



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:16 PM EDT

PDB ID : 7EKX / pdb_00007ekx
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

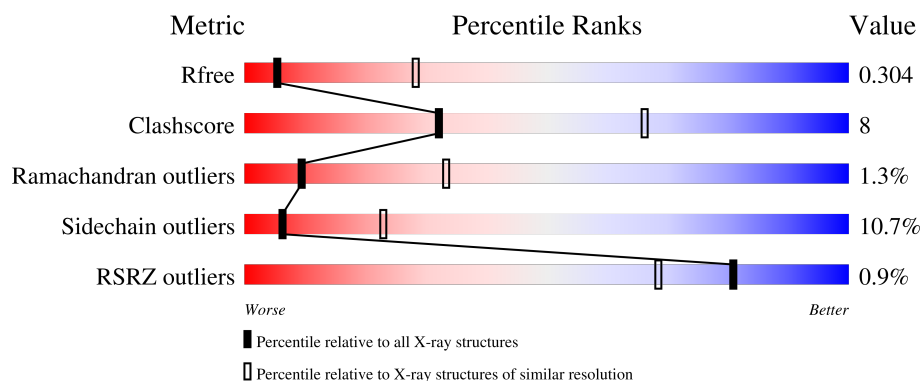
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	1536	74% 23% ..
1	B	1536	72% 24% ..
2	C	3	100%
3	D	2	50% 50%
4	E	5	60% 40%

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Mol	Chain	Length	Quality of chain
5	F	7	 100%

2 Entry composition

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	0	0	0
			34	18	16			

- 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	0	0	0
			23	12	11			

- Molecule 4 is an oligosaccharide called 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	0	0	0
			56	30	26			

- 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.

