



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 9JLR / pdb_00009jlr
Title : Crystal structure of GH57 family amylopullulanase from Aquifex aeolicus mutant E256Q in complex with maltopentaose
Authors : Zhu, Z.M.; Wang, W.W.; Li, M.J.; Xu, Q.; Zhou, H.; Huang, L.Q.; Wang, Q.S.; Yu, F.
Deposited on : 2024-09-19
Resolution : 2.79 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:

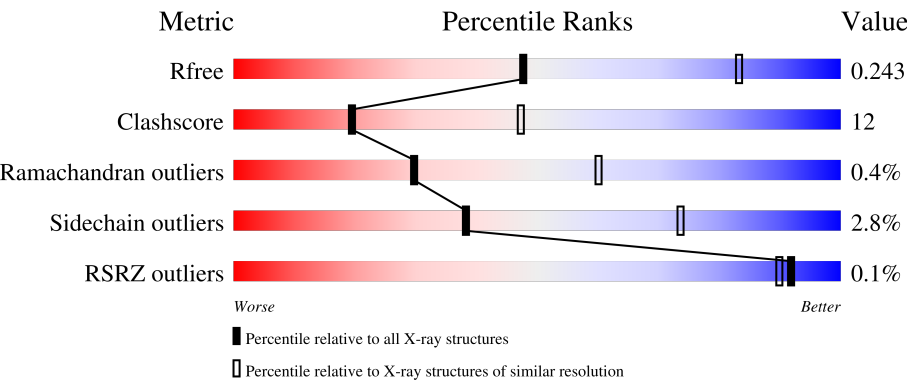
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	485	74%24%.
1	B	485	69%28%..
1	C	485	67%31%.
1	D	485	66%33%.
2	E	5	100%

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Mol	Chain	Length	Quality of chain
2	F	5	20% 80%
2	G	5	40% 60%
2	H	5	20% 60% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16627 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 Glycoside hydrolase family 57 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			4052	2651	649	742	10			
1	B	477	Total	C	N	O	S	0	0	0
			4052	2651	649	742	10			
1	C	484	Total	C	N	O	S	0	0	0
			4119	2692	666	751	10			
1	D	485	Total	C	N	O	S	0	0	0
			4129	2698	669	752	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	GLN	GLU	engineered mutation	UNP O66934
A	478	LEU	-	expression tag	UNP O66934
A	479	GLU	-	expression tag	UNP O66934
A	480	HIS	-	expression tag	UNP O66934
A	481	HIS	-	expression tag	UNP O66934
A	482	HIS	-	expression tag	UNP O66934
A	483	HIS	-	expression tag	UNP O66934
A	484	HIS	-	expression tag	UNP O66934
A	485	HIS	-	expression tag	UNP O66934
B	256	GLN	GLU	engineered mutation	UNP O66934
B	478	LEU	-	expression tag	UNP O66934
B	479	GLU	-	expression tag	UNP O66934
B	480	HIS	-	expression tag	UNP O66934
B	481	HIS	-	expression tag	UNP O66934
B	482	HIS	-	expression tag	UNP O66934
B	483	HIS	-	expression tag	UNP O66934
B	484	HIS	-	expression tag	UNP O66934
B	485	HIS	-	expression tag	UNP O66934
C	256	GLN	GLU	engineered mutation	UNP O66934
C	478	LEU	-	expression tag	UNP O66934

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Chain	Residue	Modelled	Actual	Comment	Reference
C	479	GLU	-	expression tag	UNP O66934
C	480	HIS	-	expression tag	UNP O66934
C	481	HIS	-	expression tag	UNP O66934
C	482	HIS	-	expression tag	UNP O66934
C	483	HIS	-	expression tag	UNP O66934
C	484	HIS	-	expression tag	UNP O66934
C	485	HIS	-	expression tag	UNP O66934
D	256	GLN	GLU	engineered mutation	UNP O66934
D	478	LEU	-	expression tag	UNP O66934
D	479	GLU	-	expression tag	UNP O66934
D	480	HIS	-	expression tag	UNP O66934
D	481	HIS	-	expression tag	UNP O66934
D	482	HIS	-	expression tag	UNP O66934
D	483	HIS	-	expression tag	UNP O66934
D	484	HIS	-	expression tag	UNP O66934
D	485	HIS	-	expression tag	UNP O66934

- Molecule 2 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
2	E	5	Total	C	O	0	0	0
			56	30	26			
2	F	5	Total	C	O	0	0	0
			56	30	26			
2	G	5	Total	C	O	0	0	0
			56	30	26			
2	H	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	10	Total	O	0	0
			10	10		

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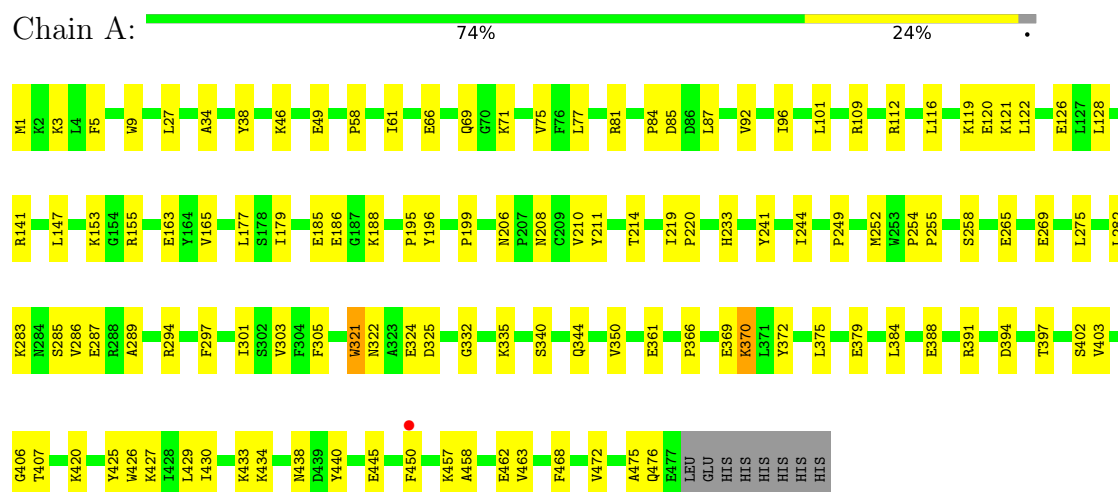
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	8	Total	O	0	0
			8	8		
3	D	12	Total	O	0	0
			12	12		

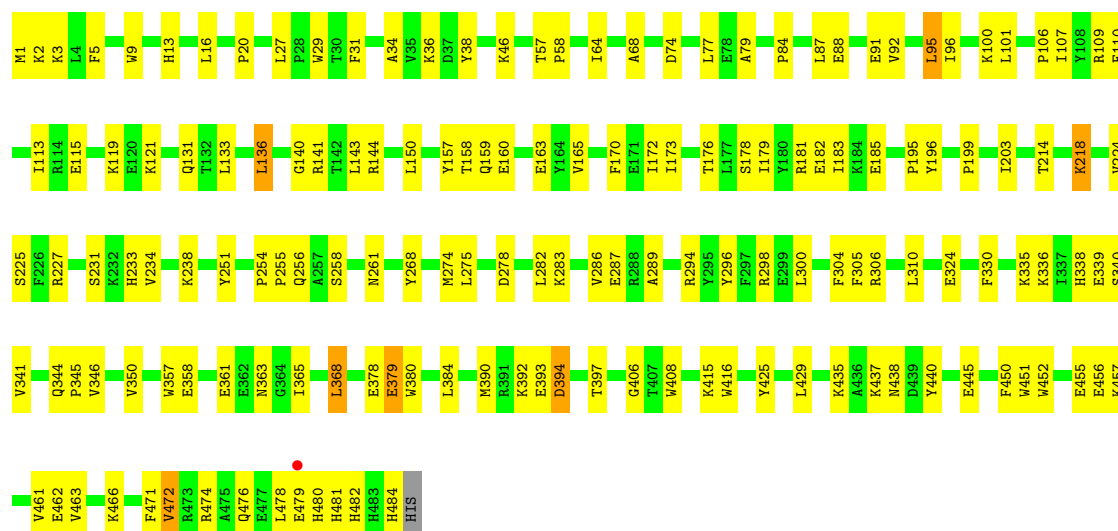
3 Residue-property plots

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: Glycoside hydrolase family 57 N-terminal domain-containing protein

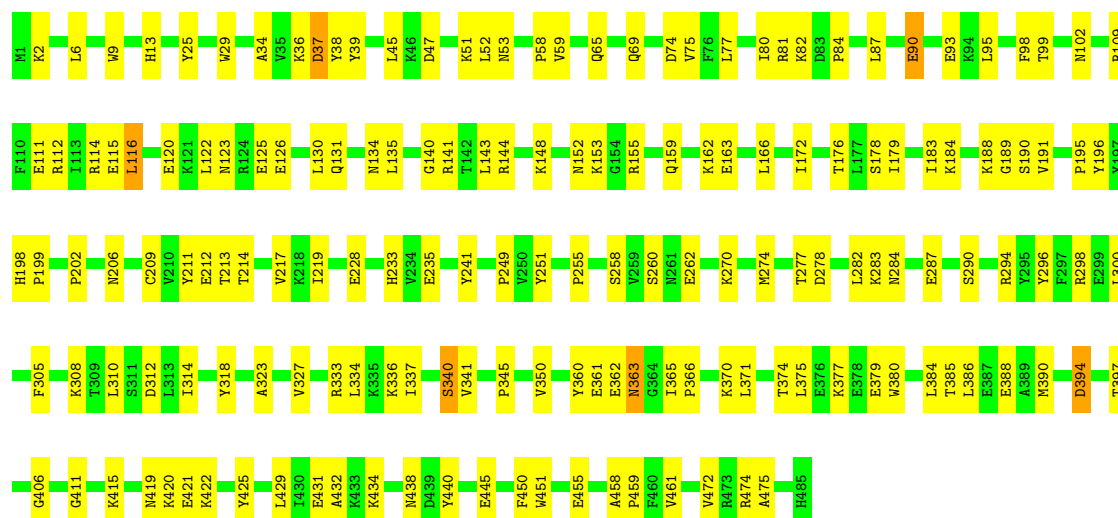


Chain C:  67% 31% .

