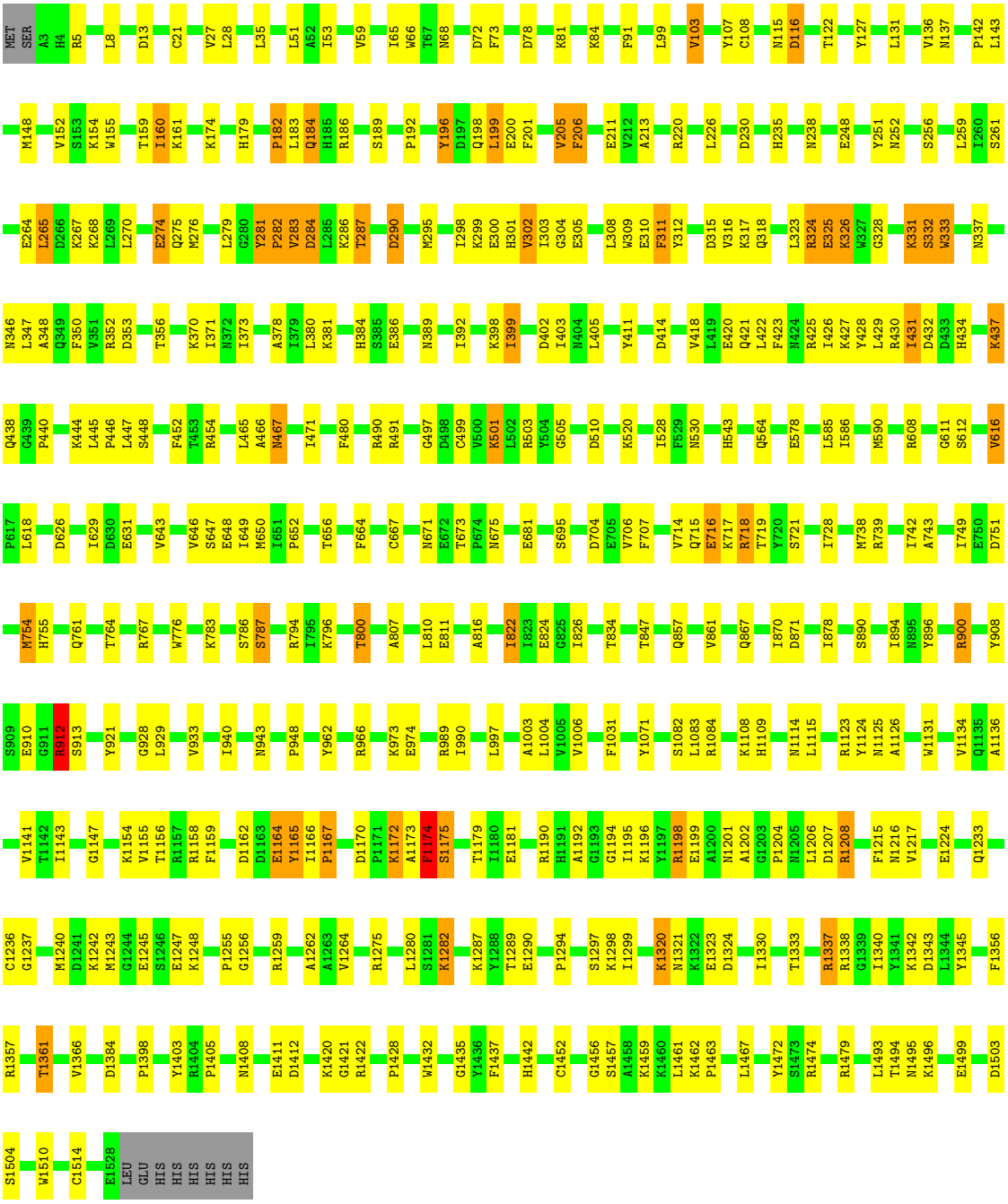
- Molecule 1: 4-alpha-glucanotransferase

Chain A:



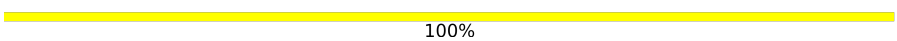
• Molecule 1: 4-alpha-glucanotransferase

Chain B:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

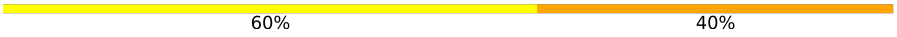


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

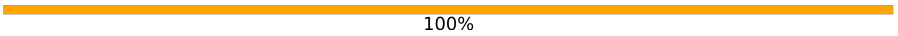
• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:



• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	160.65Å 206.28Å 258.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.15 – 3.40 46.15 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.15-3.40) 99.6 (46.15-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.272 , 0.303 0.272 , 0.303	Depositor DCC
R_{free} test set	2929 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	98.4	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 25.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	24729	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: GLC