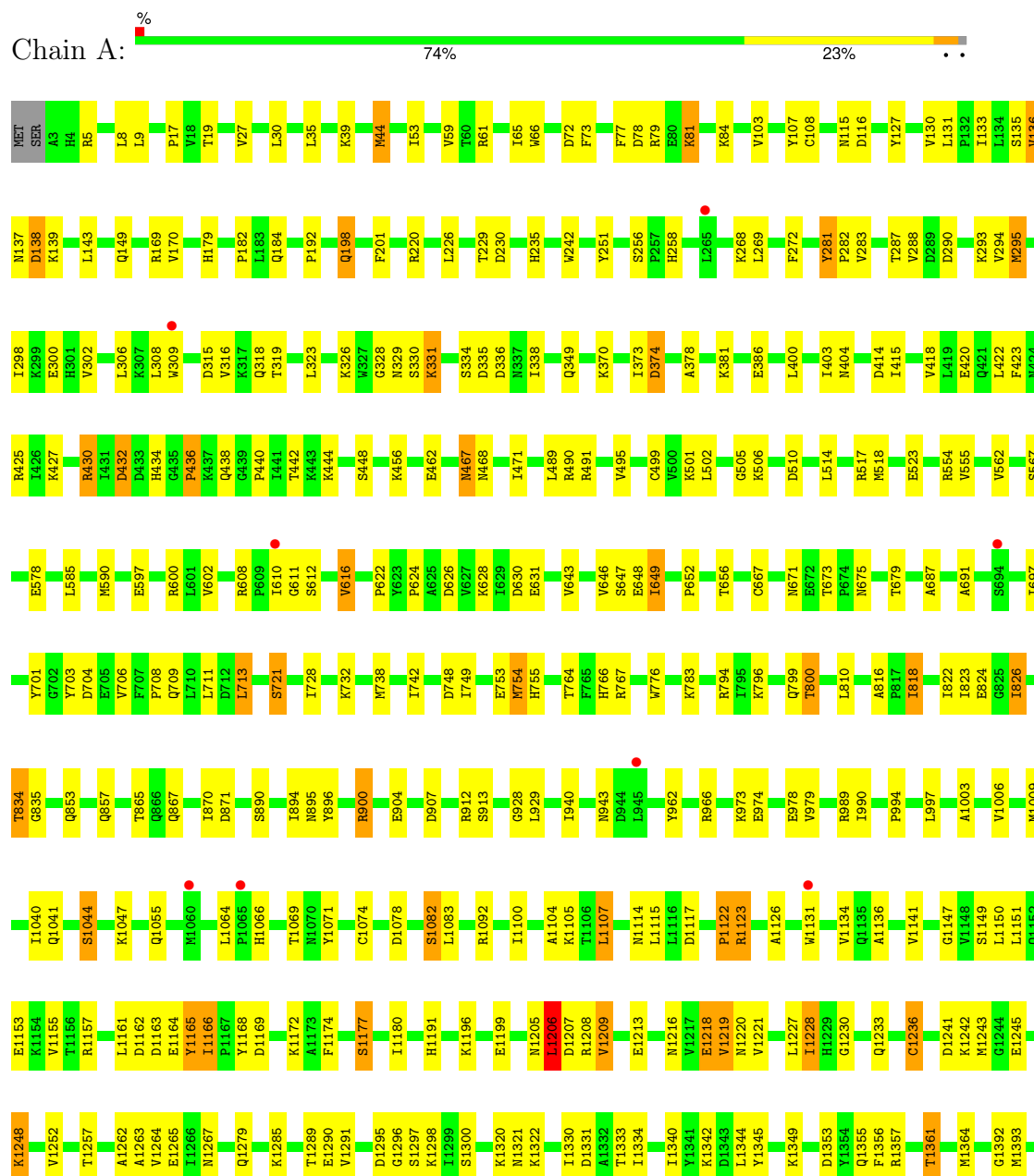


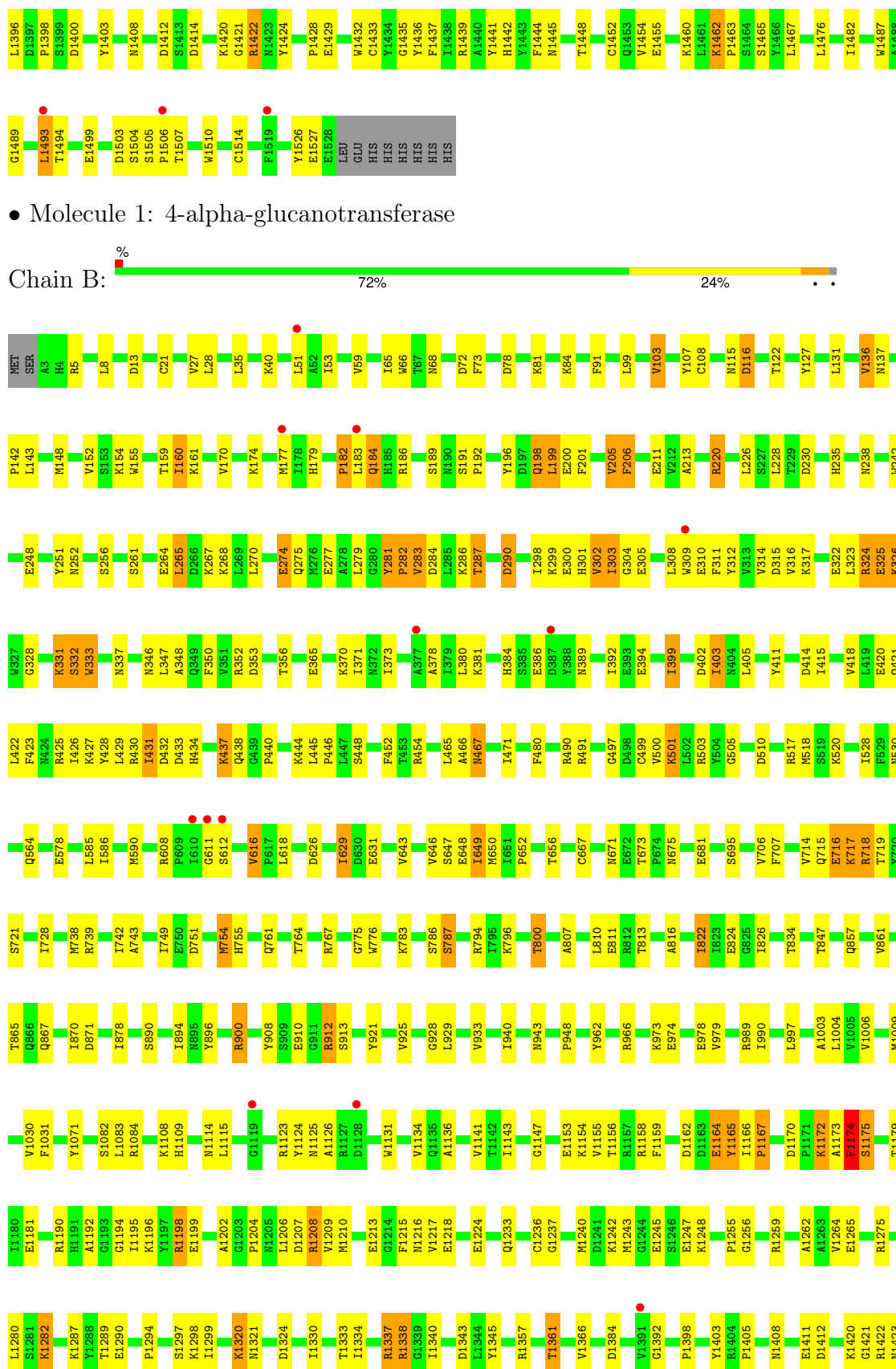
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	F	7	Total	C	O	0	0	0
			78	42	36			

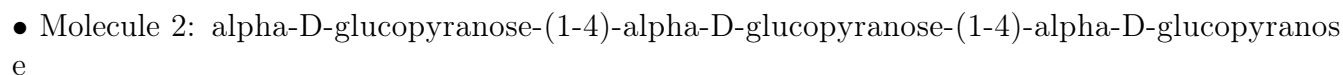
3 Residue-property plots

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: 4-alpha-glucanotransferase







GLC1
GLC2
GLC3

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

GLC1	GLC2
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
23	23
24	24
25	25
26	26
27	27
28	28
29	29
30	30
31	31
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41	41
42	42
43	43
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45	45
46	46
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48	48
49	49
50	50
51	51
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66	66
67	67
68	68
69	69
70	70
71	71
72	72
73	73
74	74
75	75
76	76
77	77
78	78
79	79
80	80
81	81
82	82
83	83
84	84
85	85
86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

- 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

GLC1	GLC2	GLC3	GLC4	GLC5
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- 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

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.272 , 0.303 0.272 , 0.304	Depositor DCC
R_{free} test set	2937 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)	0.31 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.09	0/12578	0.29	0/17055
1	B	0.11	0/12578	0.31	0/17055
All	All	0.10	0/25156	0.30	0/34110

There are no bond length outliers.

There are no bond angle outliers.