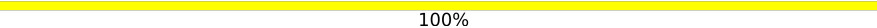


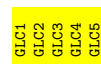
- Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain D:  66% 33% .

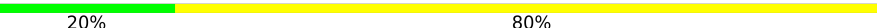


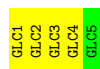
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  100%



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

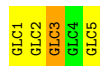
Chain F:  20% 80%



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.17Å 165.17Å 98.01Å 90.00° 109.46° 90.00°	Depositor
Resolution (Å)	46.01 – 2.79 46.01 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.01-2.79) 98.1 (46.01-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.188 , 0.245 0.189 , 0.243	Depositor DCC
R_{free} test set	2615 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16627	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/4165	0.40	0/5633
1	B	0.26	0/4165	0.41	0/5633
1	C	0.21	0/4237	0.38	0/5731
1	D	0.21	0/4248	0.39	0/5746
All	All	0.23	0/16815	0.40	0/22743

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4052	0	3989	74	0
1	B	4052	0	3989	97	1
1	C	4119	0	4041	105	1
1	D	4129	0	4048	108	0
2	E	56	0	48	1	0
2	F	56	0	48	2	0
2	G	56	0	48	6	0
2	H	56	0	48	1	0
3	A	21	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	3	0
3	C	8	0	0	2	0
3	D	12	0	0	2	0
All	All	16627	0	16259	382	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:HE22	2:G:1:GLC:H1	1.06	1.13
1:C:256:GLN:NE2	2:G:1:GLC:H1	1.75	1.01
1:C:256:GLN:HE22	2:G:1:GLC:C1	1.91	0.81
1:B:214:THR:OG1	3:B:501:HOH:O	2.01	0.79
1:B:403:VAL:O	3:B:502:HOH:O	2.02	0.77
1:B:438:ASN:ND2	1:B:474:ARG:O	2.18	0.76
1:C:415:LYS:NZ	1:C:455:GLU:OE1	2.22	0.72
1:B:401:GLU:OE1	3:B:503:HOH:O	2.09	0.71
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.55	0.70
1:C:101:LEU:HD11	2:G:4:GLC:H2	1.74	0.70
1:B:101:LEU:HD12	1:B:460:PHE:CE2	2.28	0.68
1:B:297:PHE:HB3	1:B:301:ILE:HG22	1.75	0.68
1:D:99:THR:HG22	1:D:134:ASN:HD21	1.56	0.68
2:G:1:GLC:O3	2:G:2:GLC:C1	2.41	0.67
1:D:120:GLU:CD	1:D:120:GLU:H	2.02	0.66
1:C:110:PHE:HB2	1:C:113:ILE:HD12	1.77	0.65
1:D:84:PRO:HA	1:D:87:LEU:HD12	1.79	0.65
1:B:199:PRO:HG2	1:B:201:ILE:CD1	2.26	0.65
1:D:362:GLU:O	1:D:365:ILE:HD12	1.98	0.64
1:D:340:SER:O	3:D:501:HOH:O	2.15	0.63
1:A:391:ARG:NH2	3:A:507:HOH:O	2.32	0.63
1:B:96:ILE:HG23	1:B:117:MET:HE1	1.80	0.63
1:A:210:VAL:HG21	1:A:219:ILE:HG21	1.81	0.63
1:D:115:GLU:OE2	1:D:155:ARG:NH2	2.31	0.63
1:B:327:VAL:HG21	1:B:370:LYS:HB3	1.79	0.63
1:D:34:ALA:HA	1:D:38:TYR:HB2	1.80	0.62
1:C:294:ARG:HG3	1:C:304:PHE:CZ	2.35	0.62
1:B:427:LYS:O	1:B:431:GLU:HG2	2.00	0.62
1:C:195:PRO:HB3	1:C:233:HIS:HB3	1.81	0.62
1:D:195:PRO:HB3	1:D:233:HIS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PRO:HB3	1:A:233:HIS:HB3	1.82	0.61
1:C:181:ARG:O	1:C:185:GLU:HG2	2.00	0.61
1:B:101:LEU:HD21	2:F:4:GLC:H2	1.82	0.61
1:D:95:LEU:O	1:D:99:THR:HG23	1.99	0.61
1:C:435:LYS:HB2	1:C:476:GLN:HE21	1.65	0.61
1:B:258:SER:HB3	1:B:407:THR:HG22	1.83	0.61
1:C:390:MET:HE2	1:C:390:MET:HA	1.82	0.61
1:D:379:GLU:H	1:D:379:GLU:CD	2.07	0.61
1:C:452:TRP:HB3	1:C:461:VAL:HG22	1.82	0.60
1:B:423:ASN:O	1:B:427:LYS:HG3	2.02	0.60
1:A:468:PHE:O	1:A:472:VAL:HG23	2.01	0.60
1:C:143:LEU:HG	1:C:172:ILE:HD11	1.84	0.60
1:B:262:GLU:N	1:B:262:GLU:OE2	2.35	0.60
1:D:9:TRP:HB3	1:D:350:VAL:HG22	1.83	0.60
1:B:101:LEU:HD12	1:B:460:PHE:HE2	1.65	0.60
1:A:49:GLU:OE1	3:A:503:HOH:O	2.17	0.59
1:B:264:LEU:HD23	1:B:275:LEU:HD21	1.84	0.59
1:B:19:GLU:HB3	1:B:22:THR:HG22	1.85	0.59
1:D:74:ASP:HB3	1:D:77:LEU:HB2	1.85	0.59
1:A:3:LYS:H	1:A:344:GLN:HE21	1.49	0.59
1:A:366:PRO:O	1:A:370:LYS:HD2	2.03	0.59
1:A:85:ASP:OD1	3:A:504:HOH:O	2.17	0.58
1:C:394:ASP:OD1	1:C:394:ASP:N	2.36	0.58
1:D:294:ARG:HH12	1:D:390:MET:HA	1.67	0.58
1:B:46:LYS:HD2	1:B:179:ILE:HD11	1.85	0.58
1:D:209:CYS:O	1:D:212:GLU:HG3	2.04	0.58
1:C:378:GLU:OE2	1:C:380:TRP:NE1	2.36	0.58
1:C:484:HIS:ND1	3:C:502:HOH:O	2.31	0.58
1:D:65:GLN:O	1:D:69:GLN:HG3	2.04	0.58
1:A:120:GLU:CD	1:A:120:GLU:H	2.11	0.57
1:D:116:LEU:HD13	1:D:122:LEU:HD22	1.84	0.57
1:D:176:THR:O	1:D:179:ILE:HG22	2.04	0.57
1:B:199:PRO:HG2	1:B:201:ILE:HD12	1.86	0.57
1:B:111:GLU:CD	1:B:111:GLU:H	2.12	0.56
1:C:68:ALA:HB2	1:C:173:ILE:HG22	1.87	0.56
1:D:143:LEU:HG	1:D:172:ILE:HD11	1.87	0.56
1:A:430:ILE:HG22	1:A:434:LYS:NZ	2.20	0.56
1:B:255:PRO:O	1:B:258:SER:OG	2.22	0.56
1:B:324:GLU:HG2	1:B:370:LYS:HE3	1.88	0.56
1:B:344:GLN:NE2	1:B:394:ASP:HB3	2.21	0.56
1:C:150:LEU:O	1:C:157:TYR:OH	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PRO:HB2	1:C:199:PRO:HD2	1.87	0.56
1:B:9:TRP:HB3	1:B:350:VAL:HG22	1.88	0.56
1:C:119:LYS:HD2	1:C:121:LYS:O	2.06	0.56
1:D:53:ASN:ND2	1:D:190:SER:H	2.03	0.56
1:B:104:GLU:OE2	1:B:104:GLU:N	2.34	0.55
1:C:136:LEU:HD11	1:C:165:VAL:HG21	1.89	0.55
1:C:92:VAL:O	1:C:96:ILE:HG12	2.07	0.55
1:C:462:GLU:CD	1:C:462:GLU:H	2.15	0.55
1:D:141:ARG:HG3	1:D:365:ILE:HG12	1.88	0.55
1:B:420:LYS:O	1:B:424:GLU:HG3	2.07	0.54
1:A:429:LEU:HD21	1:A:445:GLU:HG2	1.90	0.54
1:D:6:LEU:HD22	1:D:334:LEU:HD21	1.90	0.54
1:D:159:GLN:O	1:D:163:GLU:HG3	2.08	0.54
1:A:332:GLY:O	1:A:335:LYS:HG2	2.08	0.54
1:C:384:LEU:HD11	1:C:392:LYS:HE2	1.89	0.54
1:A:220:PRO:HB3	1:A:427:LYS:HE3	1.89	0.54
1:A:147:LEU:HD13	1:A:165:VAL:HG22	1.90	0.54
1:A:425:TYR:HB3	1:A:450:PHE:CE1	2.43	0.54
1:D:294:ARG:HD2	1:D:296:TYR:CZ	2.43	0.53
1:D:36:LYS:HG2	1:D:363:ASN:HD21	1.74	0.53
1:C:254:PRO:HG3	1:C:275:LEU:HD13	1.90	0.53
1:D:2:LYS:NZ	1:D:341:VAL:O	2.41	0.53
1:A:195:PRO:HB2	1:A:199:PRO:HD2	1.89	0.53
1:D:90:GLU:HA	1:D:93:GLU:OE2	2.08	0.53
1:D:228:GLU:CD	1:D:228:GLU:H	2.17	0.53
1:B:242:PHE:HB2	1:B:248:HIS:HD2	1.74	0.53
1:B:282:LEU:HB2	1:B:305:PHE:CD2	2.44	0.52
1:B:374:THR:O	1:B:378:GLU:HG2	2.09	0.52
1:C:29:TRP:CD2	2:G:3:GLC:H2	2.43	0.52
1:C:141:ARG:HD3	1:C:365:ILE:HG12	1.91	0.52
1:A:34:ALA:HA	1:A:38:TYR:HB2	1.92	0.52
1:D:13:HIS:CE1	1:D:198:HIS:HB2	2.44	0.52
1:C:435:LYS:HD2	1:C:476:GLN:HE22	1.75	0.52
1:C:3:LYS:HG3	1:C:344:GLN:HE21	1.75	0.51
1:C:34:ALA:HA	1:C:38:TYR:HB2	1.91	0.51
1:D:211:TYR:OH	1:D:219:ILE:HG12	2.10	0.51