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	0.24	0/12578	0.40	0/17055
1	B	0.24	0/12578	0.41	1/17055 (0.0%)
All	All	0.24	0/25156	0.40	1/34110 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	912	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	12269	0	11957	174	0
1	B	12269	0	11957	193	3
2	C	34	0	30	0	0
3	D	23	0	21	0	0
4	E	56	0	48	5	3
5	F	78	0	66	7	0
All	All	24729	0	24079	371	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (371) 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:B:268:LYS:HE2	1:B:305:GLU:HB3	1.58	0.85
1:B:816:ALA:HB2	1:B:826:ILE:HG13	1.61	0.81
1:B:1207:ASP:HA	5:F:5:GLC:H2	1.63	0.80
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.64	0.80
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.65	0.78
1:A:1248:LYS:HE2	1:A:1412:ASP:HB2	1.65	0.78
1:B:1123:ARG:HH22	1:B:1207:ASP:HB2	1.47	0.77
4:E:4:GLC:O3	4:E:5:GLC:O2	2.03	0.77
1:A:794:ARG:HD2	1:A:796:LYS:HE2	1.67	0.77
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.68	0.76
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.68	0.76
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.69	0.74
1:A:78:ASP:HB3	1:A:81:LYS:HB2	1.70	0.74
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.70	0.73
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.70	0.73
1:B:380:LEU:HB3	1:B:392:ILE:HD12	1.69	0.72
1:A:268:LYS:HG3	1:A:302:VAL:HG12	1.72	0.72
1:A:1123:ARG:HH21	4:E:4:GLC:H62	1.56	0.70
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.23	0.69
1:B:1208:ARG:HH21	5:F:6:GLC:H2	1.57	0.69
1:A:198:GLN:HG2	1:A:517:ARG:HH21	1.57	0.68
1:B:325:GLU:HG2	1:B:326:LYS:HG2	1.73	0.68
1:B:1384:ASP:OD1	1:B:1474:ARG:NH1	2.25	0.68
1:A:1245:GLU:HG3	1:A:1420:LYS:HB3	1.75	0.68
1:A:1083:LEU:HD22	1:A:1136:ALA:HB1	1.75	0.68
1:A:1196:LYS:HD2	1:A:1218:GLU:HG2	1.74	0.68
1:B:1240:MET:HE1	1:B:1357:ARG:HD3	1.74	0.68
1:A:816:ALA:HB2	1:A:826:ILE:HG13	1.77	0.67
1:A:1342:LYS:HE2	1:A:1353:ASP:HB3	1.77	0.67
1:A:766:HIS:HE1	1:A:865:THR:HG21	1.61	0.66
1:B:1115:LEU:HB3	1:B:1123:ARG:HB3	1.78	0.65
1:A:374:ASP:OD1	1:A:374:ASP:N	2.21	0.65
1:A:169:ARG:NH1	1:A:721:SER:O	2.29	0.64
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.78	0.64
1:B:647:SER:OG	1:B:648:GLU:N	2.31	0.64
1:A:430:ARG:HB3	1:A:438:GLN:HG3	1.80	0.64
1:B:184:GLN:HA	1:B:201:PHE:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.80	0.63
1:B:220:ARG:NH1	1:B:530:ASN:OD1	2.33	0.62
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.82	0.62
1:B:1154:LYS:HG2	1:B:1179:THR:HG22	1.82	0.62
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.80	0.62
1:B:1452:CYS:HB3	1:B:1467:LEU:HB2	1.82	0.62
1:B:186:ARG:HG2	1:B:192:PRO:HA	1.81	0.61
1:B:452:PHE:HA	1:B:466:ALA:HA	1.81	0.61
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.66	0.61
1:B:466:ALA:H	1:B:501:LYS:HD2	1.66	0.61
1:A:323:LEU:HD23	1:A:373:ILE:HG23	1.82	0.60
1:B:629:ILE:HG22	1:B:649:ILE:HA	1.82	0.60
1:A:691:ALA:HA	1:A:697:ILE:HG21	1.84	0.60
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.84	0.60
1:B:1248:LYS:HG3	1:B:1412:ASP:HB2	1.84	0.59
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	1.83	0.59
1:A:251:TYR:CE1	1:A:501:LYS:HG3	2.37	0.59
1:B:287:THR:HB	1:B:290:ASP:HB3	1.84	0.59
1:A:1331:ASP:OD1	1:A:1333:THR:OG1	2.19	0.59
1:A:136:VAL:HG13	1:A:137:ASN:H	1.68	0.59
1:B:612:SER:OG	1:B:943:ASN:ND2	2.36	0.59
1:B:1405:PRO:HB2	1:B:1496:LYS:HB2	1.85	0.58
1:A:673:THR:HG22	1:A:675:ASN:H	1.69	0.58
1:B:616:VAL:HA	1:B:646:VAL:HG11	1.84	0.58
1:B:328:GLY:H	1:B:331:LYS:HE2	1.68	0.57
1:A:1436:TYR:HE1	1:A:1439:ARG:HH21	1.51	0.57
1:A:1455:GLU:HA	1:A:1462:LYS:H	1.67	0.57
1:A:1503:ASP:O	4:E:1:GLC:O2	2.20	0.57
1:B:418:VAL:HG22	1:B:490:ARG:HA	1.86	0.57
1:B:1275:ARG:NH2	1:B:1366:VAL:O	2.38	0.57
1:B:590:MET:HB2	1:B:671:ASN:HD22	1.69	0.56
1:B:611:GLY:HA2	1:B:997:LEU:HD23	1.87	0.56
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.87	0.56
1:B:5:ARG:HA	1:B:643:VAL:HG12	1.86	0.56
1:B:238:ASN:ND2	1:B:497:GLY:O	2.39	0.56
1:A:1209:VAL:HG12	1:A:1252:VAL:HG13	1.87	0.56
1:B:564:GLN:HG3	1:B:586:ILE:HD12	1.88	0.56
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.33	0.56
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.88	0.56
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.88	0.56
1:B:68:ASN:ND2	1:B:108:CYS:SG	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.89	0.55
1:A:647:SER:OG	1:A:648:GLU:N	2.38	0.55
1:B:384:HIS:HB3	1:B:392:ILE:HD11	1.88	0.55
1:A:315:ASP:O	1:A:319:THR:OG1	2.19	0.55
1:A:77:PHE:O	1:A:554:ARG:NH1	2.40	0.55
1:B:673:THR:HG22	1:B:675:ASN:H	1.72	0.55
1:A:425:ARG:HH22	1:A:491:ARG:HB3	1.72	0.54
1:A:1355:GLN:OE1	1:A:1357:ARG:NH1	2.40	0.54
1:A:667:CYS:HA	1:A:671:ASN:HD21	1.72	0.54
1:A:5:ARG:HA	1:A:643:VAL:HG12	1.90	0.53
1:A:381:LYS:HD3	1:A:386:GLU:HG2	1.90	0.53
1:B:940:ILE:HD11	1:B:1003:ALA:HB1	1.90	0.53
1:A:1064:LEU:O	1:A:1505:SER:OG	2.20	0.53
1:B:264:GLU:HB2	1:B:309:TRP:HH2	1.74	0.53
1:B:179:HIS:NE2	1:B:230:ASP:OD1	2.41	0.53
1:A:400:LEU:O	1:A:404:ASN:ND2	2.41	0.53
1:A:251:TYR:HE1	1:A:501:LYS:HG3	1.74	0.53
1:B:309:TRP:HB2	1:B:411:TYR:HE1	1.73	0.53
1:B:199:LEU:HD11	1:B:520:LYS:HB2	1.90	0.53
1:B:27:VAL:HG22	1:B:578:GLU:HG3	1.91	0.53
1:B:1071:TYR:CE1	5:F:7:GLC:H3	2.44	0.53
1:A:9:LEU:HD11	1:A:17:PRO:HB3	1.92	0.52
1:A:1322:LYS:H	1:A:1322:LYS:HD2	1.74	0.52
1:B:286:LYS:HG2	1:B:431:ILE:HG23	1.91	0.52
1:A:335:ASP:OD1	1:A:336:ASP:N	2.41	0.52
1:A:425:ARG:NH2	1:A:491:ARG:HB3	2.25	0.52
1:A:1141:VAL:HA	1:A:1147:GLY:HA3	1.92	0.52
1:B:1435:GLY:HA3	1:B:1514:CYS:HB3	1.91	0.52
1:A:456:LYS:HG3	1:A:462:GLU:HG2	1.91	0.52
1:A:738:MET:HB3	1:A:776:TRP:CH2	2.45	0.52
1:B:152:VAL:HG12	1:B:154:LYS:HG2	1.92	0.52
1:A:115:ASN:OD1	1:A:116:ASP:N	2.43	0.52
1:B:300:GLU:HA	1:B:304:GLY:HA3	1.92	0.52
1:B:1503:ASP:O	5:F:2:GLC:O2	2.26	0.52
1:B:115:ASN:OD1	1:B:116:ASP:N	2.42	0.52
1:B:1242:LYS:HE3	1:B:1421:GLY:O	2.10	0.51