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	181	0
1	B	12269	0	11957	206	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	391	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 (391) 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: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:B:1243:MET:HE2	1:B:1255:PRO:HG3	1.75	0.67
1:A:979:VAL:HG13	1:A:1009:MET:HE3	1.78	0.66
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
1:B:1240:MET:HE1	1:B:1357:ARG:HD3	1.79	0.64
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.80	0.63
1:B:198:GLN:HG3	1:B:518:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:198:GLN:HG3	1:A:518:MET:HE1	1.85	0.58
1:B:242:TRP:CG	1:B:517:ARG:HH12	2.21	0.58
1:B:616:VAL:HA	1:B:646:VAL:HG11	1.84	0.58
1:A:1503:ASP:O	4:E:1:GLC:O2	2.20	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASN:ND2	1:B:108:CYS:SG	2.78	0.56
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:B:800:THR:O	1:B:847:THR:OG1	2.24	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:1173:ALA:C	1:B:1175:SER:H	2.17	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:1210:MET:HE3	1:B:1243:MET:HE1	1.92	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:979:VAL:HG13	1:B:1009:MET:HE3	1.91	0.51
1:B:1242:LYS:HE3	1:B:1421:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:242:TRP:CG	1:A:517:ARG:HH12	2.30	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:1259:ARG:HH12	1:B:1343:ASP:CG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1487:TRP:CD1	1:A:1487:TRP:H	2.31	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: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:242:TRP:NE1	1:A:517:ARG:HH22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:HE2	1:A:230:ASP:CG	2.21	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:1392:GLY:C	1:A:1429:GLU:HB3	2.40	0.46
1:B:177:MET:HE3	1:B:177:MET:HB2	1.86	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
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:A:895:ASN:CG	1:A:1044:SER:HB3	2.41	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:1392:GLY:C	1:B:1429:GLU:HB3	2.42	0.45
1:A:1131:TRP:HA	1:A:1134:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:738:MET:HE2	1:B:776:TRP:CE2	2.53	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:717:LYS:O	1:B:718:ARG:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:148:MET:HE2	1:B:228:LEU:HD21	2.00	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
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:B:1207:ASP:CG	1:B:1210:MET:HB2	2.44	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:B:1492:GLU:HB2	1:B:1508:GLN:CD	2.44	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:189:SER:C	1:B:191:SER:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:738:MET:HE2	1:A:776:TRP:CE2	2.54	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
1:B:1243:MET:HA	1:B:1255:PRO:HA	2.02	0.41
1:A:44:MET:HE2	1:A:44:MET:HB2	1.74	0.41
1:A:302:VAL:O	1:A:306:LEU:HD12	2.20	0.41
1:B:281:TYR:O	1:B:282:PRO:C	2.63	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: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:1421:GLY:C	1:B:1423:ASN:H	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:807:ALA:HB2	1:B:861:VAL:HG23	2.03	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
1:B:775:GLY:C	1:B:865:THR:HG22	2.47	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	14	42
1	B	1524/1536 (99%)	1365 (90%)	133 (9%)	26 (2%)	7	28
All	All	3048/3072 (99%)	2744 (90%)	264 (9%)	40 (1%)	9	33

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	1207 (90%)	136 (10%)	7	25
1	B	1343/1353 (99%)	1192 (89%)	151 (11%)	6	21
All	All	2686/2706 (99%)	2399 (89%)	287 (11%)	6	23

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	59	VAL
1	A	79	ARG
1	A	81	LYS
1	A	135	SER
1	A	136	VAL
1	A	138	ASP
1	A	139	LYS
1	A	198	GLN
1	A	220	ARG
1	A	229	THR
1	A	281	TYR
1	A	283	VAL
1	A	287	THR
1	A	288	VAL
1	A	290	ASP
1	A	293	LYS

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Mol	Chain	Res	Type
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
1	A	471	ILE
1	A	489	LEU
1	A	495	VAL
1	A	562	VAL
1	A	567	SER
1	A	585	LEU
1	A	602	VAL
1	A	616	VAL
1	A	628	LYS
1	A	630	ASP
1	A	631	GLU
1	A	649	ILE
1	A	706	VAL
1	A	709	GLN
1	A	711	LEU
1	A	713	LEU
1	A	721	SER
1	A	742	ILE
1	A	754	MET
1	A	764	THR
1	A	767	ARG
1	A	800	THR
1	A	818	ILE
1	A	822	ILE
1	A	823	ILE

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Mol	Chain	Res	Type
1	A	824	GLU
1	A	826	ILE
1	A	834	THR
1	A	853	GLN
1	A	913	SER
1	A	974	GLU
1	A	978	GLU
1	A	990	ILE
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	1123	ARG
1	A	1149	SER
1	A	1153	GLU
1	A	1161	LEU
1	A	1162	ASP
1	A	1165	TYR
1	A	1166	ILE
1	A	1169	ASP
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	1206	LEU
1	A	1208	ARG
1	A	1209	VAL
1	A	1213	GLU
1	A	1216	ASN
1	A	1218	GLU
1	A	1219	VAL
1	A	1220	ASN
1	A	1227	LEU
1	A	1228	ILE
1	A	1233	GLN
1	A	1236	CYS

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Mol	Chain	Res	Type
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	1291	VAL
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	1330	ILE
1	A	1334	ILE
1	A	1340	ILE
1	A	1349	LYS
1	A	1356	PHE
1	A	1361	THR
1	A	1408	ASN
1	A	1414	ASP
1	A	1422	ARG
1	A	1424	TYR
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	40	LYS
1	B	59	VAL
1	B	103	VAL
1	B	116	ASP
1	B	122	THR
1	B	136	VAL

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Mol	Chain	Res	Type
1	B	159	THR
1	B	160	ILE
1	B	170	VAL
1	B	183	LEU
1	B	184	GLN
1	B	198	GLN
1	B	199	LEU
1	B	200	GLU
1	B	205	VAL
1	B	206	PHE
1	B	220	ARG
1	B	261	SER
1	B	265	LEU
1	B	267	LYS
1	B	274	GLU
1	B	275	GLN
1	B	277	GLU
1	B	279	LEU
1	B	283	VAL
1	B	287	THR
1	B	290	ASP
1	B	298	ILE
1	B	302	VAL
1	B	303	ILE
1	B	308	LEU
1	B	310	GLU
1	B	312	TYR
1	B	314	VAL
1	B	316	VAL
1	B	317	LYS
1	B	322	GLU
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

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Mol	Chain	Res	Type
1	B	353	ASP
1	B	356	THR
1	B	365	GLU
1	B	371	ILE
1	B	373	ILE
1	B	389	ASN
1	B	394	GLU
1	B	399	ILE
1	B	403	ILE
1	B	415	ILE
1	B	421	GLN
1	B	426	ILE
1	B	431	ILE
1	B	433	ASP
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	500	VAL
1	B	585	LEU
1	B	616	VAL
1	B	629	ILE
1	B	631	GLU
1	B	649	ILE
1	B	650	MET
1	B	715	GLN
1	B	716	GLU
1	B	717	LYS
1	B	742	ILE
1	B	751	ASP
1	B	754	MET
1	B	764	THR
1	B	767	ARG
1	B	787	SER
1	B	800	THR
1	B	811	GLU
1	B	813	THR
1	B	822	ILE
1	B	824	GLU
1	B	834	THR