1:D:318:TYR:HB2	1:D:360:TYR:OH	2.11	0.51
1:A:92:VAL:O	1:A:96:ILE:HG13	2.10	0.51
1:B:27:LEU:HD22	1:B:29:TRP:NE1	2.26	0.51
1:C:20:PRO:HD3	1:C:471:PHE:CE1	2.45	0.51
1:C:294:ARG:HD2	1:C:296:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:LYS:HB2	1:C:476:GLN:NE2	2.26	0.51
1:D:458:ALA:HB1	1:D:459:PRO:HD2	1.93	0.51
1:B:74:ASP:HB3	1:B:77:LEU:HB2	1.91	0.51
1:D:189:GLY:HA2	1:D:385:THR:HG22	1.93	0.51
1:D:51:LYS:HD2	1:D:385:THR:HG23	1.94	0.50
1:A:325:ASP:OD2	1:B:283:LYS:HD2	2.12	0.50
1:C:2:LYS:C	1:C:338:HIS:HE2	2.19	0.50
1:C:88:GLU:HB2	1:C:91:GLU:HG3	1.93	0.50
1:D:425:TYR:HB3	1:D:450:PHE:CE2	2.46	0.50
1:D:283:LYS:HE3	1:D:284:ASN:OD1	2.11	0.50
1:A:457:LYS:HD2	1:A:458:ALA:N	2.26	0.50
1:D:99:THR:CG2	1:D:134:ASN:HD21	2.23	0.50
1:A:375:LEU:O	3:A:505:HOH:O	2.20	0.50
1:D:29:TRP:CD2	2:H:3:GLC:H2	2.47	0.50
1:D:45:LEU:HD13	1:D:188:LYS:HB3	1.93	0.50
1:C:9:TRP:HB3	1:C:350:VAL:HG22	1.93	0.49
1:C:438:ASN:HB3	1:C:479:GLU:HG2	1.94	0.49
1:A:5:PHE:HB3	1:A:384:LEU:HD12	1.93	0.49
1:C:261:ASN:HB3	1:C:298:ARG:HH22	1.76	0.49
1:B:140:GLY:O	1:B:144:ARG:HG3	2.12	0.49
1:C:5:PHE:HB2	1:C:346:VAL:HG22	1.93	0.49
1:D:183:ILE:HG13	1:D:184:LYS:N	2.27	0.49
1:B:141:ARG:HB2	1:B:365:ILE:HG12	1.94	0.49
1:A:384:LEU:HD22	1:A:388:GLU:HB3	1.94	0.49
1:A:241:TYR:HB3	1:A:249:PRO:HD3	1.95	0.49
1:C:170:PHE:HA	1:C:173:ILE:HD12	1.95	0.49
1:D:81:ARG:HD2	1:D:81:ARG:C	2.38	0.49
1:C:159:GLN:O	1:C:163:GLU:HG3	2.13	0.48
1:D:81:ARG:NH1	1:D:82:LYS:HG3	2.27	0.48
1:A:112:ARG:HH12	1:A:119:LYS:NZ	2.11	0.48
1:C:341:VAL:HG21	1:C:345:PRO:HB3	1.95	0.48
1:D:80:ILE:O	1:D:162:LYS:NZ	2.46	0.48
1:A:61:ILE:HD13	1:A:244:ILE:HG13	1.94	0.48
1:B:116:LEU:CD2	1:B:126:GLU:HB3	2.43	0.48
1:D:419:ASN:HD21	1:D:422:LYS:HE3	1.77	0.48
1:D:421:GLU:H	1:D:421:GLU:CD	2.21	0.48
1:B:287:GLU:HG3	1:B:288:ARG:H	1.77	0.48
1:D:294:ARG:NH1	1:D:390:MET:HA	2.29	0.48
1:A:9:TRP:HB3	1:A:350:VAL:HG22	1.95	0.48
1:A:66:GLU:HG3	1:A:71:LYS:HB2	1.95	0.48
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ILE:O	1:B:183:ILE:HG23	2.13	0.48
1:C:79:ALA:O	1:C:131:GLN:NE2	2.47	0.48
1:A:58:PRO:HG2	1:A:196:TYR:HA	1.94	0.48
1:C:437:LYS:HD2	1:C:478:LEU:HD23	1.94	0.48
1:B:120:GLU:OE2	1:B:120:GLU:N	2.39	0.48
1:C:176:THR:O	1:C:179:ILE:HG22	2.14	0.48
1:D:112:ARG:O	1:D:116:LEU:HD23	2.14	0.48
1:D:377:LYS:HD3	1:D:377:LYS:C	2.39	0.48
1:B:258:SER:HA	1:B:406:GLY:O	2.14	0.47
1:B:362:GLU:HB2	1:B:366:PRO:HD3	1.96	0.47
1:C:74:ASP:HB3	1:C:77:LEU:HB2	1.95	0.47
1:A:297:PHE:HB3	1:A:301:ILE:HG22	1.95	0.47
1:A:321:TRP:CD1	1:A:321:TRP:N	2.82	0.47
1:C:415:LYS:HB3	1:C:416:TRP:CZ3	2.49	0.47
1:D:99:THR:HG21	1:D:130:LEU:HD11	1.96	0.47
1:D:251:TYR:HB3	1:D:274:MET:HE3	1.97	0.47
1:A:372:TYR:OH	3:A:502:HOH:O	2.10	0.47
1:D:36:LYS:NZ	1:D:37:ASP:OD1	2.47	0.47
1:D:415:LYS:HE3	1:D:451:TRP:CD2	2.49	0.47
1:A:186:GLU:HB3	1:A:188:LYS:HG3	1.95	0.47
1:A:275:LEU:HD22	1:A:301:ILE:HD13	1.97	0.47
1:B:101:LEU:HD12	1:B:460:PHE:CD2	2.49	0.47
1:C:107:ILE:HD13	1:C:358:GLU:HB2	1.95	0.47
1:C:113:ILE:HD11	1:C:133:LEU:HB3	1.97	0.47
1:C:258:SER:HA	1:C:406:GLY:O	2.15	0.47
1:D:195:PRO:HB2	1:D:199:PRO:HD2	1.96	0.47
1:A:101:LEU:HD11	2:E:4:GLC:H2	1.96	0.47
1:B:36:LYS:HG2	1:B:363:ASN:ND2	2.30	0.47
1:C:335:LYS:HG3	1:C:380:TRP:CZ2	2.49	0.47
1:D:123:ASN:HD22	1:D:125:GLU:H	1.63	0.47
1:D:431:GLU:HA	1:D:434:LYS:HD2	1.97	0.47
1:B:440:TYR:HA	1:B:443:VAL:HG23	1.96	0.47
1:A:27:LEU:HG	1:A:463:VAL:HG11	1.97	0.46
1:B:27:LEU:HD22	1:B:29:TRP:HE1	1.79	0.46
1:C:140:GLY:O	1:C:144:ARG:HG3	2.15	0.46
1:D:310:LEU:O	1:D:314:ILE:HG13	2.15	0.46
1:B:421:GLU:HA	1:B:424:GLU:OE1	2.15	0.46
1:C:182:GLU:HG3	1:C:183:ILE:N	2.29	0.46
1:D:135:LEU:HD11	1:D:166:LEU:HG	1.96	0.46
1:D:235:GLU:HG2	1:D:270:LYS:HD2	1.97	0.46
1:B:13:HIS:CE1	1:B:198:HIS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:180:TYR:CD1	2.50	0.46
1:A:81:ARG:HH12	1:A:163:GLU:HG2	1.80	0.46
1:B:52:LEU:O	1:B:189:GLY:HA3	2.16	0.46
1:C:218:LYS:H	1:C:218:LYS:HG2	1.58	0.46
1:C:379:GLU:H	1:C:379:GLU:HG3	1.42	0.46
1:A:438:ASN:OD1	1:A:440:TYR:HB2	2.16	0.46
1:A:220:PRO:HG3	1:A:426:TRP:HB2	1.97	0.46
1:B:155:ARG:HG3	1:B:156:ASN:OD1	2.15	0.46
1:C:36:LYS:HD2	1:C:363:ASN:OD1	2.15	0.46
1:C:438:ASN:CB	1:C:479:GLU:HG2	2.46	0.46
1:D:123:ASN:ND2	1:D:126:GLU:HG3	2.31	0.46
1:D:152:ASN:O	3:D:502:HOH:O	2.20	0.46
1:B:79:ALA:O	1:B:131:GLN:NE2	2.49	0.46
1:B:313:LEU:HA	1:B:317:SER:HB2	1.96	0.46
1:B:462:GLU:O	1:B:466:LYS:HG2	2.15	0.46
1:C:440:TYR:CD2	1:C:474:ARG:HG2	2.51	0.46
1:D:440:TYR:CD2	1:D:474:ARG:HG3	2.51	0.46
1:C:115:GLU:OE1	3:C:501:HOH:O	2.20	0.46
1:A:81:ARG:HD3	1:A:81:ARG:C	2.41	0.46
1:B:101:LEU:CD2	2:F:4:GLC:H2	2.45	0.46
1:C:472:VAL:O	1:C:476:GLN:HG3	2.16	0.46
1:B:259:VAL:O	1:B:405:ALA:HA	2.16	0.45
1:B:144:ARG:NH2	1:B:363:ASN:HB2	2.31	0.45
1:B:199:PRO:HG3	1:B:233:HIS:CG	2.51	0.45
1:B:234:VAL:O	1:B:238:LYS:HG3	2.17	0.45
1:C:425:TYR:HB3	1:C:450:PHE:CE1	2.51	0.45
1:B:438:ASN:OD1	1:B:440:TYR:HB2	2.16	0.45
1:C:160:GLU:OE2	1:C:160:GLU:N	2.32	0.45
1:D:109:ARG:NH2	1:D:361:GLU:OE1	2.50	0.45
1:D:206:ASN:HB3	1:D:262:GLU:OE2	2.17	0.45
1:B:5:PHE:CD1	1:B:384:LEU:HD11	2.51	0.45
1:D:214:THR:HB	1:D:217:VAL:HG13	1.99	0.45
1:A:46:LYS:HE2	1:A:179:ILE:HD11	1.98	0.45
1:A:109:ARG:NH2	1:A:361:GLU:OE2	2.50	0.45
1:B:120:GLU:H	1:B:120:GLU:CD	2.24	0.45
1:C:294:ARG:CD	1:C:296:TYR:HE1	2.30	0.45
1:D:140:GLY:O	1:D:144:ARG:HG2	2.16	0.45
1:A:322:ASN:HD21	1:B:288:ARG:HB3	1.80	0.45
1:D:432:ALA:HB2	1:D:472:VAL:HG13	1.98	0.45
1:C:234:VAL:O	1:C:238:LYS:HG3	2.17	0.44
1:D:99:THR:HG22	1:D:134:ASN:ND2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LYS:O	1:D:312:ASP:HB2	2.17	0.44
1:B:379:GLU:OE2	1:D:148:LYS:HE2	2.17	0.44
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.85	0.44
1:C:294:ARG:HD2	1:C:296:TYR:CE1	2.52	0.44
1:A:121:LYS:HG3	1:A:122:LEU:N	2.33	0.44
1:A:457:LYS:HD2	1:A:458:ALA:H	1.82	0.44
1:B:235:GLU:HG2	1:B:270:LYS:HD2	1.99	0.44
1:C:478:LEU:HD12	1:C:482:HIS:CD2	2.52	0.44
1:A:84:PRO:HA	1:A:87:LEU:HD12	2.00	0.44
1:D:258:SER:HA	1:D:406:GLY:O	2.17	0.44
1:B:16:LEU:HD23	1:B:443:VAL:HG11	1.99	0.44