1:B:1108:LYS:HB3	1:B:1124:TYR:CZ	2.46	0.51
1:B:721:SER:HB3	1:B:822:ILE:HG23	1.93	0.51
1:A:136:VAL:HA	1:A:226:LEU:HD21	1.92	0.51
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.46	0.51
1:A:1066:HIS:CG	4:E:1:GLC:H1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:THR:O	1:B:847:THR:OG1	2.24	0.51
1:A:53:ILE:HD11	1:A:65:ILE:HD11	1.92	0.50
1:A:1493:LEU:HB3	1:A:1504:SER:HB2	1.94	0.50
1:B:116:ASP:N	1:B:116:ASP:OD1	2.45	0.50
1:B:428:TYR:HA	1:B:432:ASP:HA	1.92	0.50
1:A:295:MET:HA	1:A:298:ILE:HB	1.92	0.50
1:B:235:HIS:HB2	1:B:499:CYS:HB3	1.93	0.50
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.47	0.50
1:B:1320:LYS:HA	1:B:1338:ARG:HB3	1.93	0.50
1:B:870:ILE:HD11	1:B:997:LEU:HD13	1.94	0.50
1:A:306:LEU:HD13	1:A:309:TRP:CZ2	2.46	0.50
1:A:1452:CYS:HB3	1:A:1467:LEU:HD22	1.94	0.50
5:F:1:GLC:H61	5:F:2:GLC:O5	2.11	0.49
1:A:679:THR:OG1	1:A:783:LYS:HG2	2.12	0.49
1:B:72:ASP:OD1	1:B:73:PHE:N	2.42	0.49
1:B:160:ILE:HG12	1:B:205:VAL:HG12	1.94	0.49
1:B:754:MET:HG2	1:B:755:HIS:N	2.26	0.49
1:A:748:ASP:OD1	1:A:749:ILE:N	2.43	0.49
1:B:422:LEU:HD23	1:B:425:ARG:HE	1.77	0.49
1:A:418:VAL:HG22	1:A:490:ARG:HA	1.94	0.49
1:B:738:MET:HB3	1:B:776:TRP:CH2	2.47	0.49
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.94	0.49
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.95	0.49
1:B:466:ALA:HB3	1:B:501:LYS:HE3	1.94	0.49
1:B:1108:LYS:HE2	1:B:1109:HIS:CE1	2.47	0.49
1:B:1083:LEU:HD22	1:B:1136:ALA:HB1	1.95	0.49
1:B:206:PHE:HB3	1:B:211:GLU:HB3	1.93	0.48
1:A:468:ASN:HB3	1:A:501:LYS:HD3	1.94	0.48
1:A:1221:VAL:HG22	1:A:1228:ILE:HA	1.95	0.48
1:B:1192:ALA:O	1:B:1294:PRO:HD3	2.14	0.48
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.48	0.48
1:A:754:MET:HG2	1:A:755:HIS:N	2.27	0.48
1:A:1236:CYS:HB3	1:A:1241:ASP:HA	1.95	0.48
1:B:425:ARG:HH22	1:B:491:ARG:HB3	1.77	0.48
1:B:1158:ARG:HD3	1:B:1174:PHE:HB3	1.93	0.48
1:B:1167:PRO:HB2	1:B:1170:ASP:HB3	1.96	0.48
1:B:103:VAL:O	1:B:107:TYR:OH	2.18	0.48
1:B:213:ALA:HA	1:B:528:ILE:HG23	1.96	0.48
1:A:1078:ASP:O	1:A:1082:SER:OG	2.30	0.48
1:A:1206:LEU:O	4:E:4:GLC:H4	2.12	0.48
1:B:718:ARG:O	1:B:719:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HA	1:A:272:PHE:HB3	1.95	0.48
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.94	0.48
1:A:1393:MET:HB3	1:A:1433:CYS:HB2	1.95	0.48
1:B:281:TYR:N	1:B:282:PRO:HD2	2.29	0.48
1:B:420:GLU:HA	1:B:423:PHE:CE2	2.49	0.48
1:B:921:TYR:HB2	1:B:948:PRO:HB2	1.96	0.48
1:B:1173:ALA:C	1:B:1175:SER:H	2.17	0.48
1:B:299:LYS:HD2	1:B:300:GLU:HG2	1.96	0.47
1:A:505:GLY:HA3	1:A:510:ASP:HB2	1.96	0.47
1:A:612:SER:OG	1:A:943:ASN:ND2	2.46	0.47
1:A:687:ALA:HB2	1:A:703:TYR:HE2	1.78	0.47
1:A:432:ASP:HB2	1:A:436:PRO:HB3	1.96	0.47
1:B:466:ALA:N	1:B:501:LYS:HD2	2.30	0.47
1:B:281:TYR:H	1:B:282:PRO:HD2	1.79	0.47
1:B:66:TRP:CH2	1:B:84:LYS:HE2	2.49	0.47
1:B:189:SER:HB3	1:B:714:VAL:HG13	1.97	0.47
1:B:717:LYS:HD2	1:B:717:LYS:HA	1.73	0.47
1:A:907:ASP:O	1:A:1047:LYS:HE2	2.15	0.47
1:B:929:LEU:HD22	1:B:1006:VAL:HG13	1.97	0.47
1:A:1422:ARG:HE	1:A:1422:ARG:HB3	1.44	0.47
1:B:136:VAL:HA	1:B:226:LEU:HD21	1.95	0.47
5:F:3:GLC:O6	5:F:4:GLC:O5	2.30	0.47
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.50	0.46
1:A:149:GLN:HG2	1:A:170:VAL:HG11	1.97	0.46
1:A:523:GLU:HB2	1:A:555:VAL:HG21	1.97	0.46
1:B:248:GLU:HA	1:B:252:ASN:ND2	2.29	0.46
1:A:39:LYS:HD2	1:A:44:MET:HG2	1.97	0.46
1:B:466:ALA:HB3	1:B:501:LYS:CE	2.46	0.46
1:B:1282:LYS:HB3	1:B:1282:LYS:HE3	1.75	0.46
1:B:324:ARG:H	1:B:324:ARG:HG3	1.56	0.46
1:B:681:GLU:HB2	1:B:783:LYS:HD3	1.96	0.46
1:B:928:GLY:HA2	1:B:966:ARG:NH2	2.30	0.46
1:B:78:ASP:HB3	1:B:81:LYS:HB3	1.96	0.46
1:B:155:TRP:NE1	1:B:716:GLU:O	2.48	0.46
1:A:182:PRO:HG2	1:A:192:PRO:O	2.15	0.46
1:A:326:LYS:HE2	1:A:329:ASN:H	1.79	0.46
1:A:818:ILE:H	1:A:818:ILE:HG12	1.61	0.46
1:B:452:PHE:CE1	1:B:466:ALA:HB2	2.50	0.46
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.81	0.46
1:A:66:TRP:CH2	1:A:84:LYS:HE2	2.50	0.46
1:B:154:LYS:HG3	1:B:155:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:MET:HB3	1:A:1444:PHE:HE2	1.81	0.46
1:B:912:ARG:HA	1:B:912:ARG:HD3	1.62	0.46
1:B:1174:PHE:HD2	1:B:1174:PHE:N	2.14	0.46
1:B:783:LYS:HD2	1:B:857:GLN:HB2	1.98	0.46
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.49	0.46
1:A:834:THR:HG22	1:A:835:GLY:H	1.81	0.46
1:B:324:ARG:HE	1:B:324:ARG:HB2	1.48	0.46
1:B:467:ASN:HB3	1:B:499:CYS:O	2.16	0.46
1:A:27:VAL:HG22	1:A:578:GLU:HG3	1.97	0.45
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.98	0.45
1:A:61:ARG:HG3	1:A:1465:SER:HB2	1.99	0.45
1:A:420:GLU:HA	1:A:423:PHE:CE2	2.51	0.45
1:B:51:LEU:HD11	1:B:99:LEU:HD11	1.99	0.45
1:B:270:LEU:O	1:B:274:GLU:HB2	2.16	0.45
1:A:331:LYS:HG2	1:A:381:LYS:HD2	1.98	0.45
1:A:890:SER:O	1:A:894:ILE:HG13	2.17	0.45
1:B:21:CYS:H	1:B:656:THR:HG21	1.81	0.45
1:B:309:TRP:HB2	1:B:411:TYR:CE1	2.52	0.45
1:B:425:ARG:NH2	1:B:491:ARG:HB3	2.31	0.45
1:A:414:ASP:O	1:A:418:VAL:HG23	2.17	0.45
1:B:136:VAL:HG13	1:B:137:ASN:H	1.82	0.45
1:B:331:LYS:HB3	1:B:332:SER:H	1.51	0.45
1:B:452:PHE:HB2	1:B:454:ARG:HH21	1.80	0.45
1:A:1242:LYS:HD2	1:A:1242:LYS:HA	1.70	0.45
1:A:370:LYS:HD2	1:A:370:LYS:HA	1.59	0.45
1:A:616:VAL:HA	1:A:646:VAL:HG11	1.98	0.45
1:B:286:LYS:HA	1:B:431:ILE:HD13	1.99	0.45
1:B:761:GLN:HE22	1:B:787:SER:HB2	1.81	0.45
1:B:1242:LYS:HZ1	1:B:1422:ARG:HA	1.82	0.45
1:A:1131:TRP:HA	1:A:1134:VAL:HG12	1.99	0.44
1:B:429:LEU:HB3	1:B:430:ARG:NH1	2.31	0.44
1:B:471:ILE:HD11	1:B:480:PHE:HB3	1.99	0.44
1:B:505:GLY:HA3	1:B:510:ASP:HB2	2.00	0.44
1:B:1125:ASN:O	1:B:1237:GLY:HA2	2.17	0.44
1:A:282:PRO:HG2	1:A:294:VAL:HG23	1.99	0.44
1:A:427:LYS:HB2	1:A:427:LYS:HE3	1.90	0.44
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.52	0.44
1:B:1259:ARG:HH12	1:B:1343:ASP:CG	2.19	0.44
1:A:622:PRO:O	1:A:624:PRO:HD3	2.18	0.44
1:A:713:LEU:H	1:A:713:LEU:HG	1.49	0.44