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Mol	Chain	Res	Type
1	B	908	TYR
1	B	910	GLU
1	B	912	ARG
1	B	925	VAL
1	B	973	LYS
1	B	974	GLU
1	B	978	GLU
1	B	990	ILE
1	B	1030	VAL
1	B	1082	SER
1	B	1153	GLU
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	1206	LEU
1	B	1208	ARG
1	B	1209	VAL
1	B	1213	GLU
1	B	1216	ASN
1	B	1217	VAL
1	B	1218	GLU
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	1265	GLU
1	B	1280	LEU
1	B	1282	LYS
1	B	1289	THR
1	B	1290	GLU

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Mol	Chain	Res	Type
1	B	1298	LYS
1	B	1299	ILE
1	B	1320	LYS
1	B	1321	ASN
1	B	1324	ASP
1	B	1330	ILE
1	B	1333	THR
1	B	1334	ILE
1	B	1337	ARG
1	B	1338	ARG
1	B	1361	THR
1	B	1408	ASN
1	B	1442	HIS
1	B	1455	GLU
1	B	1459	LYS
1	B	1461	LEU
1	B	1462	LYS
1	B	1527	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	246	HIS
1	A	369	ASN
1	A	467	ASN
1	A	669	HIS
1	A	758	HIS
1	A	766	HIS
1	A	876	HIS
1	A	1152	GLN
1	A	1205	ASN
1	A	1216	ASN
1	A	1220	ASN
1	A	1309	GLN
1	A	1408	ASN
1	B	185	HIS
1	B	239	ASN
1	B	354	ASN
1	B	372	ASN
1	B	384	HIS
1	B	424	ASN

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Mol	Chain	Res	Type
1	B	468	ASN
1	B	758	HIS
1	B	785	HIS
1	B	957	HIS
1	B	1201	ASN
1	B	1408	ASN
1	B	1453	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1.03	1 (5%)
2	GLC	C	2	2	11,11,12	1.27	2 (18%)	15,15,17	1.12	0
2	GLC	C	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.18	1 (6%)
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	0.76	0	15,15,17	1.23	1 (6%)
4	GLC	E	1	4	12,12,12	0.79	0	17,17,17	1.02	0
4	GLC	E	2	4	11,11,12	1.09	1 (9%)	15,15,17	1.22	1 (6%)
4	GLC	E	3	4	11,11,12	1.06	0	15,15,17	1.97	4 (26%)
4	GLC	E	4	4	11,11,12	0.98	1 (9%)	15,15,17	2.18	6 (40%)
4	GLC	E	5	4	11,11,12	0.84	0	15,15,17	2.53	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	F	1	5	12,12,12	1.56	2 (16%)	17,17,17	1.11	1 (5%)
5	GLC	F	2	5	11,11,12	1.13	2 (18%)	15,15,17	1.36	2 (13%)
5	GLC	F	3	5	11,11,12	1.55	1 (9%)	15,15,17	1.72	4 (26%)
5	GLC	F	4	5	11,11,12	0.97	0	15,15,17	1.69	3 (20%)
5	GLC	F	5	5	11,11,12	1.26	1 (9%)	15,15,17	1.16	1 (6%)
5	GLC	F	6	5	11,11,12	1.22	2 (18%)	15,15,17	1.08	2 (13%)
5	GLC	F	7	5	11,11,12	0.94	0	15,15,17	1.41	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
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	4.05	1.61	1.53
5	F	1	GLC	C4-C5	3.49	1.60	1.53
5	F	1	GLC	O4-C4	3.29	1.51	1.43
4	E	2	GLC	O4-C4	2.81	1.49	1.43
4	E	4	GLC	O4-C4	2.68	1.49	1.43
2	C	3	GLC	O5-C1	2.51	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	5	GLC	O5-C5	2.27	1.47	1.43
5	F	2	GLC	C4-C3	2.24	1.58	1.52
2	C	2	GLC	O5-C5	2.20	1.47	1.43
5	F	6	GLC	C4-C5	2.13	1.57	1.53
2	C	1	GLC	O1-C1	2.07	1.46	1.39
2	C	2	GLC	O3-C3	2.02	1.48	1.43
5	F	2	GLC	O4-C4	2.02	1.48	1.43
5	F	6	GLC	O5-C5	2.02	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	GLC	C1-O5-C5	5.51	119.57	112.19
4	E	5	GLC	C6-C5-C4	5.39	126.25	113.02
4	E	5	GLC	C1-O5-C5	-4.94	105.56	112.19
4	E	4	GLC	O4-C4-C3	4.68	121.40	110.38
5	F	4	GLC	C1-O5-C5	-4.56	106.07	112.19
4	E	5	GLC	C1-C2-C3	-4.51	103.07	109.64
5	F	3	GLC	O4-C4-C5	4.33	120.00	109.32
4	E	4	GLC	C1-O5-C5	4.33	117.99	112.19
5	F	7	GLC	O5-C5-C6	4.26	115.95	107.66
4	E	5	GLC	O4-C4-C3	-3.39	102.39	110.38
4	E	2	GLC	O4-C4-C3	3.20	117.93	110.38
2	C	3	GLC	O5-C5-C6	3.14	113.77	107.66
5	F	1	GLC	O4-C4-C5	3.08	116.92	109.32
5	F	2	GLC	C2-C3-C4	-2.87	105.81	110.86
4	E	3	GLC	O5-C1-C2	-2.74	104.26	110.79
5	F	3	GLC	O4-C4-C3	-2.72	103.95	110.38
5	F	4	GLC	C2-C3-C4	-2.69	106.13	110.86
4	E	4	GLC	O5-C5-C6	-2.69	102.43	107.66
3	D	2	GLC	O5-C5-C6	2.66	112.84	107.66
4	E	4	GLC	C2-C3-C4	-2.56	106.37	110.86
5	F	3	GLC	C6-C5-C4	2.50	119.17	113.02
5	F	4	GLC	C6-C5-C4	-2.46	106.98	113.02
4	E	3	GLC	O2-C2-C1	2.44	114.80	109.22
5	F	6	GLC	O4-C4-C5	2.32	115.05	109.32
4	E	4	GLC	O5-C1-C2	-2.31	105.28	110.79
5	F	5	GLC	O4-C4-C5	2.28	114.94	109.32
2	C	1	GLC	O3-C3-C2	-2.24	105.09	110.38
4	E	4	GLC	C1-C2-C3	2.20	112.85	109.64
4	E	3	GLC	C1-C2-C3	2.12	112.73	109.64
5	F	6	GLC	O5-C5-C6	2.08	111.72	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	GLC	C6-C5-C4	-2.07	107.94	113.02
5	F	3	GLC	C1-C2-C3	2.01	112.57	109.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