1:C:274:MET:HE3	1:C:274:MET:HB3	1.90	0.44
1:B:218:LYS:HE3	1:B:218:LYS:HB3	1.86	0.44
1:B:296:TYR:CE1	1:B:302:SER:HB2	2.53	0.44
1:C:2:LYS:HG3	1:C:344:GLN:HG3	1.99	0.44
1:C:457:LYS:HD2	1:C:457:LYS:C	2.43	0.44
1:D:52:LEU:C	1:D:53:ASN:HD22	2.26	0.44
1:A:294:ARG:O	1:A:397:THR:HA	2.18	0.44
1:B:414:LEU:HA	1:B:417:ILE:O	2.18	0.44
1:C:451:TRP:HD1	1:C:452:TRP:CD2	2.36	0.44
1:B:274:MET:HE1	1:B:386:LEU:HD22	1.99	0.43
1:C:1:MET:HB2	1:C:1:MET:HE2	1.65	0.43
1:D:25:TYR:HB2	1:D:74:ASP:HA	1.99	0.43
1:A:177:LEU:H	1:A:177:LEU:HD12	1.83	0.43
1:A:438:ASN:OD1	1:A:475:ALA:HA	2.17	0.43
1:B:279:GLU:O	1:B:283:LYS:HG2	2.18	0.43
1:A:285:SER:HB3	1:A:403:VAL:HA	1.99	0.43
1:B:57:THR:HG22	1:B:194:SER:HB2	1.99	0.43
1:B:195:PRO:HB3	1:B:233:HIS:HB3	2.00	0.43
1:D:111:GLU:HA	1:D:114:ARG:HG3	2.00	0.43
1:A:199:PRO:HG3	1:A:233:HIS:CG	2.54	0.43
1:C:160:GLU:H	1:C:160:GLU:CD	2.24	0.43
1:B:6:LEU:O	1:B:383:THR:HA	2.17	0.43
1:B:195:PRO:HB2	1:B:199:PRO:HD2	2.00	0.43
1:C:225:SER:OG	1:C:227:ARG:HD2	2.18	0.43
1:B:22:THR:HG23	1:B:24:GLU:H	1.84	0.43
1:B:323:ALA:O	1:B:327:VAL:HG23	2.17	0.43
1:C:106:PRO:HB3	1:C:109:ARG:NH2	2.34	0.43
1:D:36:LYS:HG2	1:D:363:ASN:ND2	2.34	0.43
1:D:241:TYR:HB3	1:D:249:PRO:HD3	2.01	0.43
1:D:298:ARG:HB2	1:D:300:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ALA:HB1	1:B:367:PHE:HA	2.01	0.43
1:C:268:TYR:CE2	1:C:300:LEU:HD13	2.54	0.43
1:D:323:ALA:O	1:D:327:VAL:HG23	2.19	0.43
1:A:69:GLN:O	1:A:71:LYS:HE3	2.19	0.43
1:D:420:LYS:HB3	1:D:420:LYS:HE2	1.75	0.43
1:A:283:LYS:HA	1:A:283:LYS:HD3	1.77	0.42
1:A:402:SER:OG	3:A:506:HOH:O	2.22	0.42
1:A:472:VAL:O	1:A:476:GLN:HG3	2.19	0.42
1:B:34:ALA:HA	1:B:38:TYR:HB2	1.99	0.42
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.85	0.42
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.79	0.42
1:A:282:LEU:HB2	1:A:305:PHE:CD2	2.54	0.42
1:B:261:ASN:O	1:B:265:GLU:HG3	2.18	0.42
1:D:202:PRO:HB3	1:D:260:SER:HB3	2.01	0.42
1:A:81:ARG:NH1	1:A:163:GLU:OE2	2.50	0.42
1:B:55:ASN:ND2	1:B:253:TRP:HB3	2.35	0.42
1:C:100:LYS:HB2	1:C:100:LYS:HE3	1.70	0.42
1:D:282:LEU:HB2	1:D:305:PHE:CD1	2.54	0.42
1:A:141:ARG:NH1	1:A:369:GLU:OE2	2.48	0.42
1:A:265:GLU:O	1:A:269:GLU:HG3	2.19	0.42
1:C:310:LEU:HG	1:C:330:PHE:CE1	2.54	0.42
1:C:415:LYS:HB3	1:C:416:TRP:CE3	2.55	0.42
1:D:294:ARG:HD2	1:D:296:TYR:CE1	2.54	0.42
1:A:275:LEU:HD21	1:A:303:VAL:HG22	2.01	0.42
1:B:56:LEU:HD11	1:B:180:TYR:CE1	2.55	0.42
1:B:106:PRO:HD2	1:B:359:TYR:HA	2.01	0.42
1:B:396:LYS:HE3	1:B:396:LYS:HB3	1.85	0.42
1:D:429:LEU:HD21	1:D:445:GLU:HG3	2.02	0.42
1:C:27:LEU:HG	1:C:463:VAL:HG11	2.02	0.42
1:C:84:PRO:HA	1:C:87:LEU:HG	2.01	0.42
1:C:238:LYS:HB3	1:C:238:LYS:HE2	1.74	0.42
1:C:304:PHE:HE2	1:C:390:MET:HE3	1.84	0.42
1:D:198:HIS:CD2	1:D:255:PRO:HB3	2.55	0.42
1:D:370:LYS:O	1:D:374:THR:OG1	2.28	0.42
1:D:384:LEU:HD23	1:D:388:GLU:HB3	2.01	0.42
1:A:433:LYS:HA	1:A:433:LYS:HD2	1.89	0.42
1:C:13:HIS:HB2	1:C:57:THR:CG2	2.50	0.42
1:C:91:GLU:O	1:C:95:LEU:HD13	2.20	0.42
1:D:277:THR:OG1	1:D:278:ASP:N	2.52	0.42
1:C:282:LEU:HB2	1:C:305:PHE:CD1	2.55	0.42
1:D:458:ALA:HB3	1:D:461:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:PRO:HG2	1:C:196:TYR:HA	2.01	0.42
1:C:357:TRP:CZ2	1:C:368:LEU:HD21	2.55	0.42
1:D:153:LYS:HB3	1:D:153:LYS:HE3	1.67	0.42
1:A:258:SER:HA	1:A:406:GLY:O	2.19	0.42
1:B:419:ASN:OD1	1:B:419:ASN:C	2.63	0.42
1:B:462:GLU:H	1:B:462:GLU:CD	2.28	0.42
1:C:251:TYR:CD1	1:C:274:MET:HE3	2.55	0.42
1:C:278:ASP:OD1	1:C:306:ARG:NE	2.48	0.41
1:D:80:ILE:HG23	1:D:131:GLN:HB3	2.01	0.41
1:D:333:ARG:O	1:D:337:ILE:HG13	2.20	0.41
1:D:336:LYS:O	1:D:340:SER:HB3	2.20	0.41
1:D:341:VAL:HG21	1:D:345:PRO:HB3	2.01	0.41
1:D:98:PHE:O	1:D:102:ASN:ND2	2.54	0.41
1:D:394:ASP:OD1	1:D:394:ASP:N	2.53	0.41
1:D:438:ASN:ND2	1:D:475:ALA:HA	2.36	0.41
1:A:1:MET:HE1	1:A:379:GLU:HB3	2.01	0.41
1:A:195:PRO:HD3	1:A:252:MET:HE3	2.01	0.41
1:B:153:LYS:HE3	1:B:155:ARG:O	2.21	0.41
1:B:254:PRO:HA	1:B:255:PRO:HD3	1.92	0.41
1:C:13:HIS:HB2	1:C:57:THR:HG21	2.02	0.41
1:D:47:ASP:OD1	1:D:47:ASP:N	2.53	0.41
1:B:120:GLU:N	1:B:120:GLU:CD	2.79	0.41
1:C:195:PRO:HD2	1:C:255:PRO:HD3	2.02	0.41
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.96	0.41
1:D:334:LEU:HB3	1:D:380:TRP:CH2	2.56	0.41
1:D:371:LEU:O	1:D:375:LEU:HD23	2.20	0.41
1:A:116:LEU:HD22	1:A:126:GLU:HB3	2.03	0.41
1:C:96:ILE:HG12	1:C:96:ILE:H	1.72	0.41
1:D:184:LYS:HD2	1:D:191:VAL:HG12	2.01	0.41
1:A:254:PRO:HA	1:A:255:PRO:HD3	1.98	0.41
1:C:64:ILE:HG23	1:C:173:ILE:HG23	2.02	0.41
1:C:109:ARG:NH2	1:C:361:GLU:OE2	2.54	0.41
1:A:286:VAL:CG1	1:A:289:ALA:HB2	2.51	0.41
1:B:2:LYS:HG2	1:B:338:HIS:NE2	2.36	0.41
1:B:45:LEU:HD11	1:B:52:LEU:HB2	2.02	0.41
1:B:254:PRO:HD3	1:B:275:LEU:HB2	2.02	0.41
1:C:3:LYS:O	1:C:344:GLN:HG2	2.20	0.41
1:C:16:LEU:HD12	1:C:16:LEU:HA	1.90	0.41
1:D:213:THR:HG21	1:D:411:GLY:O	2.21	0.41
1:B:7:VAL:HG11	1:B:348:PHE:CZ	2.56	0.41
1:B:239:GLU:O	1:B:243:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:TYR:HD1	1:B:274:MET:HB3	1.85	0.41
1:B:335:LYS:HG3	1:B:380:TRP:CZ2	2.56	0.41
1:D:39:TYR:CD1	1:D:39:TYR:C	2.98	0.41
1:D:53:ASN:OD1	1:D:386:LEU:N	2.54	0.41
1:D:334:LEU:HB3	1:D:380:TRP:HH2	1.86	0.41
1:D:362:GLU:HG2	1:D:366:PRO:HD3	2.03	0.41
1:A:153:LYS:HE2	1:A:155:ARG:O	2.21	0.41
1:A:462:GLU:H	1:A:462:GLU:HG2	1.68	0.41
1:B:368:LEU:HA	1:B:368:LEU:HD23	1.80	0.41
1:C:286:VAL:CG1	1:C:289:ALA:HB2	2.51	0.41
1:C:429:LEU:HD11	1:C:445:GLU:HG3	2.03	0.41
1:D:314:ILE:HG13	1:D:314:ILE:H	1.63	0.41
1:A:211:TYR:OH	1:A:219:ILE:HG12	2.21	0.40
1:C:31:PHE:CD2	1:C:77:LEU:HD21	2.57	0.40
1:C:278:ASP:HB2	1:C:408:TRP:HB3	2.04	0.40
1:C:456:GLU:O	1:C:457:LYS:C	2.63	0.40
1:D:274:MET:HE3	1:D:274:MET:HB3	1.80	0.40
1:A:258:SER:HB3	1:A:407:THR:HG22	2.04	0.40
1:C:336:LYS:O	1:C:340:SER:HB3	2.21	0.40
1:D:58:PRO:HG2	1:D:196:TYR:HA	2.02	0.40
1:B:293:LEU:HD23	1:B:396:LYS:HB3	2.03	0.40
1:C:283:LYS:HA	1:C:283:LYS:HD3	1.70	0.40
1:C:466:LYS:C	1:C:466:LYS:HD3	2.47	0.40
1:D:120:GLU:CD	1:D:120:GLU:N	2.76	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLU:OE2	1:C:480:HIS:ND1[2_656]	2.16	0.04