1:B:467:ASN:OD1	1:B:467:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLN:HB2	1:A:994:PRO:HG3	2.00	0.44
1:A:35:LEU:HG	1:A:133:ILE:HD13	2.00	0.44
1:A:800:THR:HG23	1:A:867:GLN:HA	2.00	0.44
1:A:1242:LYS:HE3	1:A:1421:GLY:O	2.18	0.44
1:B:414:ASP:O	1:B:418:VAL:HG23	2.17	0.44
1:A:608:ARG:HD2	1:A:749:ILE:HG12	1.99	0.44
1:A:1151:LEU:HA	1:A:1180:ILE:HB	1.99	0.44
1:A:1463:PRO:HD3	1:A:1526:TYR:CE1	2.53	0.44
1:B:265:LEU:HD13	1:B:265:LEU:HA	1.89	0.44
1:A:235:HIS:CG	1:A:499:CYS:HB3	2.53	0.44
1:B:251:TYR:HB2	1:B:501:LYS:NZ	2.32	0.44
1:B:1174:PHE:N	1:B:1174:PHE:CD2	2.84	0.44
1:B:1131:TRP:HA	1:B:1134:VAL:HG12	2.00	0.44
1:B:1141:VAL:HA	1:B:1147:GLY:HA3	1.99	0.44
1:A:19:THR:HA	1:A:656:THR:HG23	1.99	0.43
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.17	0.43
1:B:673:THR:HG21	1:B:707:PHE:O	2.17	0.43
1:B:1108:LYS:HB3	1:B:1124:TYR:CE2	2.53	0.43
1:B:1256:GLY:HA2	1:B:1422:ARG:NH1	2.33	0.43
1:B:695:SER:O	1:B:739:ARG:NH2	2.51	0.43
1:B:1411:GLU:O	1:B:1420:LYS:N	2.47	0.43
1:A:72:ASP:OD1	1:A:73:PHE:N	2.43	0.43
1:A:611:GLY:HA2	1:A:997:LEU:HD23	2.00	0.43
1:A:912:ARG:HA	1:A:912:ARG:HD3	1.90	0.43
1:B:427:LYS:HE3	1:B:427:LYS:HB3	1.77	0.43
1:B:878:ILE:HG21	1:B:1004:LEU:HD23	2.00	0.43
1:B:1432:TRP:CG	1:B:1510:TRP:CD1	3.07	0.43
1:B:1495:ASN:HB2	1:B:1499:GLU:HB3	2.01	0.43
1:A:649:ILE:H	1:A:649:ILE:HG13	1.64	0.43
1:B:53:ILE:HD11	1:B:65:ILE:HD11	2.00	0.43
1:B:328:GLY:HA2	1:B:331:LYS:HB2	2.00	0.43
1:B:251:TYR:HA	1:B:503:ARG:HD3	2.00	0.43
1:B:794:ARG:HD2	1:B:796:LYS:HE2	2.01	0.43
1:B:890:SER:O	1:B:894:ILE:HG13	2.18	0.43
1:A:1206:LEU:HB3	1:A:1207:ASP:H	1.74	0.43
1:B:402:ASP:HA	1:B:405:LEU:HG	2.01	0.43
1:B:1202:ALA:HB1	1:B:1215:PHE:CG	2.54	0.43
1:A:103:VAL:O	1:A:107:TYR:OH	2.22	0.43
1:A:896:TYR:CE2	1:A:973:LYS:HD3	2.53	0.43
1:A:928:GLY:HA2	1:A:966:ARG:NH2	2.34	0.43
1:B:1181:GLU:OE2	1:B:1287:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1242:LYS:HA	1:B:1242:LYS:HD2	1.66	0.43
1:B:148:MET:SD	1:B:179:HIS:HB2	2.59	0.42
1:A:400:LEU:HD23	1:A:403:ILE:HD12	2.00	0.42
1:A:783:LYS:HD2	1:A:857:GLN:HB2	2.00	0.42
1:B:284:ASP:HB2	1:B:438:GLN:HG2	2.01	0.42
1:A:30:LEU:HD22	1:A:130:VAL:HG22	2.00	0.42
1:A:331:LYS:CD	1:A:378:ALA:HA	2.49	0.42
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.54	0.42
1:B:142:PRO:HG2	1:B:743:ALA:HB1	2.01	0.42
1:B:174:LYS:HA	1:B:174:LYS:HD3	1.74	0.42
1:A:1071:TYR:HD2	1:A:1115:LEU:HD11	1.85	0.42
1:B:1198:ARG:HG3	1:B:1199:GLU:N	2.34	0.42
1:A:871:ASP:OD2	1:A:989:ARG:NH2	2.53	0.42
1:A:1441:TYR:O	1:A:1445:ASN:HB2	2.20	0.42
1:B:286:LYS:HB2	1:B:438:GLN:OE1	2.19	0.42
1:B:626:ASP:OD1	1:B:626:ASP:N	2.50	0.42
1:B:667:CYS:HA	1:B:671:ASN:HD21	1.85	0.42
1:A:610:ILE:HA	1:A:753:GLU:HB3	2.01	0.42
1:B:381:LYS:HD3	1:B:386:GLU:HA	2.00	0.42
1:A:1107:LEU:HB3	1:A:1157:ARG:NH1	2.34	0.42
1:B:182:PRO:HD3	1:B:230:ASP:HB2	2.01	0.42
1:B:1084:ARG:HH11	1:B:1143:ILE:HD11	1.85	0.42
1:A:35:LEU:HD12	1:A:35:LEU:H	1.85	0.42
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.84	0.42
1:A:1420:LYS:HD3	1:A:1420:LYS:HA	1.81	0.42
1:B:276:MET:HE3	1:B:447:LEU:HD22	2.02	0.42
1:B:871:ASP:OD2	1:B:989:ARG:NH2	2.53	0.42
1:B:1031:PHE:HB2	1:B:1479:ARG:HG3	2.01	0.42
5:F:1:GLC:H61	5:F:2:GLC:C5	2.50	0.42
1:A:506:LYS:HE3	1:A:506:LYS:HB2	1.93	0.42
1:A:597:GLU:HG2	1:A:600:ARG:NH2	2.33	0.42
1:A:1100:ILE:HG21	1:A:1150:LEU:HD21	2.01	0.42
1:A:1117:ASP:H	1:A:1122:PRO:HB3	1.84	0.42
1:B:399:ILE:HA	1:B:402:ASP:HB2	2.02	0.42
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.46	0.42
1:A:895:ASN:HB2	1:A:1040:ILE:O	2.20	0.42
1:A:895:ASN:OD1	1:A:1044:SER:HB3	2.19	0.42
1:B:1337:ARG:HG3	1:B:1340:ILE:HD11	2.02	0.42
1:A:900:ARG:CZ	1:A:904:GLU:HB3	2.50	0.41
1:A:1104:ALA:HB3	1:A:1155:VAL:HG11	2.01	0.41
1:A:184:GLN:HA	1:A:201:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1243:MET:HA	1:B:1255:PRO:HA	2.02	0.41
1:A:302:VAL:O	1:A:306:LEU:HD12	2.20	0.41
1:A:415:ILE:HD13	1:A:415:ILE:HA	1.93	0.41
1:A:1435:GLY:HA3	1:A:1514:CYS:HB3	2.02	0.41
1:B:161:LYS:HD2	1:B:161:LYS:HA	1.89	0.41
1:A:44:MET:HE2	1:A:44:MET:HB2	1.96	0.41
1:A:1157:ARG:H	1:A:1177:SER:HA	1.85	0.41
1:A:1165:TYR:HB2	1:A:1166:ILE:H	1.80	0.41
1:A:1482:ILE:HD12	1:A:1489:GLY:HA2	2.03	0.41
1:B:91:PHE:HE1	1:B:1472:TYR:HB2	1.85	0.41
1:B:303:ILE:H	1:B:303:ILE:HG13	1.64	0.41
1:B:333:TRP:HB2	1:B:378:ALA:O	2.20	0.41
1:B:370:LYS:HD2	1:B:370:LYS:HA	1.68	0.41
1:B:1199:GLU:HG3	1:B:1215:PHE:HA	2.01	0.41
1:A:626:ASP:OD1	1:A:626:ASP:N	2.49	0.41
1:A:671:ASN:OD1	1:A:671:ASN:N	2.44	0.41
1:A:467:ASN:HB3	1:A:499:CYS:O	2.20	0.41
1:A:1452:CYS:HB3	1:A:1467:LEU:HB2	2.02	0.41
1:B:800:THR:HG23	1:B:867:GLN:HA	2.02	0.41
1:B:1493:LEU:HB3	1:B:1504:SER:HB2	2.02	0.41
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.21	0.41
1:A:1392:GLY:C	1:A:1429:GLU:HB3	2.40	0.41
1:A:1432:TRP:CG	1:A:1510:TRP:CD1	3.09	0.41
1:B:962:TYR:CZ	1:B:966:ARG:HD3	2.56	0.41
1:B:1123:ARG:NH2	1:B:1207:ASP:HB2	2.27	0.41
1:B:618:LEU:HD22	1:B:933:VAL:HG13	2.02	0.41
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.36	0.41
1:A:326:LYS:HG3	1:A:328:GLY:H	1.85	0.40
1:A:502:LEU:HD13	1:A:514:LEU:HD11	2.03	0.40
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.50	0.40
1:B:184:GLN:H	1:B:184:GLN:HG2	1.64	0.40
1:B:301:HIS:HA	1:B:305:GLU:HG3	2.03	0.40
1:B:608:ARG:HD2	1:B:749:ILE:HG12	2.02	0.40
1:A:1263:ALA:HA	1:A:1344:LEU:HD23	2.03	0.40
1:B:252:ASN:O	1:B:256:SER:N	2.54	0.40
1:B:259:LEU:HD12	1:B:501:LYS:HZ3	1.87	0.40
1:B:807:ALA:HB2	1:B:861:VAL:HG23	2.03	0.40
1:A:895:ASN:CG	1:A:1044:SER:HB3	2.41	0.40
1:A:1487:TRP:CE2	1:A:1506:PRO:HG2	2.56	0.40
1:B:348:ALA:HB1	1:B:403:ILE:HG13	2.04	0.40
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:TYR:HA	1:B:900:ARG:HG2	2.02	0.40
1:B:1320:LYS:HE3	1:B:1320:LYS:HB2	1.86	0.40
1:B:1172:LYS:H	1:B:1172:LYS:HG3	1.68	0.40
1:A:940:ILE:HD11	1:A:1003:ALA:HB1	2.04	0.40
1:A:1164:GLU:HB3	1:A:1165:TYR:H	1.55	0.40
1:B:1164:GLU:HB3	1:B:1165:TYR:H	1.48	0.40