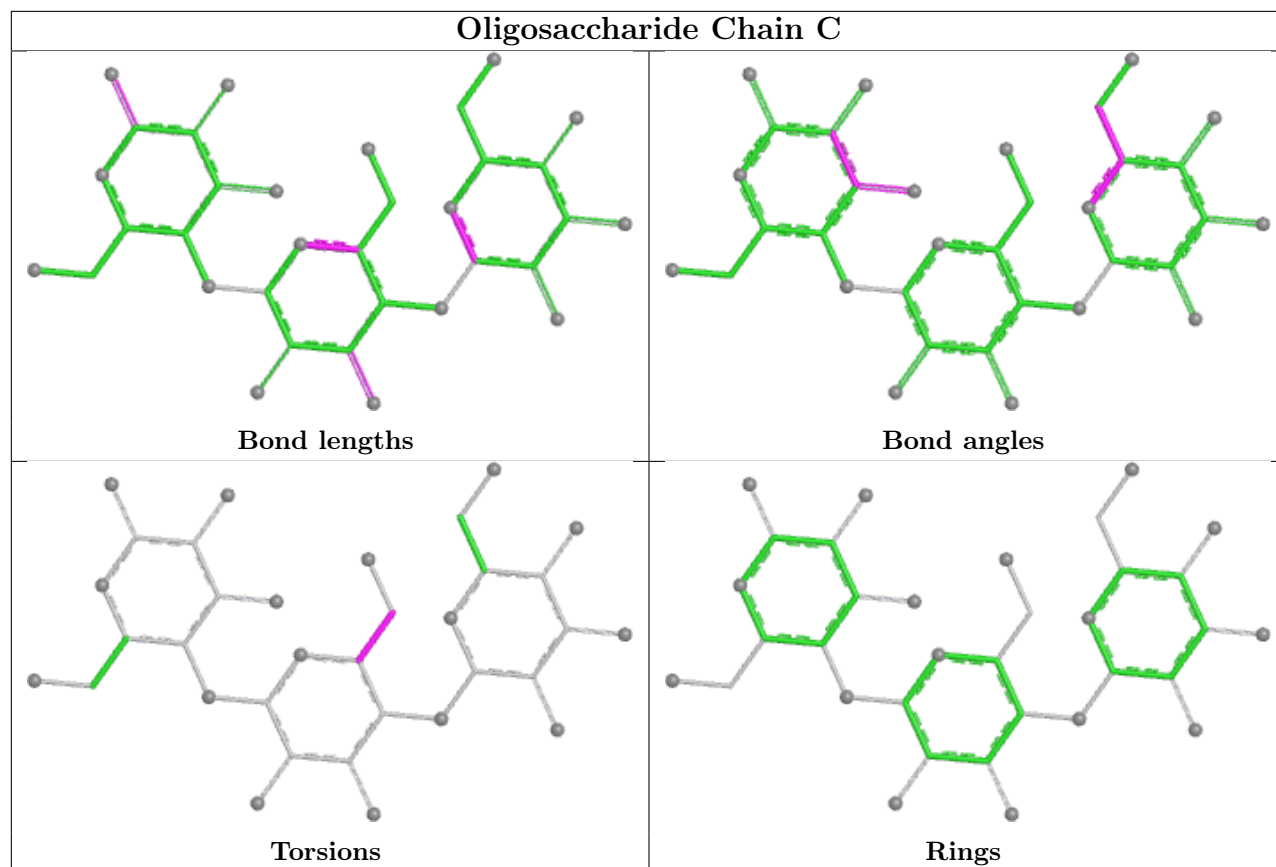
Mol	Chain	Res	Type	Atoms
4	E	5	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
4	E	2	GLC	O5-C5-C6-O6
5	F	3	GLC	O5-C5-C6-O6
4	E	4	GLC	O5-C5-C6-O6

There are no ring outliers.