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	475/485 (98%)	462 (97%)	12 (2%)	1 (0%)	43	72
1	B	475/485 (98%)	461 (97%)	12 (2%)	2 (0%)	30	60
1	C	482/485 (99%)	465 (96%)	15 (3%)	2 (0%)	30	60
1	D	483/485 (100%)	470 (97%)	10 (2%)	3 (1%)	21	51
All	All	1915/1940 (99%)	1858 (97%)	49 (3%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	GLU
1	C	287	GLU
1	D	287	GLU
1	B	287	GLU
1	D	363	ASN
1	D	455	GLU
1	A	287	GLU
1	C	481	HIS

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	437/445 (98%)	427 (98%)	10 (2%)	44	78
1	B	437/445 (98%)	426 (98%)	11 (2%)	42	76
1	C	444/445 (100%)	426 (96%)	18 (4%)	27	62
1	D	445/445 (100%)	435 (98%)	10 (2%)	45	78
All	All	1763/1780 (99%)	1714 (97%)	49 (3%)	38	73

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL

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Mol	Chain	Res	Type
1	A	128	LEU
1	A	185	GLU
1	A	214	THR
1	A	321	TRP
1	A	324	GLU
1	A	340	SER
1	A	370	LYS
1	A	394	ASP
1	A	420	LYS
1	B	59	VAL
1	B	80	ILE
1	B	158	THR
1	B	178	SER
1	B	201	ILE
1	B	213	THR
1	B	228	GLU
1	B	266	LEU
1	B	342	ASP
1	B	394	ASP
1	B	421	GLU
1	C	46	LYS
1	C	95	LEU
1	C	136	LEU
1	C	158	THR
1	C	178	SER
1	C	203	ILE
1	C	214	THR
1	C	218	LYS
1	C	224	VAL
1	C	231	SER
1	C	324	GLU
1	C	339	GLU
1	C	368	LEU
1	C	379	GLU
1	C	393	GLU
1	C	394	ASP
1	C	397	THR
1	C	472	VAL
1	D	37	ASP
1	D	59	VAL
1	D	75	VAL
1	D	90	GLU