All (3) 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:912:ARG:NH1	4:E:5:GLC:C5[5_445]	1.44	0.76
1:B:912:ARG:NH1	4:E:5:GLC:C6[5_445]	1.57	0.63
1:B:912:ARG:NH1	4:E:5:GLC:C4[5_445]	1.65	0.55

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	1524/1536 (99%)	1379 (90%)	131 (9%)	14 (1%)	17 49
1	B	1524/1536 (99%)	1365 (90%)	133 (9%)	26 (2%)	9 34
All	All	3048/3072 (99%)	2744 (90%)	264 (9%)	40 (1%)	12 39

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	PRO
1	B	196	TYR
1	B	281	TYR
1	B	1167	PRO
1	A	432	ASP

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Mol	Chain	Res	Type
1	A	1163	ASP
1	B	283	VAL
1	B	718	ARG
1	B	1456	GLY
1	A	138	ASP
1	A	281	TYR
1	A	1168	TYR
1	A	1454	VAL
1	B	28	LEU
1	B	282	PRO
1	B	440	PRO
1	B	913	SER
1	B	1164	GLU
1	A	708	PRO
1	A	900	ARG
1	A	1206	LEU
1	A	1296	GLY
1	B	446	PRO
1	B	786	SER
1	B	1174	PHE
1	A	1448	THR
1	B	311	PHE
1	B	332	SER
1	B	501	LYS
1	B	706	VAL
1	B	900	ARG
1	B	1297	SER
1	A	440	PRO
1	A	1122	PRO
1	B	315	ASP
1	B	434	HIS
1	B	1194	GLY
1	B	1204	PRO
1	B	182	PRO
1	B	302	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	1343/1353 (99%)	1217 (91%)	126 (9%)	8 30
1	B	1343/1353 (99%)	1208 (90%)	135 (10%)	7 27
All	All	2686/2706 (99%)	2425 (90%)	261 (10%)	8 28

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	79	ARG
1	A	81	LYS
1	A	135	SER
1	A	138	ASP
1	A	139	LYS
1	A	185	HIS
1	A	198	GLN
1	A	207	LYS
1	A	229	THR
1	A	281	TYR
1	A	283	VAL
1	A	284	ASP
1	A	287	THR
1	A	288	VAL
1	A	290	ASP
1	A	293	LYS
1	A	295	MET
1	A	300	GLU
1	A	308	LEU
1	A	316	VAL
1	A	318	GLN
1	A	330	SER
1	A	331	LYS
1	A	334	SER
1	A	338	ILE
1	A	349	GLN
1	A	374	ASP
1	A	430	ARG
1	A	434	HIS
1	A	442	THR
1	A	444	LYS
1	A	448	SER
1	A	467	ASN

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Mol	Chain	Res	Type
1	A	471	ILE
1	A	495	VAL
1	A	567	SER
1	A	616	VAL
1	A	628	LYS
1	A	630	ASP
1	A	664	PHE
1	A	704	ASP
1	A	709	GLN
1	A	711	LEU
1	A	713	LEU
1	A	721	SER
1	A	754	MET
1	A	761	GLN
1	A	767	ARG
1	A	800	THR
1	A	818	ILE
1	A	822	ILE
1	A	823	ILE
1	A	824	GLU
1	A	834	THR
1	A	853	GLN
1	A	913	SER
1	A	1009	MET
1	A	1016	ARG
1	A	1044	SER
1	A	1055	GLN
1	A	1069	THR
1	A	1074	CYS
1	A	1082	SER
1	A	1092	ARG
1	A	1105	LYS
1	A	1107	LEU
1	A	1149	SER
1	A	1153	GLU
1	A	1157	ARG
1	A	1161	LEU
1	A	1162	ASP
1	A	1165	TYR
1	A	1166	ILE
1	A	1169	ASP
1	A	1170	ASP

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Mol	Chain	Res	Type
1	A	1172	LYS
1	A	1174	PHE
1	A	1177	SER
1	A	1191	HIS
1	A	1199	GLU
1	A	1205	ASN
1	A	1208	ARG
1	A	1213	GLU
1	A	1216	ASN
1	A	1218	GLU
1	A	1220	ASN
1	A	1227	LEU
1	A	1233	GLN
1	A	1236	CYS
1	A	1243	MET
1	A	1248	LYS
1	A	1257	THR
1	A	1264	VAL
1	A	1265	GLU
1	A	1267	ASN
1	A	1279	GLN
1	A	1285	LYS
1	A	1289	THR
1	A	1290	GLU
1	A	1295	ASP
1	A	1297	SER
1	A	1298	LYS
1	A	1300	SER
1	A	1320	LYS
1	A	1321	ASN
1	A	1325	ASP
1	A	1330	ILE
1	A	1334	ILE
1	A	1340	ILE
1	A	1349	LYS
1	A	1356	PHE
1	A	1361	THR
1	A	1396	LEU
1	A	1408	ASN
1	A	1414	ASP
1	A	1422	ARG
1	A	1424	TYR

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Mol	Chain	Res	Type
1	A	1442	HIS
1	A	1460	LYS
1	A	1462	LYS
1	A	1476	LEU
1	A	1493	LEU
1	A	1494	THR
1	A	1499	GLU
1	A	1527	GLU
1	B	35	LEU
1	B	59	VAL
1	B	103	VAL
1	B	116	ASP
1	B	122	THR
1	B	159	THR
1	B	160	ILE
1	B	183	LEU
1	B	184	GLN
1	B	196	TYR
1	B	198	GLN
1	B	199	LEU
1	B	200	GLU
1	B	205	VAL
1	B	206	PHE
1	B	261	SER
1	B	265	LEU
1	B	267	LYS
1	B	274	GLU
1	B	275	GLN
1	B	279	LEU
1	B	283	VAL
1	B	284	ASP
1	B	287	THR
1	B	290	ASP
1	B	295	MET
1	B	298	ILE
1	B	302	VAL
1	B	308	LEU
1	B	310	GLU
1	B	311	PHE
1	B	312	TYR
1	B	316	VAL
1	B	317	LYS

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Mol	Chain	Res	Type
1	B	318	GLN
1	B	323	LEU
1	B	324	ARG
1	B	325	GLU
1	B	326	LYS
1	B	331	LYS
1	B	333	TRP
1	B	337	ASN
1	B	346	ASN
1	B	347	LEU
1	B	350	PHE
1	B	352	ARG
1	B	353	ASP
1	B	356	THR
1	B	371	ILE
1	B	373	ILE
1	B	389	ASN
1	B	398	LYS
1	B	399	ILE
1	B	421	GLN
1	B	426	ILE
1	B	431	ILE
1	B	437	LYS
1	B	444	LYS
1	B	445	LEU
1	B	448	SER
1	B	465	LEU
1	B	467	ASN
1	B	543	HIS
1	B	585	LEU
1	B	616	VAL
1	B	631	GLU
1	B	650	MET
1	B	664	PHE
1	B	704	ASP
1	B	715	GLN
1	B	716	GLU
1	B	742	ILE
1	B	751	ASP
1	B	754	MET
1	B	764	THR
1	B	767	ARG

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Mol	Chain	Res	Type
1	B	787	SER
1	B	800	THR
1	B	811	GLU
1	B	822	ILE
1	B	824	GLU
1	B	834	THR
1	B	908	TYR
1	B	910	GLU
1	B	912	ARG
1	B	973	LYS
1	B	974	GLU
1	B	990	ILE
1	B	1082	SER
1	B	1155	VAL
1	B	1156	THR
1	B	1159	PHE
1	B	1162	ASP
1	B	1165	TYR
1	B	1166	ILE
1	B	1172	LYS
1	B	1174	PHE
1	B	1175	SER
1	B	1190	ARG
1	B	1195	ILE
1	B	1196	LYS
1	B	1198	ARG
1	B	1201	ASN
1	B	1206	LEU
1	B	1208	ARG
1	B	1216	ASN
1	B	1217	VAL
1	B	1224	GLU
1	B	1233	GLN
1	B	1236	CYS
1	B	1245	GLU
1	B	1247	GLU
1	B	1264	VAL
1	B	1280	LEU
1	B	1282	LYS
1	B	1289	THR
1	B	1290	GLU
1	B	1298	LYS

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Mol	Chain	Res	Type
1	B	1299	ILE
1	B	1320	LYS
1	B	1321	ASN
1	B	1323	GLU
1	B	1324	ASP
1	B	1330	ILE
1	B	1333	THR
1	B	1337	ARG
1	B	1342	LYS
1	B	1356	PHE
1	B	1361	THR
1	B	1408	ASN
1	B	1442	HIS
1	B	1457	SER
1	B	1459	LYS
1	B	1461	LEU
1	B	1462	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	766	HIS

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)