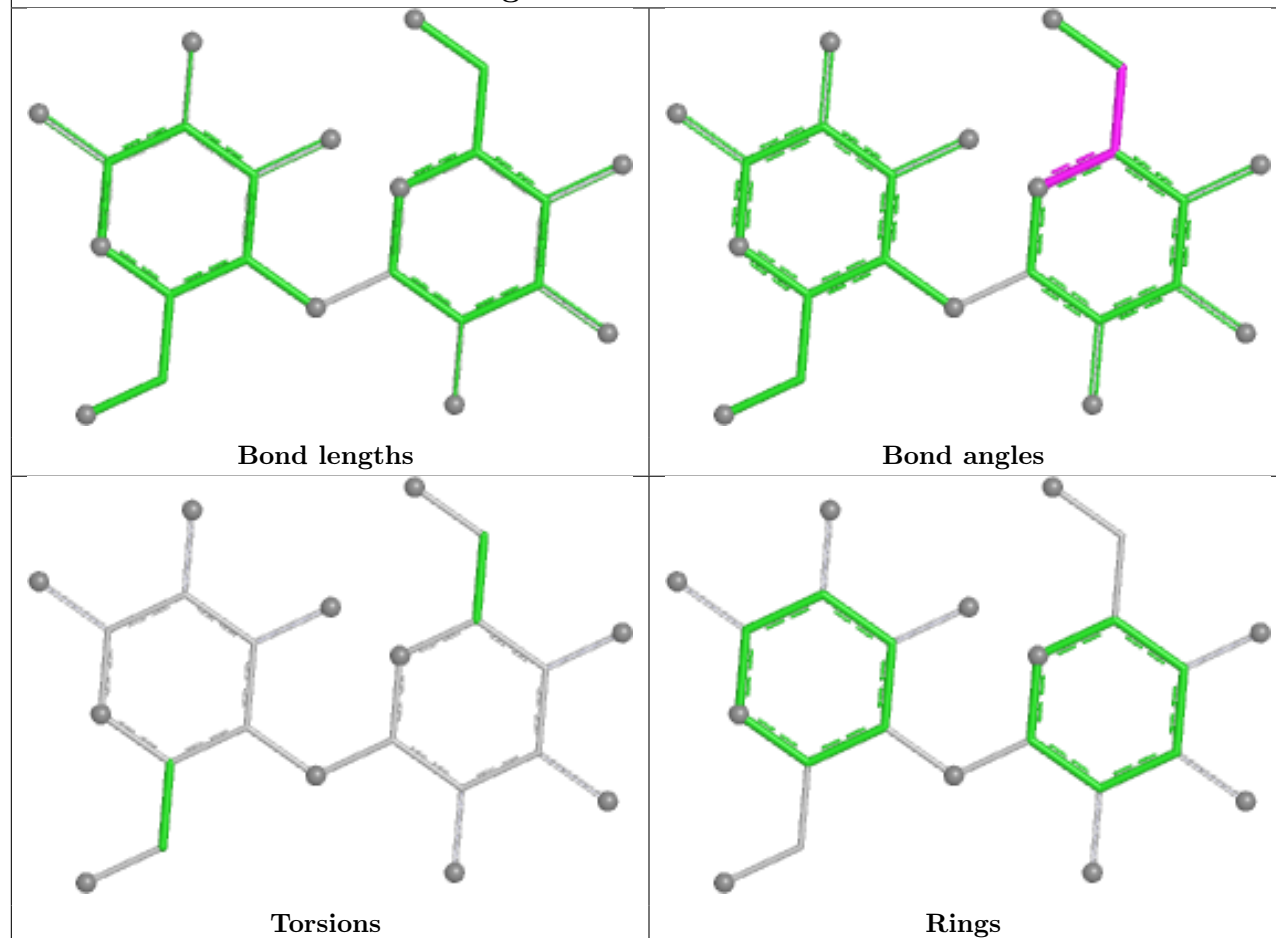
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	GLC	2	0
5	F	7	GLC	1	0
5	F	6	GLC	1	0
5	F	4	GLC	1	0
4	E	5	GLC	1	3
5	F	3	GLC	1	0
5	F	5	GLC	1	0
5	F	2	GLC	3	0
4	E	1	GLC	2	0
4	E	4	GLC	3	0

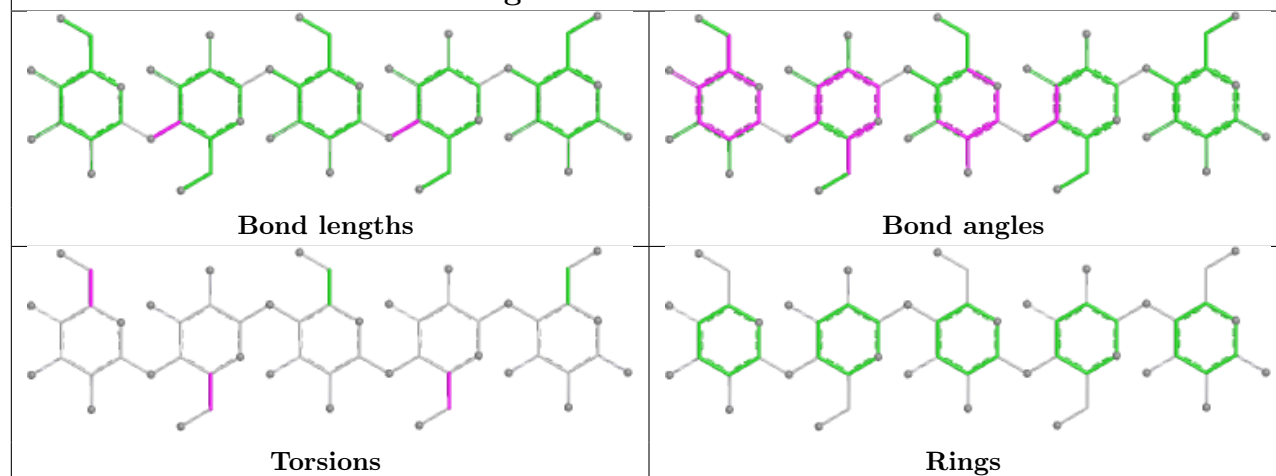
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