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Mol	Chain	Res	Type
1	D	116	LEU
1	D	178	SER
1	D	290	SER
1	D	340	SER
1	D	394	ASP
1	D	397	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	A	344	GLN
1	B	55	ASN
1	B	233	HIS
1	B	248	HIS
1	B	273	ASN
1	C	167	ASN
1	C	216	ASN
1	C	248	HIS
1	C	256	GLN
1	C	322	ASN
1	C	476	GLN
1	D	65	GLN
1	D	118	ASN
1	D	123	ASN
1	D	167	ASN
1	D	208	ASN
1	D	273	ASN
1	D	363	ASN
1	D	438	ASN
1	D	480	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	E	1	2	12,12,12	0.88	0	17,17,17	1.39	3 (17%)
2	GLC	E	2	2	11,11,12	0.59	0	15,15,17	2.64	5 (33%)
2	GLC	E	3	2	11,11,12	0.62	0	15,15,17	1.98	4 (26%)
2	GLC	E	4	2	11,11,12	0.68	0	15,15,17	1.08	0
2	GLC	E	5	2	11,11,12	0.51	0	15,15,17	1.12	1 (6%)
2	GLC	F	1	2	12,12,12	0.66	0	17,17,17	1.63	4 (23%)
2	GLC	F	2	2	11,11,12	0.65	0	15,15,17	2.41	5 (33%)
2	GLC	F	3	2	11,11,12	0.62	0	15,15,17	2.10	5 (33%)
2	GLC	F	4	2	11,11,12	0.68	0	15,15,17	0.93	0
2	GLC	F	5	2	11,11,12	0.60	0	15,15,17	0.64	0
2	GLC	G	1	2	12,12,12	0.70	0	17,17,17	2.18	7 (41%)
2	GLC	G	2	2	11,11,12	0.53	0	15,15,17	2.35	4 (26%)
2	GLC	G	3	2	11,11,12	0.60	0	15,15,17	1.82	3 (20%)
2	GLC	G	4	2	11,11,12	0.60	0	15,15,17	0.88	0
2	GLC	G	5	2	11,11,12	0.49	0	15,15,17	1.04	1 (6%)
2	GLC	H	1	2	12,12,12	0.77	0	17,17,17	1.45	5 (29%)
2	GLC	H	2	2	11,11,12	0.57	0	15,15,17	2.48	4 (26%)
2	GLC	H	3	2	11,11,12	0.60	0	15,15,17	1.80	3 (20%)
2	GLC	H	4	2	11,11,12	0.58	0	15,15,17	1.21	0
2	GLC	H	5	2	11,11,12	0.52	0	15,15,17	0.90	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	E	1	2	-	2/2/22/22	0/1/1/1

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

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GLC	O4-C4-C5	6.15	124.46	109.32
2	H	2	GLC	O4-C4-C5	6.13	124.43	109.32
2	F	2	GLC	O4-C4-C5	6.05	124.22	109.32
2	G	2	GLC	O4-C4-C5	5.80	123.61	109.32
2	F	2	GLC	C1-O5-C5	5.24	119.21	112.19
2	H	2	GLC	C1-O5-C5	5.13	119.07	112.19
2	E	2	GLC	C1-O5-C5	5.06	118.97	112.19
2	F	3	GLC	C2-C3-C4	-4.83	102.36	110.86
2	E	3	GLC	O4-C4-C3	4.59	121.21	110.38
2	G	1	GLC	O4-C4-C3	-4.58	99.59	110.38
2	G	2	GLC	C1-O5-C5	4.39	118.07	112.19
2	F	3	GLC	O4-C4-C5	4.18	119.62	109.32
2	G	3	GLC	C2-C3-C4	-4.12	103.62	110.86
2	E	2	GLC	C2-C3-C4	-3.98	103.86	110.86
2	H	3	GLC	C2-C3-C4	-3.67	104.40	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	GLC	O4-C4-C5	3.65	118.32	109.32
2	G	2	GLC	C2-C3-C4	-3.52	104.67	110.86
2	E	5	GLC	C1-O5-C5	3.48	116.84	112.19
2	G	1	GLC	C1-O5-C5	3.47	120.36	113.65
2	H	3	GLC	O4-C4-C3	3.42	118.45	110.38
2	E	3	GLC	C2-C3-C4	-3.41	104.87	110.86
2	H	2	GLC	C2-C3-C4	-3.33	105.01	110.86
2	F	1	GLC	O5-C1-C2	3.13	115.81	110.30
2	G	5	GLC	C1-O5-C5	2.98	116.17	112.19
2	F	1	GLC	O1-C1-O5	-2.92	101.74	110.41
2	G	3	GLC	O4-C4-C3	2.91	117.23	110.38
2	G	1	GLC	O5-C1-C2	2.90	115.40	110.30
2	F	2	GLC	C2-C3-C4	-2.86	105.83	110.86
2	H	3	GLC	O4-C4-C5	2.82	116.27	109.32
2	G	1	GLC	O3-C3-C4	-2.82	103.73	110.38
2	E	1	GLC	C1-O5-C5	2.79	119.06	113.65
2	F	3	GLC	O4-C4-C3	2.79	116.95	110.38
2	G	1	GLC	O2-C2-C1	-2.73	102.94	109.25
2	E	2	GLC	O5-C5-C6	-2.67	102.46	107.66
2	H	1	GLC	O6-C6-C5	-2.61	102.45	111.33
2	G	1	GLC	O5-C5-C4	2.57	114.32	109.70
2	E	3	GLC	O5-C5-C6	2.51	112.54	107.66
2	E	3	GLC	O4-C4-C5	2.50	115.48	109.32
2	G	1	GLC	O1-C1-C2	-2.40	102.03	108.98
2	F	1	GLC	O4-C4-C3	-2.38	104.77	110.38
2	F	3	GLC	O2-C2-C1	2.33	114.56	109.22
2	E	1	GLC	O6-C6-C5	-2.33	103.41	111.33
2	F	2	GLC	O5-C5-C4	-2.29	105.26	110.83
2	E	2	GLC	C1-C2-C3	2.27	112.94	109.64
2	H	5	GLC	C1-O5-C5	2.22	115.16	112.19
2	H	1	GLC	O3-C3-C2	-2.21	105.17	110.38
2	H	1	GLC	C4-C3-C2	2.17	114.64	110.83
2	H	2	GLC	C3-C4-C5	-2.13	106.38	110.23
2	H	1	GLC	C6-C5-C4	-2.12	107.81	113.02
2	F	2	GLC	O4-C4-C3	2.10	115.33	110.38
2	E	1	GLC	O5-C5-C6	-2.08	101.28	106.44
2	F	1	GLC	C3-C4-C5	2.06	113.96	110.23
2	G	2	GLC	O4-C4-C3	2.02	115.15	110.38
2	F	3	GLC	O5-C5-C4	-2.02	105.90	110.83
2	H	1	GLC	O2-C2-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	3	GLC	C4-C5-C6-O6
2	G	3	GLC	C4-C5-C6-O6
2	G	3	GLC	O5-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	E	4	GLC	C4-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	F	5	GLC	C4-C5-C6-O6
2	E	4	GLC	O5-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6
2	F	5	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	F	4	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	G	5	GLC	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 10 short contacts:

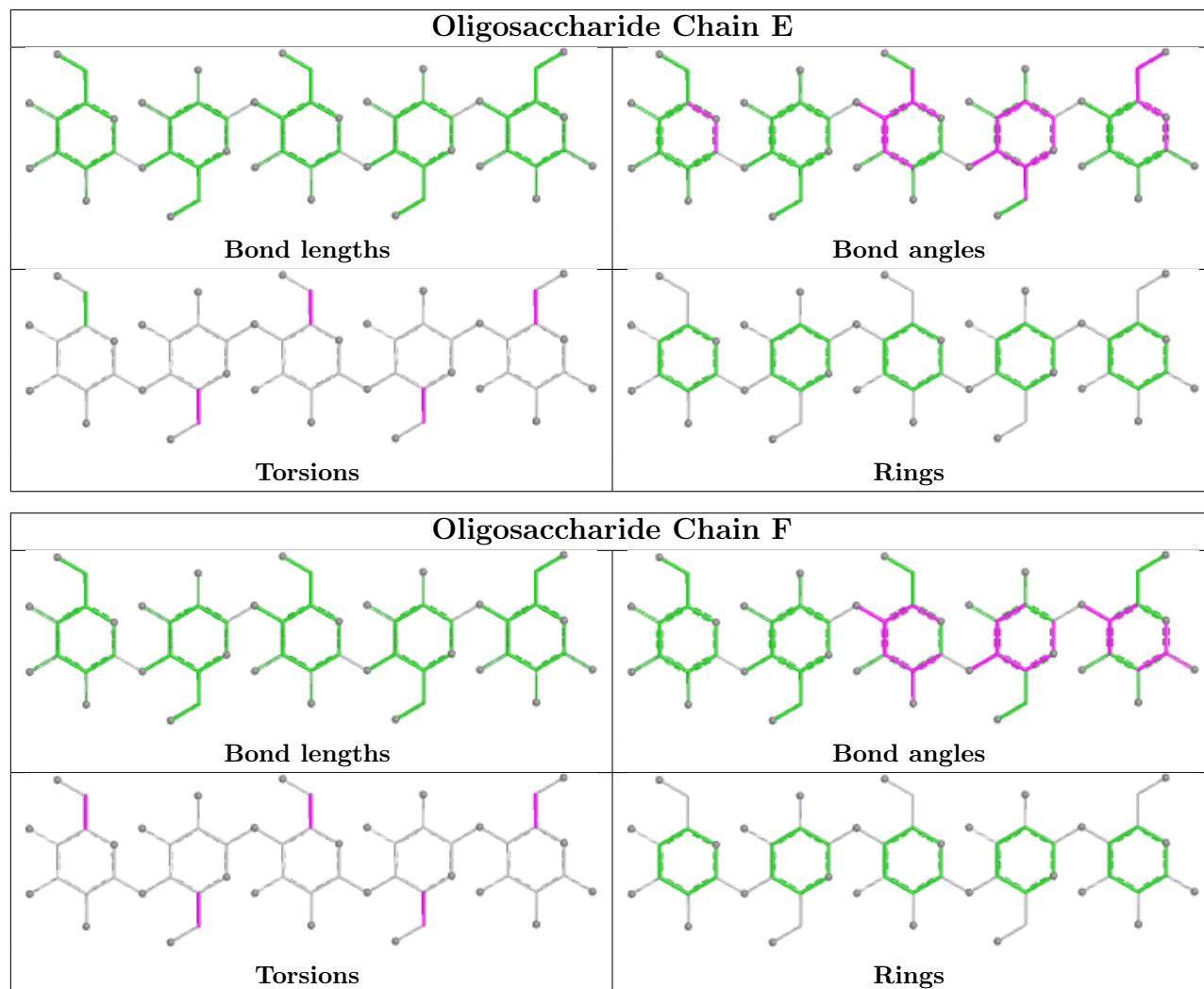
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	4	GLC	1	0
2	G	1	GLC	4	0
2	G	2	GLC	1	0
2	G	3	GLC	1	0
2	E	4	GLC	1	0
2	F	4	GLC	2	0