17 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	GLC	C	1	2	12,12,12	1.02	1 (8%)	17,17,17	1.05	1 (5%)
2	GLC	C	2	2	11,11,12	1.29	2 (18%)	15,15,17	1.22	1 (6%)
2	GLC	C	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.47	2 (13%)
3	GLC	D	1	3	12,12,12	0.59	0	17,17,17	0.60	0
3	GLC	D	2	3	11,11,12	0.75	0	15,15,17	1.44	1 (6%)
4	GLC	E	1	4	12,12,12	0.80	0	17,17,17	1.03	0
4	GLC	E	2	4	11,11,12	1.13	1 (9%)	15,15,17	1.28	1 (6%)
4	GLC	E	3	4	11,11,12	1.09	0	15,15,17	2.18	4 (26%)
4	GLC	E	4	4	11,11,12	1.02	1 (9%)	15,15,17	2.36	6 (40%)
4	GLC	E	5	4	11,11,12	0.85	0	15,15,17	2.70	4 (26%)
5	GLC	F	1	5	12,12,12	1.59	2 (16%)	17,17,17	1.11	1 (5%)
5	GLC	F	2	5	11,11,12	1.16	2 (18%)	15,15,17	1.45	3 (20%)
5	GLC	F	3	5	11,11,12	1.56	1 (9%)	15,15,17	1.81	4 (26%)
5	GLC	F	4	5	11,11,12	0.98	0	15,15,17	1.75	3 (20%)
5	GLC	F	5	5	11,11,12	1.27	2 (18%)	15,15,17	1.28	2 (13%)
5	GLC	F	6	5	11,11,12	1.23	1 (9%)	15,15,17	1.25	2 (13%)
5	GLC	F	7	5	11,11,12	0.95	0	15,15,17	1.74	1 (6%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
4	GLC	E	1	4	-	0/2/22/22	0/1/1/1
4	GLC	E	2	4	-	1/2/19/22	0/1/1/1
4	GLC	E	3	4	-	0/2/19/22	0/1/1/1
4	GLC	E	4	4	-	1/2/19/22	0/1/1/1
4	GLC	E	5	4	-	1/2/19/22	0/1/1/1
5	GLC	F	1	5	-	0/2/22/22	0/1/1/1
5	GLC	F	2	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	F	3	5	-	1/2/19/22	0/1/1/1
5	GLC	F	4	5	-	0/2/19/22	0/1/1/1
5	GLC	F	5	5	-	0/2/19/22	0/1/1/1
5	GLC	F	6	5	-	0/2/19/22	0/1/1/1
5	GLC	F	7	5	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	GLC	C4-C5	4.10	1.61	1.53
5	F	1	GLC	C4-C5	3.53	1.60	1.53
5	F	1	GLC	O4-C4	3.45	1.51	1.43
4	E	2	GLC	O4-C4	2.94	1.49	1.43
4	E	4	GLC	O4-C4	2.81	1.49	1.43
2	C	3	GLC	O5-C1	2.63	1.47	1.43
5	F	2	GLC	C4-C3	2.29	1.58	1.52
5	F	5	GLC	O5-C5	2.18	1.47	1.43
5	F	6	GLC	C4-C5	2.15	1.57	1.53
2	C	2	GLC	O3-C3	2.12	1.48	1.43
5	F	2	GLC	O4-C4	2.12	1.48	1.43
2	C	2	GLC	O5-C5	2.11	1.47	1.43
5	F	5	GLC	O4-C4	2.07	1.47	1.43
2	C	1	GLC	O1-C1	2.04	1.46	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	5	GLC	C6-C5-C4	5.66	126.25	113.00
5	F	7	GLC	O5-C5-C6	5.58	115.95	107.20
4	E	3	GLC	C1-O5-C5	5.45	119.57	112.19
4	E	5	GLC	C1-C2-C3	-5.36	103.07	109.67
4	E	5	GLC	C1-O5-C5	-4.89	105.56	112.19
4	E	4	GLC	O4-C4-C3	4.78	121.40	110.35
5	F	4	GLC	C1-O5-C5	-4.52	106.07	112.19
5	F	3	GLC	O4-C4-C5	4.31	120.00	109.30
4	E	4	GLC	C1-O5-C5	4.28	117.99	112.19
4	E	3	GLC	O5-C1-C2	-4.22	104.26	110.77
2	C	3	GLC	O5-C5-C6	4.19	113.77	107.20
3	D	2	GLC	O5-C5-C6	3.60	112.84	107.20
4	E	4	GLC	O5-C1-C2	-3.56	105.28	110.77
4	E	5	GLC	O4-C4-C3	-3.44	102.39	110.35
4	E	2	GLC	O4-C4-C3	3.28	117.93	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	GLC	O4-C4-C5	3.07	116.92	109.30
4	E	4	GLC	O5-C5-C6	-3.04	102.43	107.20
5	F	2	GLC	C2-C3-C4	-2.94	105.81	110.89
5	F	6	GLC	O5-C5-C6	2.88	111.72	107.20
5	F	3	GLC	O4-C4-C3	-2.77	103.95	110.35
4	E	3	GLC	O2-C2-C1	2.76	114.80	109.15
5	F	4	GLC	C2-C3-C4	-2.75	106.13	110.89
5	F	3	GLC	C6-C5-C4	2.63	119.17	113.00
4	E	4	GLC	C2-C3-C4	-2.62	106.37	110.89
4	E	4	GLC	C1-C2-C3	2.59	112.85	109.67
5	F	4	GLC	C6-C5-C4	-2.57	106.98	113.00
5	F	5	GLC	O5-C5-C6	2.51	111.15	107.20
4	E	3	GLC	C1-C2-C3	2.49	112.73	109.67
5	F	3	GLC	C1-C2-C3	2.37	112.57	109.67
5	F	6	GLC	O4-C4-C5	2.32	115.05	109.30
2	C	1	GLC	O3-C3-C2	-2.28	105.09	110.35
5	F	5	GLC	O4-C4-C5	2.27	114.94	109.30
2	C	3	GLC	O5-C1-C2	-2.24	107.31	110.77
5	F	2	GLC	C6-C5-C4	-2.16	107.94	113.00
2	C	2	GLC	O5-C1-C2	-2.12	107.50	110.77
5	F	2	GLC	O5-C1-C2	-2.06	107.59	110.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	5	GLC	O5-C5-C6-O6
5	F	3	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
4	E	2	GLC	O5-C5-C6-O6
4	E	4	GLC	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	GLC	3	0
5	F	6	GLC	1	0
5	F	3	GLC	1	0
4	E	5	GLC	1	3
5	F	1	GLC	2	0

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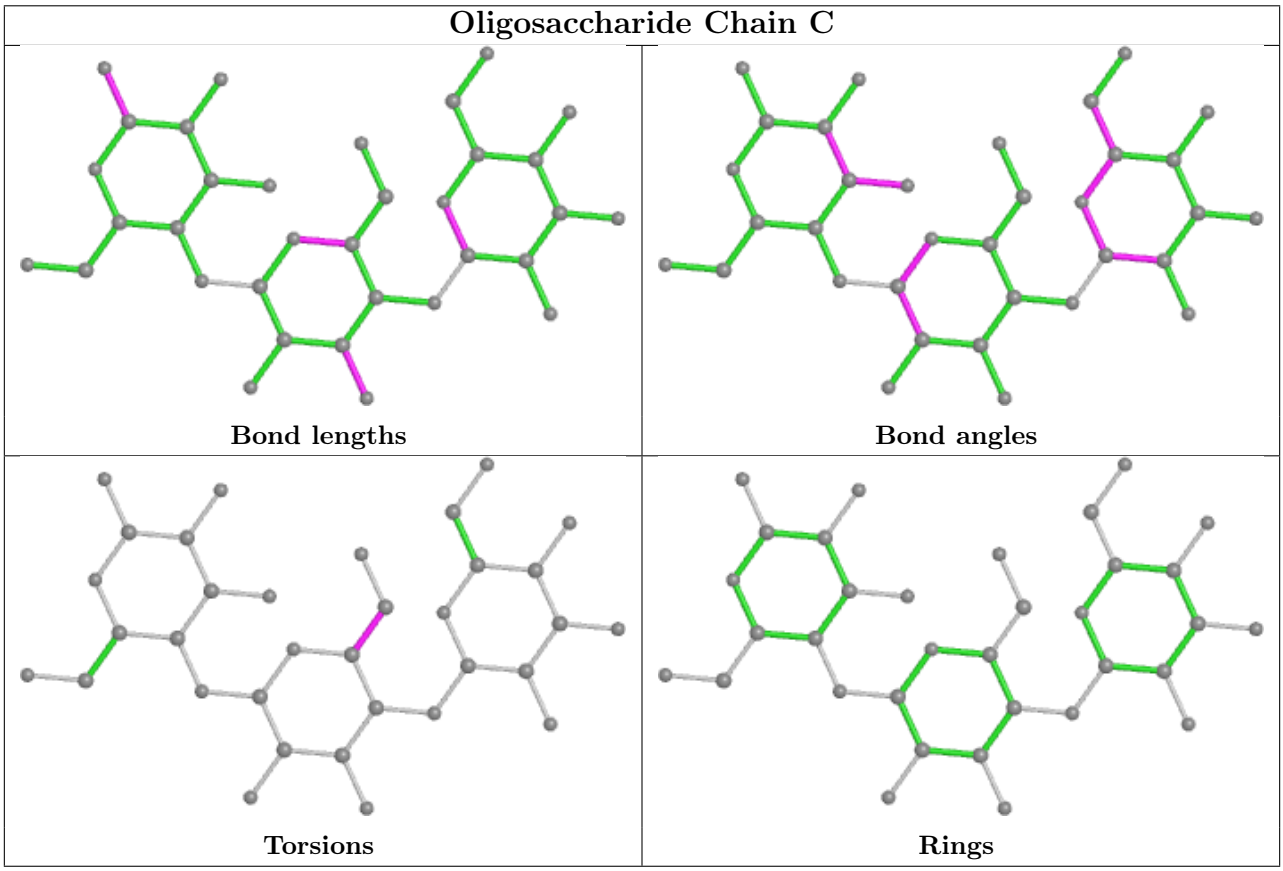
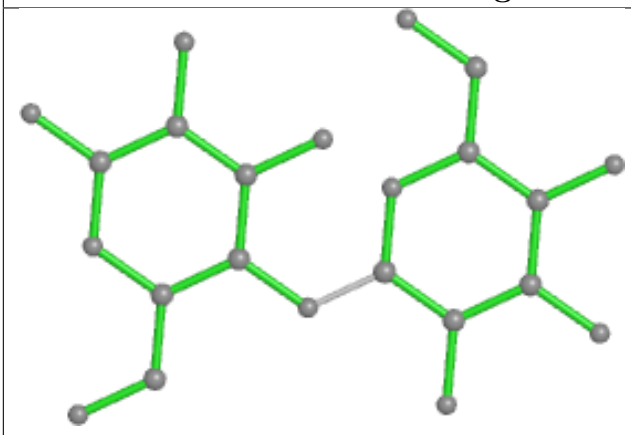
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	7	GLC	1	0
4	E	4	GLC	3	0
5	F	4	GLC	1	0
5	F	5	GLC	1	0
4	E	1	GLC	2	0