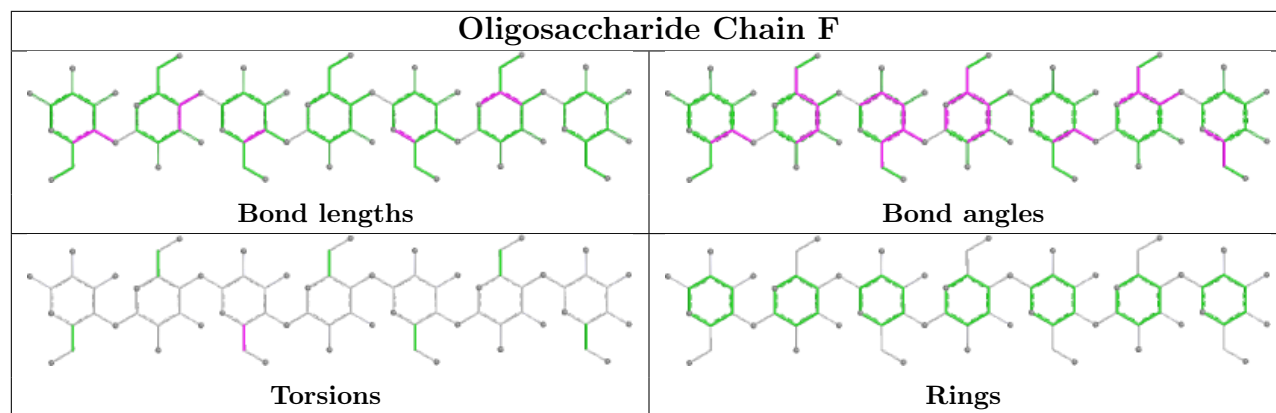


Oligosaccharide Chain D



Oligosaccharide Chain E





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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1526/1536 (99%)	-0.00	11 (0%) 84 73	79, 128, 184, 214	0
1	B	1526/1536 (99%)	0.04	16 (1%) 79 66	76, 139, 246, 294	0
All	All	3052/3072 (99%)	0.02	27 (0%) 81 68	76, 134, 220, 294	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	611	GLY	4.8
1	B	610	ILE	4.2
1	B	309	TRP	3.3
1	B	1511	SER	2.8
1	B	1128	ASP	2.8
1	A	1065	PRO	2.6
1	A	309	TRP	2.6
1	A	945	LEU	2.5
1	A	1519	PHE	2.4
1	B	1119	GLY	2.4
1	B	1506	PRO	2.4
1	A	610	ILE	2.4
1	A	1493	LEU	2.4
1	B	51	LEU	2.3
1	B	177	MET	2.3
1	B	183	LEU	2.3
1	A	1131	TRP	2.3
1	B	612	SER	2.2
1	A	1506	PRO	2.2
1	A	1060	MET	2.2
1	B	1391	VAL	2.2
1	B	387	ASP	2.2
1	B	1487	TRP	2.1
1	B	1519	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	694	SER	2.1
1	A	265	LEU	2.1
1	B	377	ALA	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](#)

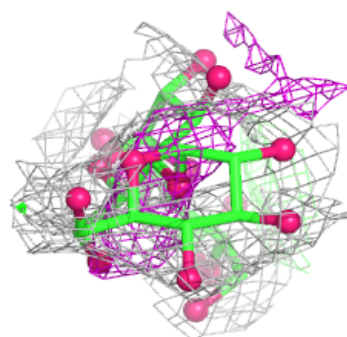
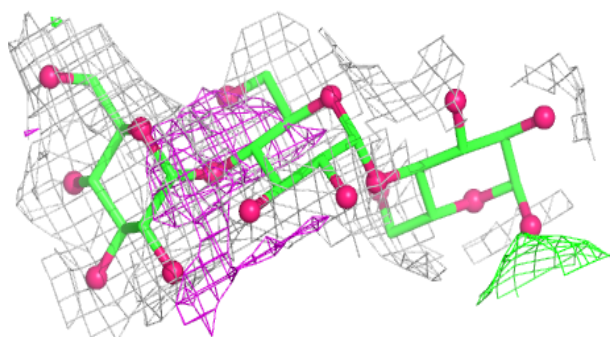
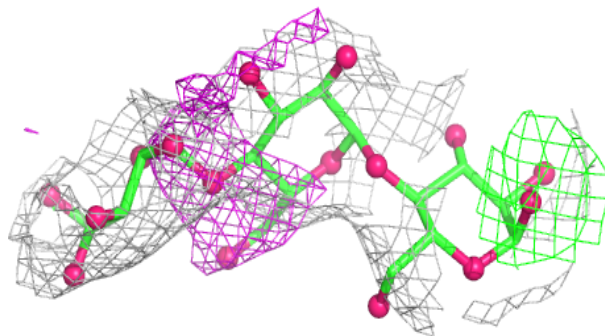
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	D	1	12/12	0.38	0.09	159,166,173,183	0
3	GLC	D	2	11/12	0.56	0.09	150,168,174,174	0
5	GLC	F	7	11/12	0.56	0.08	157,161,167,168	0
4	GLC	E	3	11/12	0.59	0.12	133,142,149,157	0
2	GLC	C	1	12/12	0.60	0.11	93,110,116,118	0
5	GLC	F	1	12/12	0.66	0.10	153,161,167,168	0
2	GLC	C	3	11/12	0.66	0.10	80,82,88,94	0
4	GLC	E	5	11/12	0.68	0.09	156,167,190,200	0
2	GLC	C	2	11/12	0.69	0.11	100,102,107,108	0
4	GLC	E	2	11/12	0.70	0.10	113,134,154,157	0
4	GLC	E	4	11/12	0.73	0.09	150,154,163,163	0
4	GLC	E	1	12/12	0.73	0.11	122,142,151,176	0
5	GLC	F	3	11/12	0.77	0.15	146,152,167,168	0
5	GLC	F	5	11/12	0.78	0.10	131,143,151,151	0
5	GLC	F	4	11/12	0.82	0.10	129,140,144,148	0
5	GLC	F	6	11/12	0.85	0.07	144,152,158,161	0
5	GLC	F	2	11/12	0.88	0.12	157,161,167,168	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.

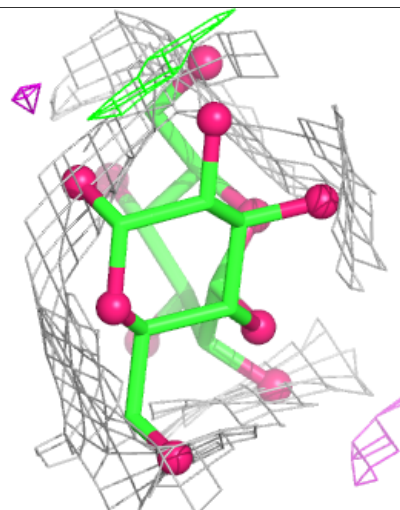
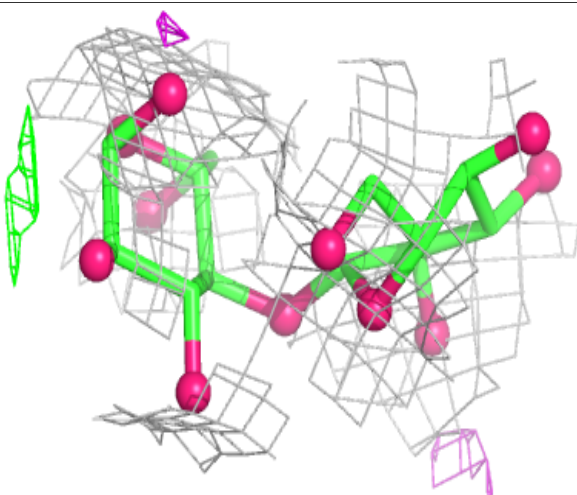
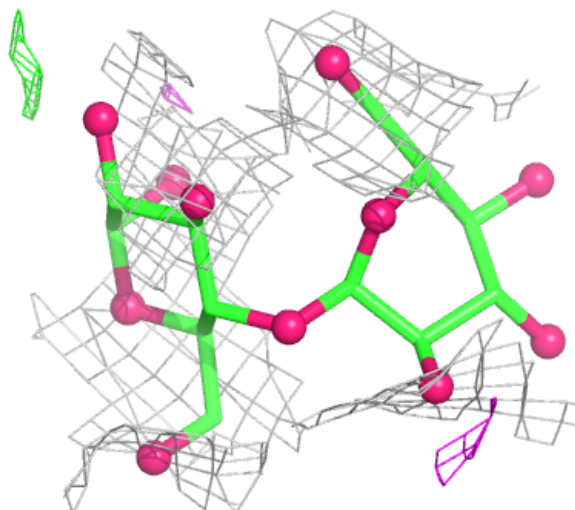
Electron density around Chain C:

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



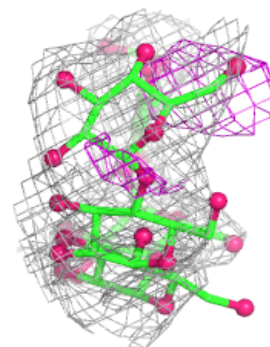
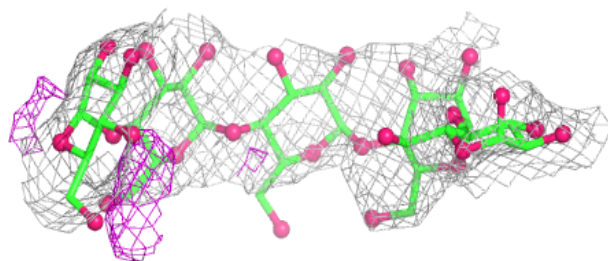
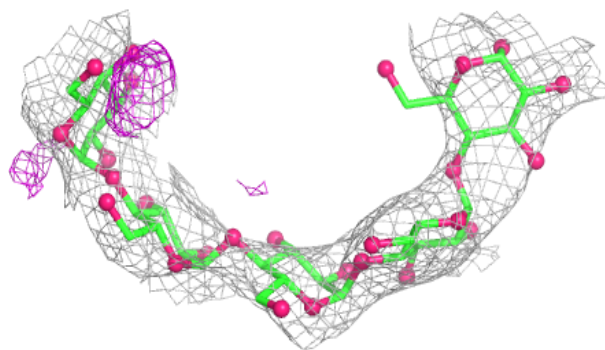
Electron density around Chain D:

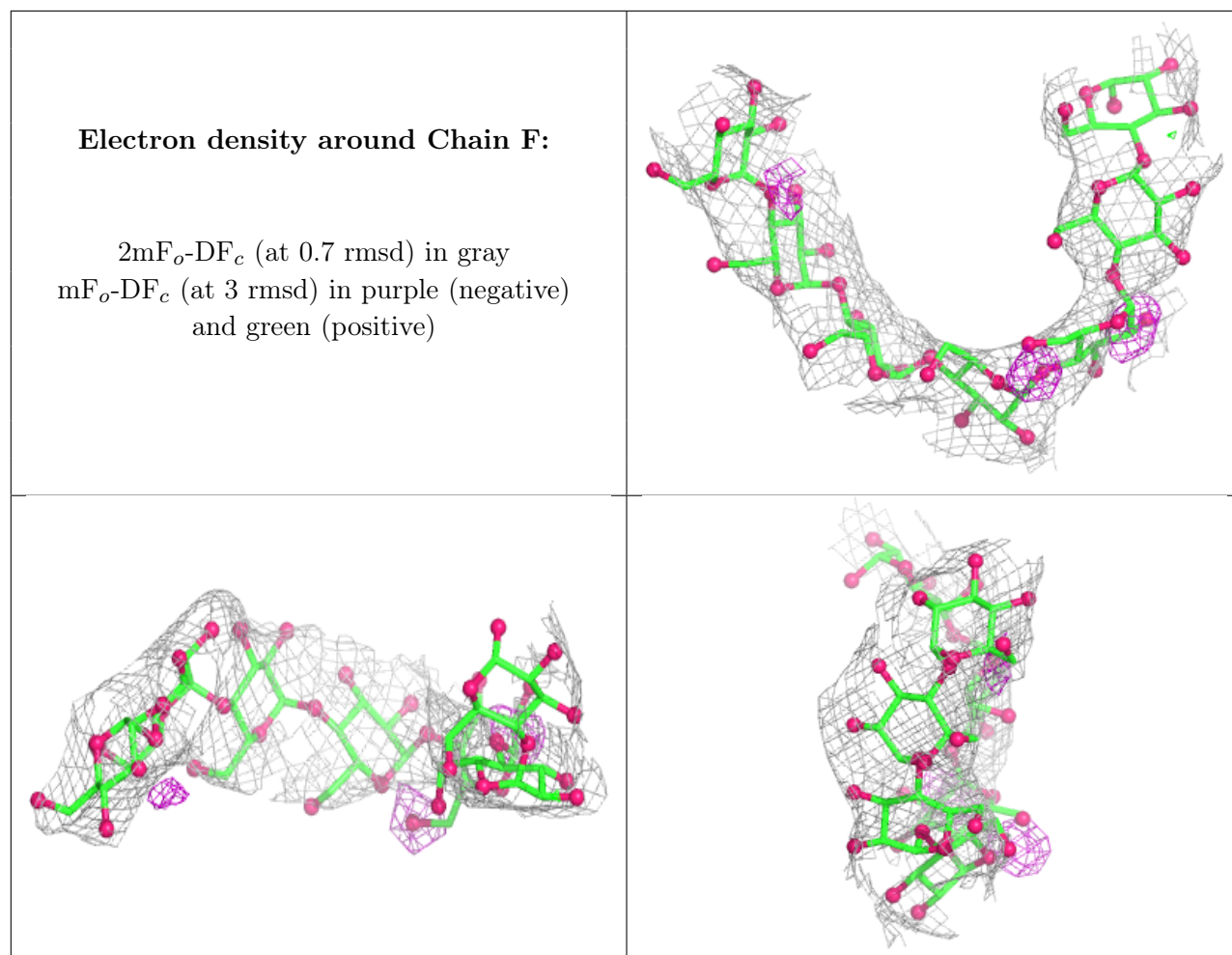
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.