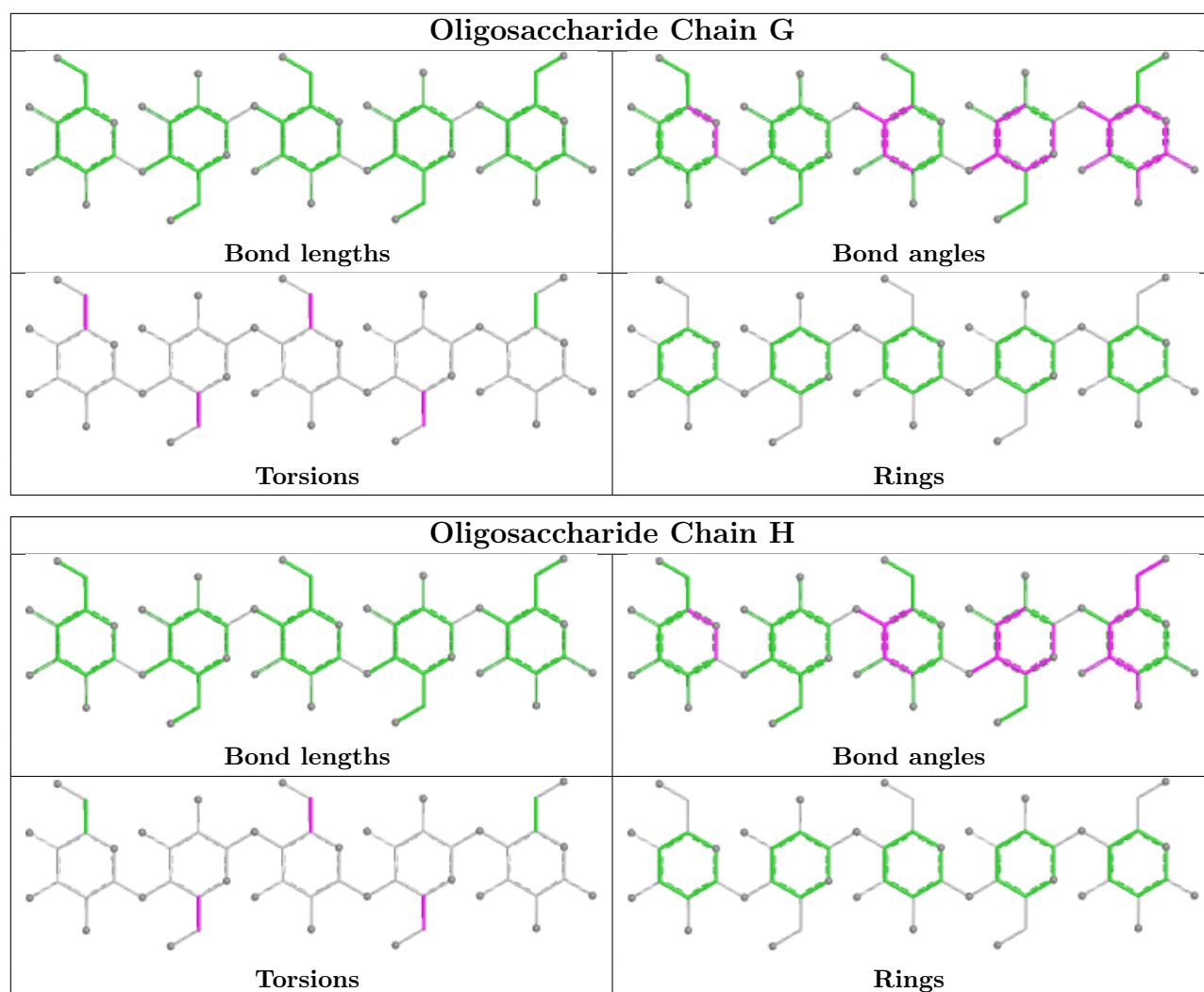
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	GLC	1	0

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	477/485 (98%)	-0.37	1 (0%) 91 88	40, 55, 76, 126	0
1	B	477/485 (98%)	-0.35	0 100 100	42, 59, 80, 107	0
1	C	484/485 (99%)	-0.26	1 (0%) 91 88	44, 66, 94, 122	0
1	D	485/485 (100%)	-0.17	0 100 100	48, 69, 90, 126	0
All	All	1923/1940 (99%)	-0.29	2 (0%) 92 90	40, 62, 88, 126	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	GLU	2.1
1	A	450	PHE	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.

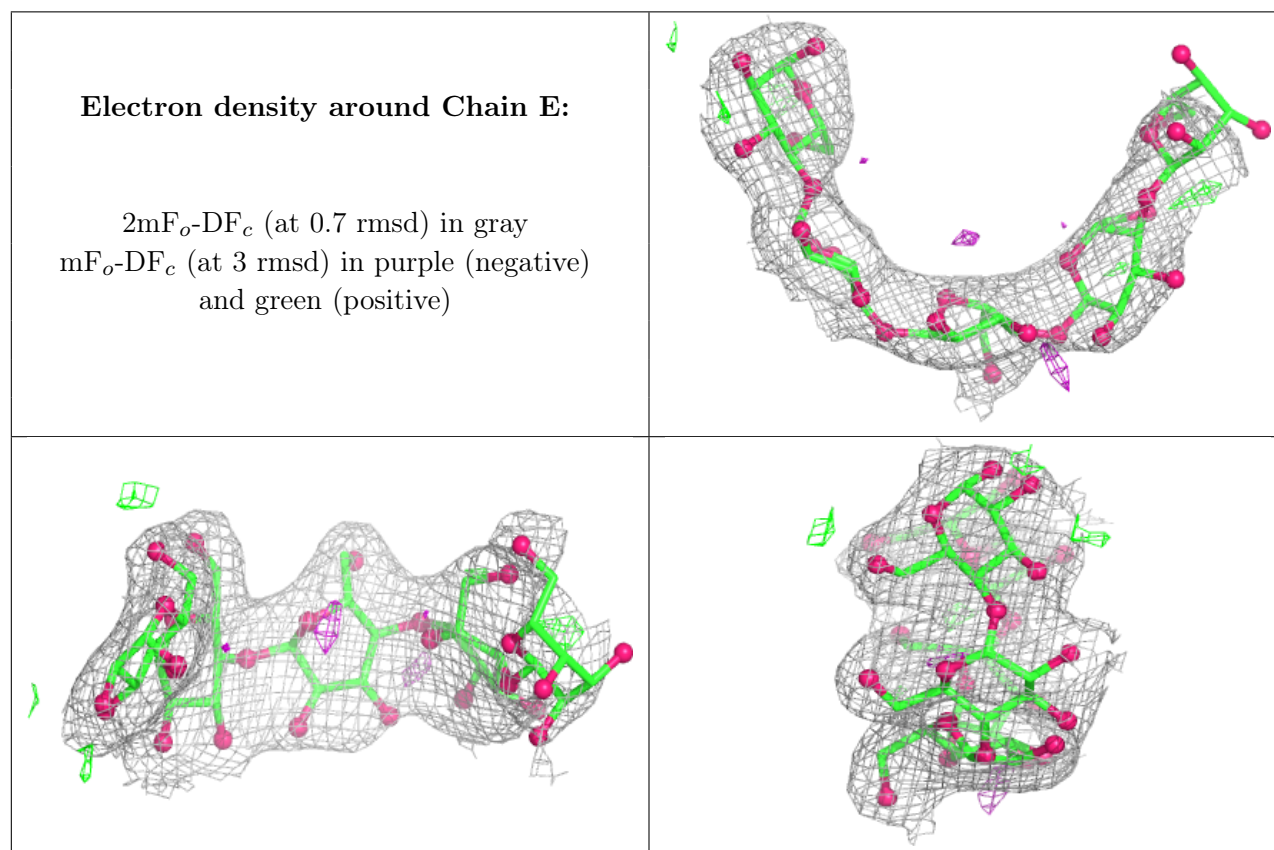
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	G	5	11/12	0.41	0.12	115,121,128,130	0
2	GLC	E	5	11/12	0.56	0.13	92,104,123,134	0
2	GLC	H	5	11/12	0.57	0.12	108,120,132,137	0
2	GLC	F	5	11/12	0.59	0.16	100,113,119,122	0
2	GLC	F	4	11/12	0.82	0.11	70,77,82,90	0