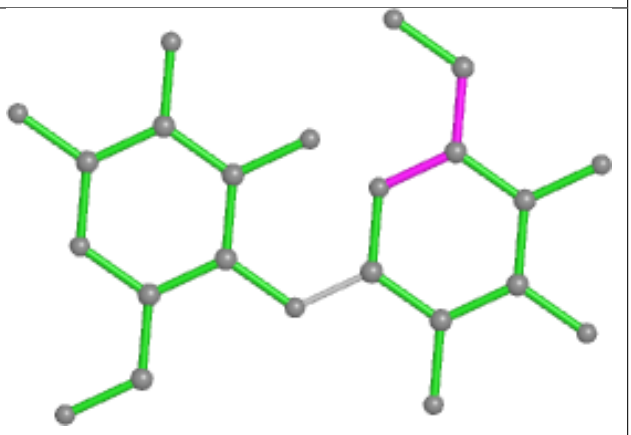
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



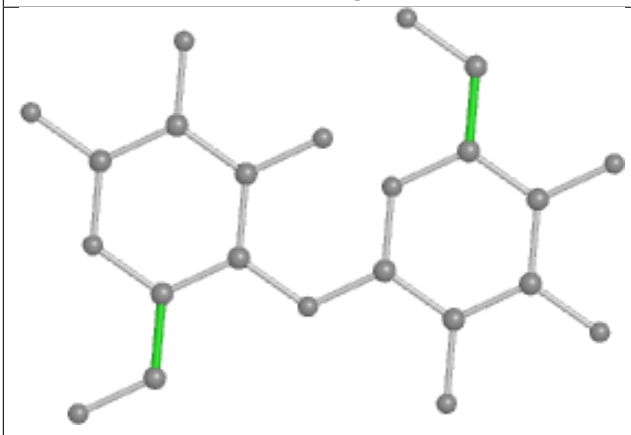
Oligosaccharide Chain D



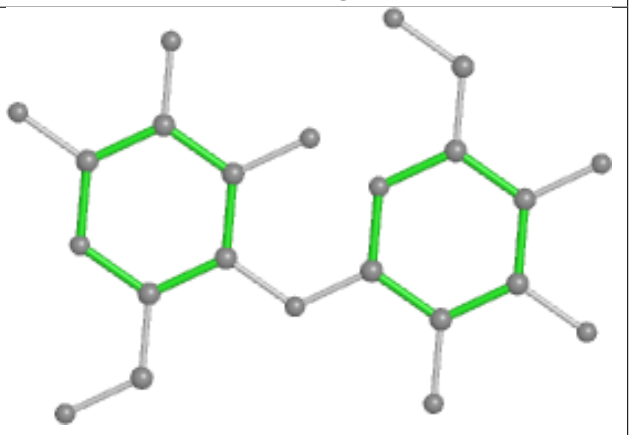
Bond lengths



Bond angles

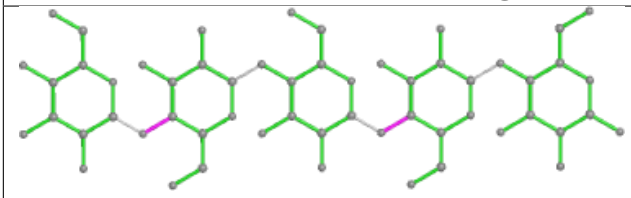


Torsions

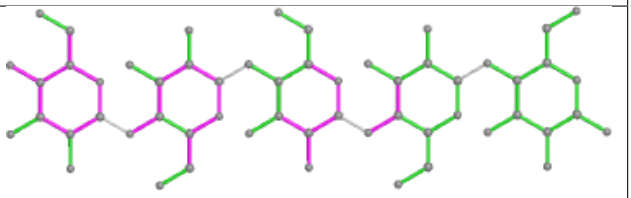


Rings

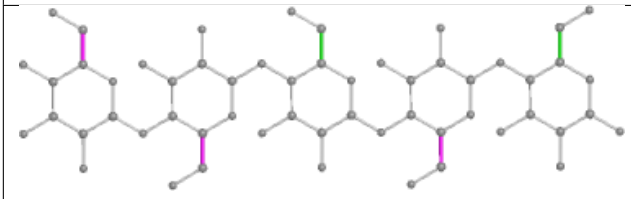
Oligosaccharide Chain E



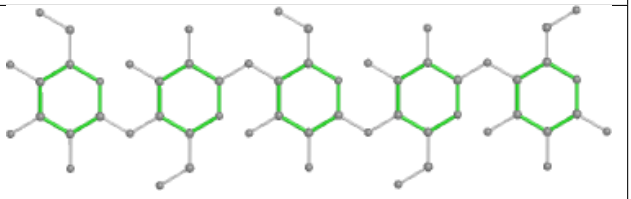
Bond lengths



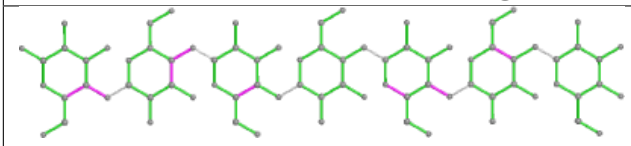
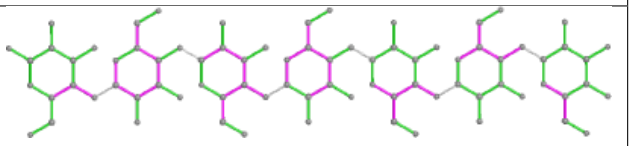
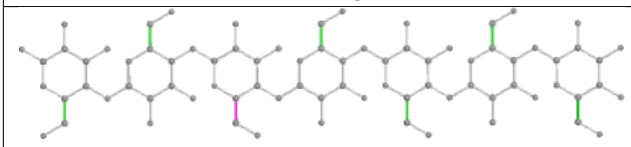
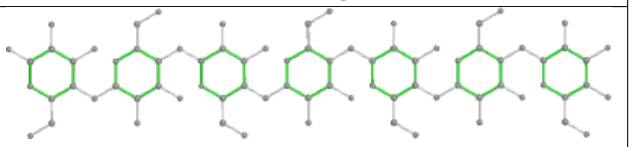
Bond angles



Torsions



Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

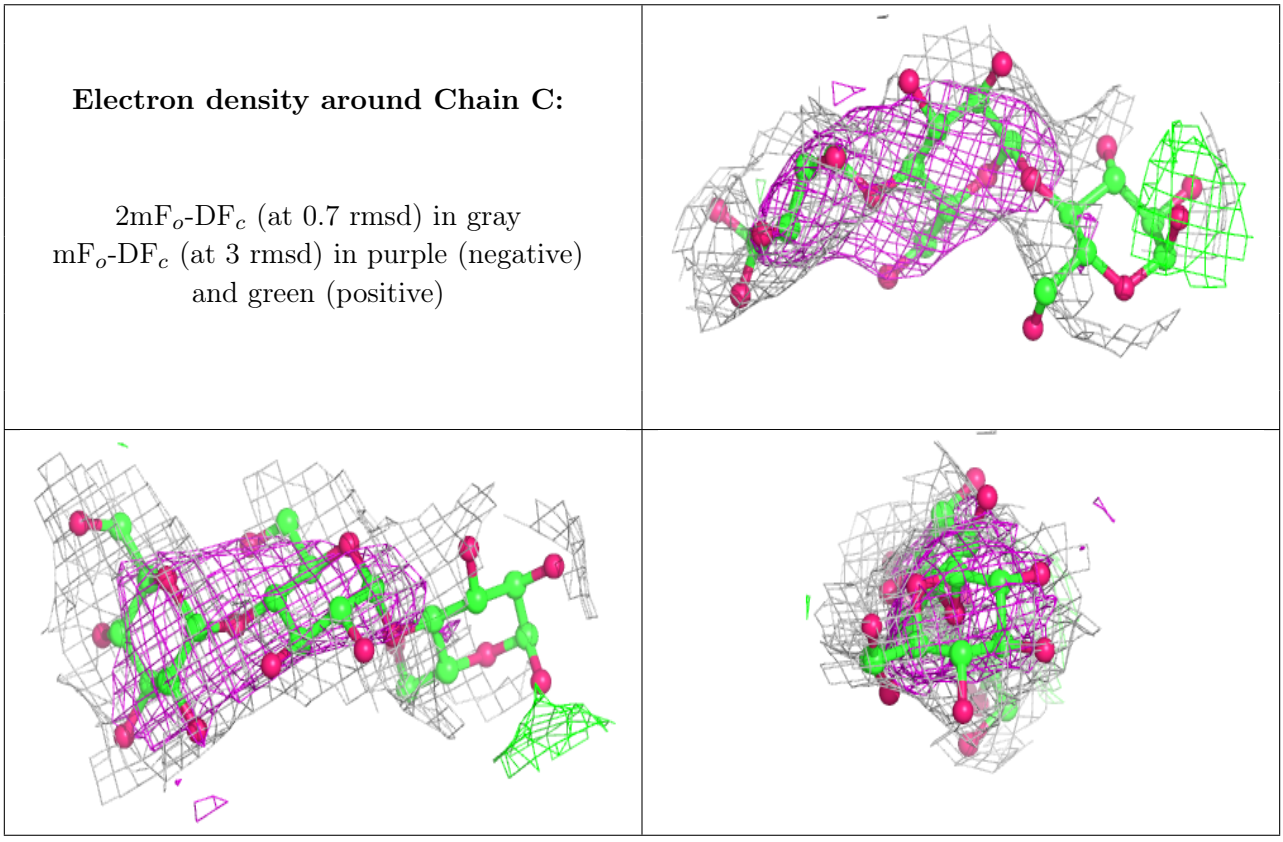
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

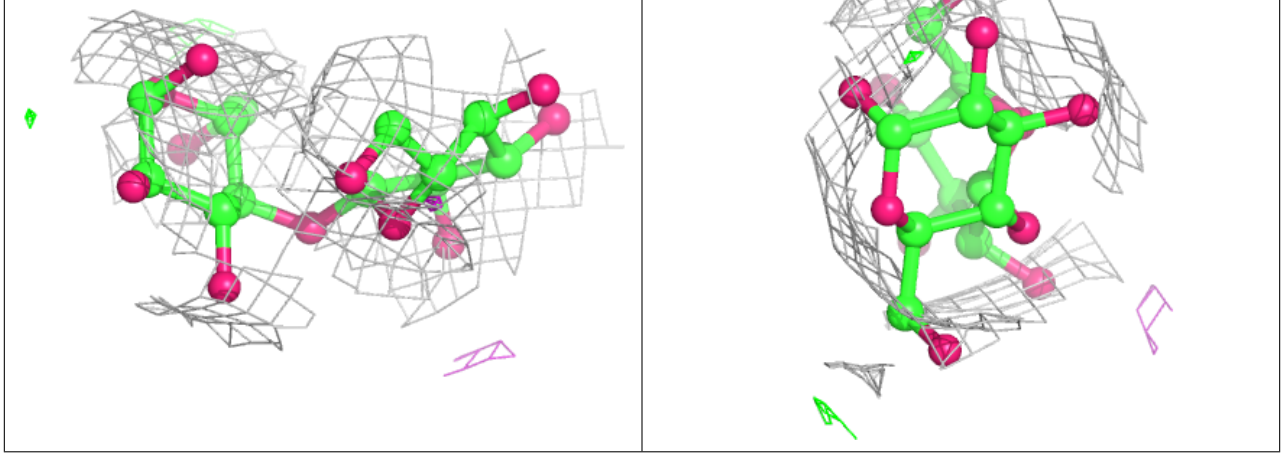
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



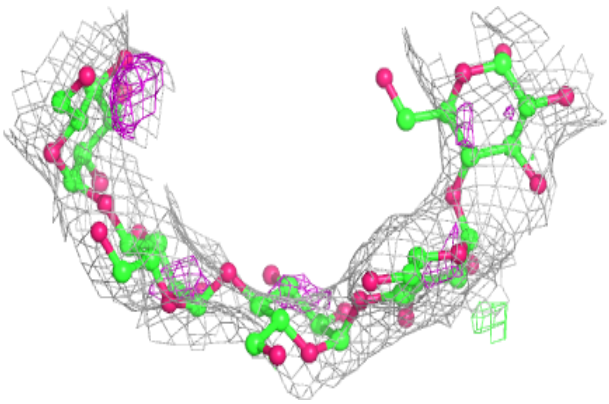
Electron density around Chain D:

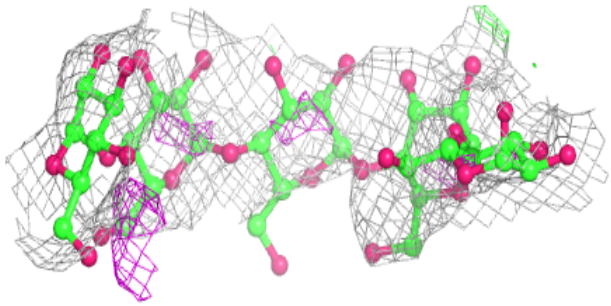
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

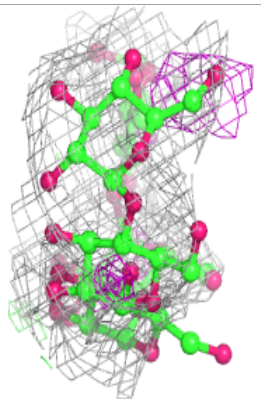


Electron density around Chain E:

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

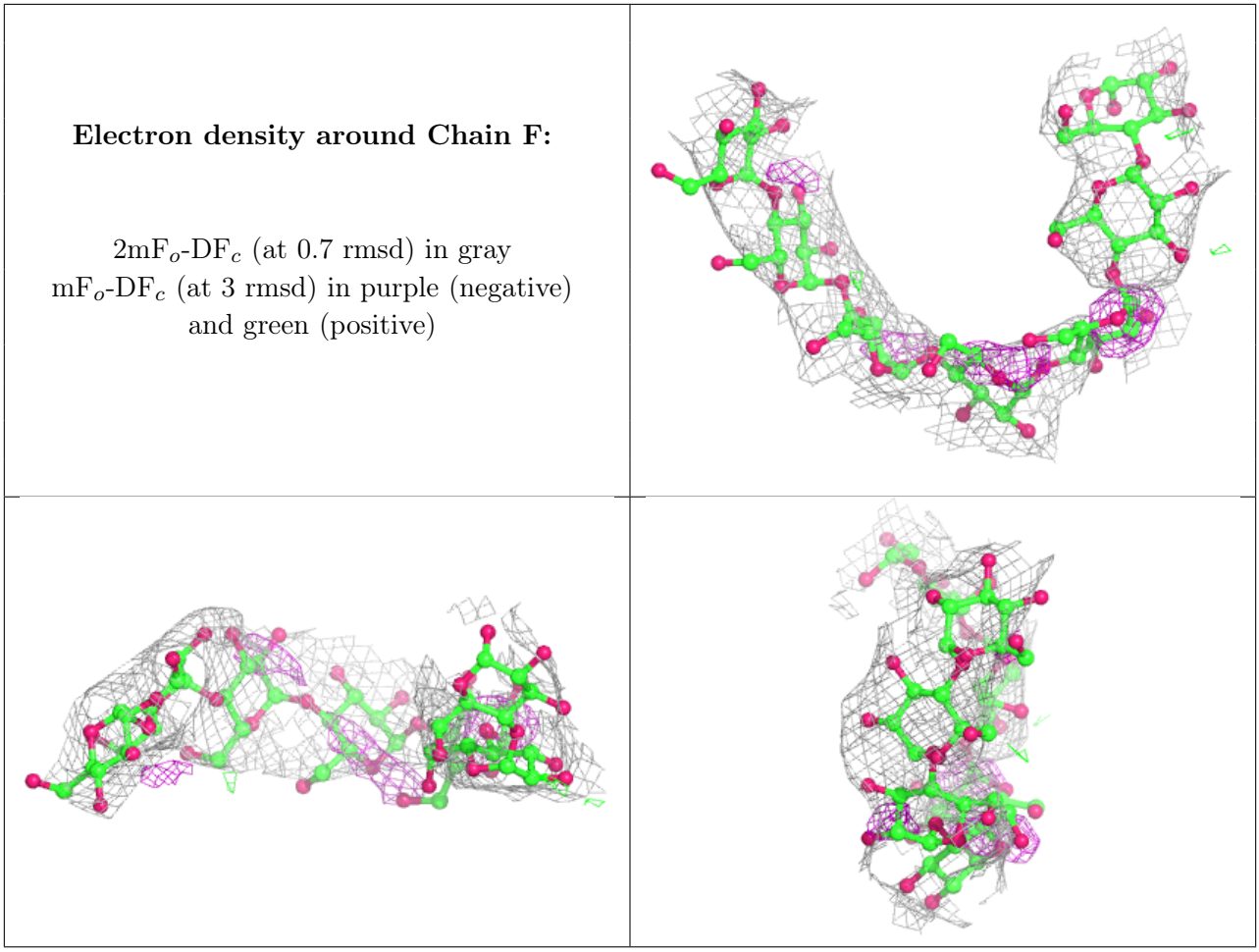






Electron density around Chain F:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.