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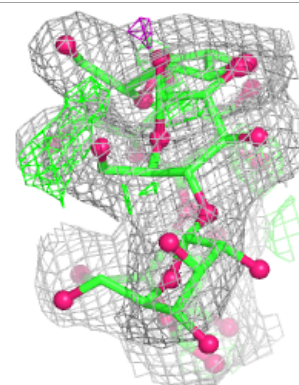
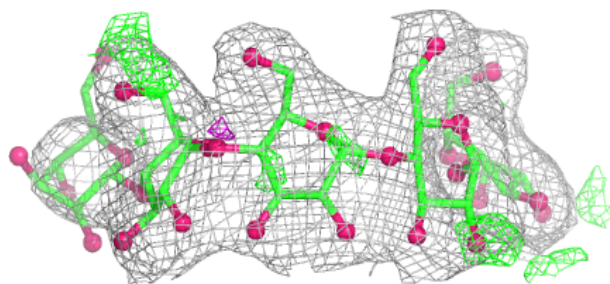
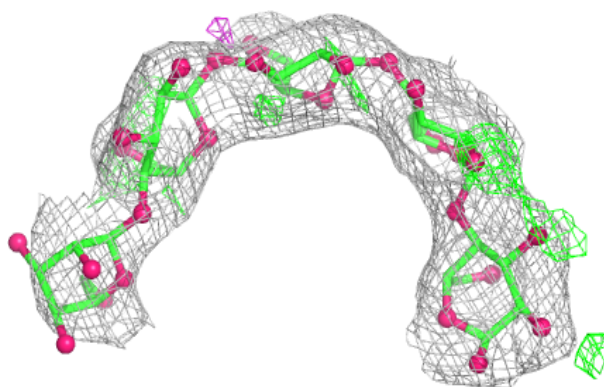
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	E	4	11/12	0.89	0.10	60,77,86,98	0
2	GLC	H	4	11/12	0.89	0.08	75,90,102,108	0
2	GLC	G	4	11/12	0.89	0.09	79,85,102,109	0
2	GLC	F	3	11/12	0.91	0.10	48,57,68,78	0
2	GLC	G	1	12/12	0.91	0.07	51,62,68,69	0
2	GLC	F	2	11/12	0.91	0.10	40,52,61,82	0
2	GLC	H	3	11/12	0.92	0.10	60,64,77,80	0
2	GLC	E	1	12/12	0.92	0.07	47,51,55,56	0
2	GLC	G	3	11/12	0.92	0.09	58,70,80,86	0
2	GLC	H	1	12/12	0.93	0.08	54,63,68,70	0
2	GLC	F	1	12/12	0.93	0.07	48,50,62,62	0
2	GLC	E	3	11/12	0.94	0.07	48,57,69,70	0
2	GLC	G	2	11/12	0.94	0.07	53,57,69,70	0
2	GLC	H	2	11/12	0.94	0.08	52,58,61,68	0
2	GLC	E	2	11/12	0.95	0.07	42,47,53,54	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.

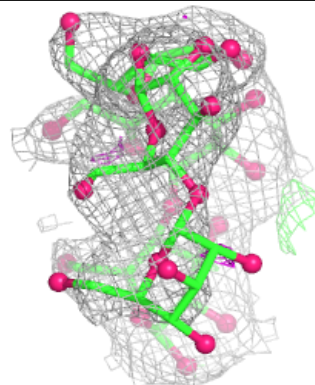
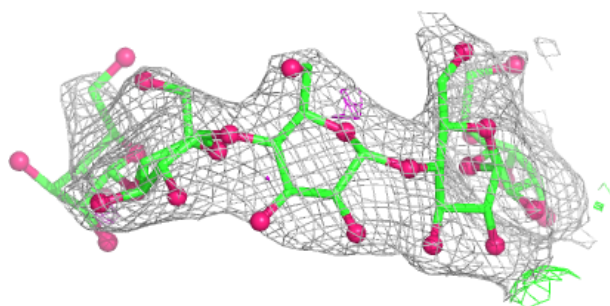
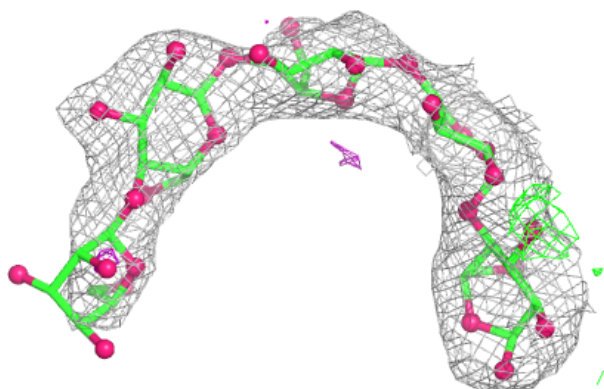


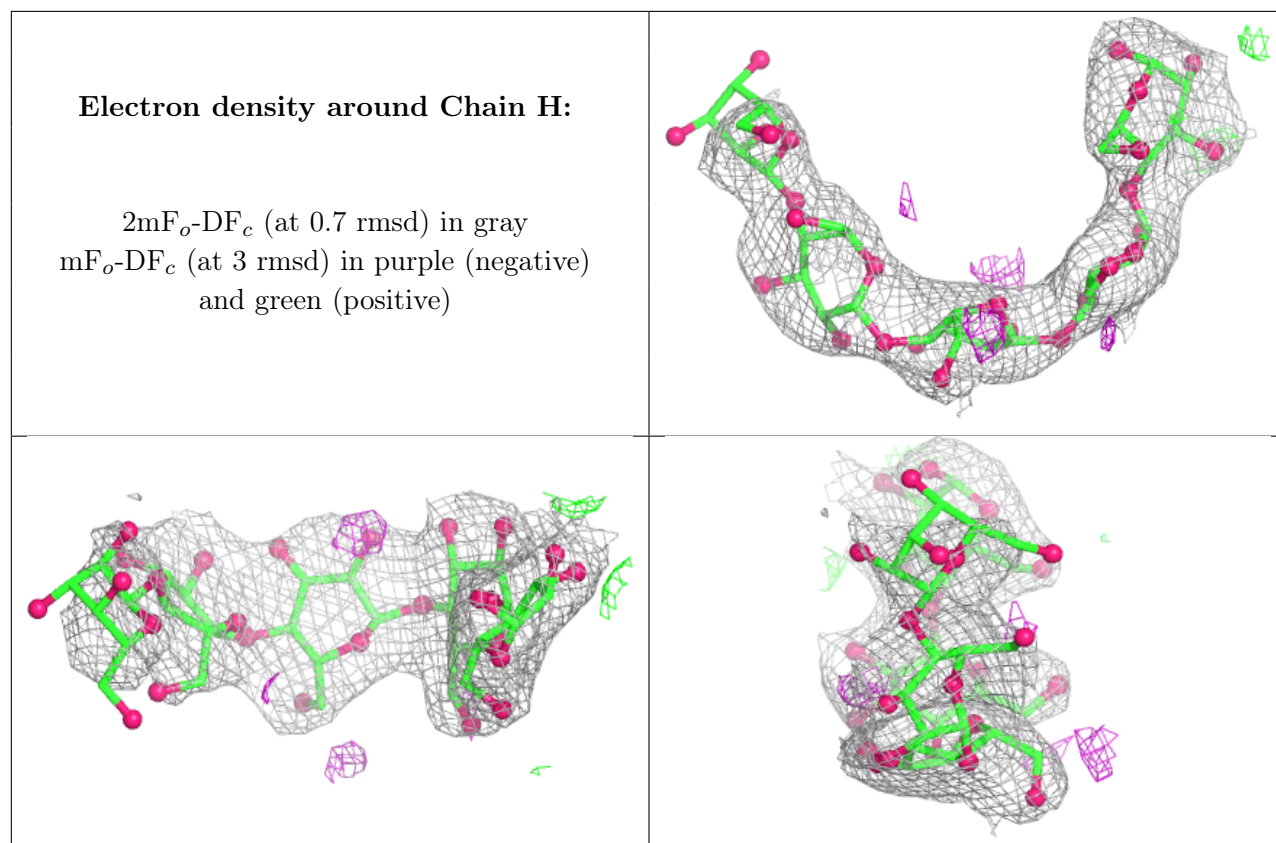
Electron density around Chain F:

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

**Electron density around Chain G:**

$2mF_o - DF_c$ (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.