



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 AM UTC

PDB ID : 4LQ1 / pdb_00004lq1
Title : Crystal Structure of E.Coli Branching Enzyme in complex with maltohexaose
Authors : Feng, L.; Geiger, J.H.
Deposited on : 2013-07-17
Resolution : 2.55 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

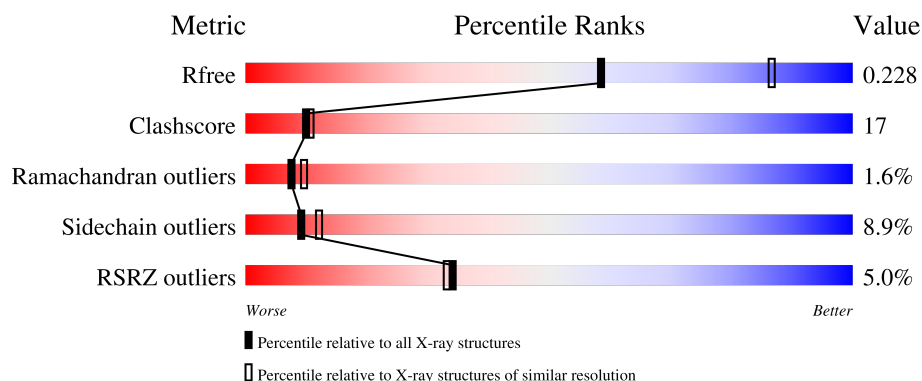
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	612	7% 62% 28% 5% .
1	B	612	7% 69% 23% 5% .
1	C	612	3% 67% 24% 5% .
1	D	612	3% 72% 20% . . .
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 50%50%
2	I	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20219 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4817	3080	854	867	16			
1	B	596	Total	C	N	O	S	0	1	0
			4904	3132	871	885	16			
1	C	589	Total	C	N	O	S	0	0	0
			4840	3094	858	872	16			
1	D	593	Total	C	N	O	S	0	8	0
			4954	3163	886	888	17			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

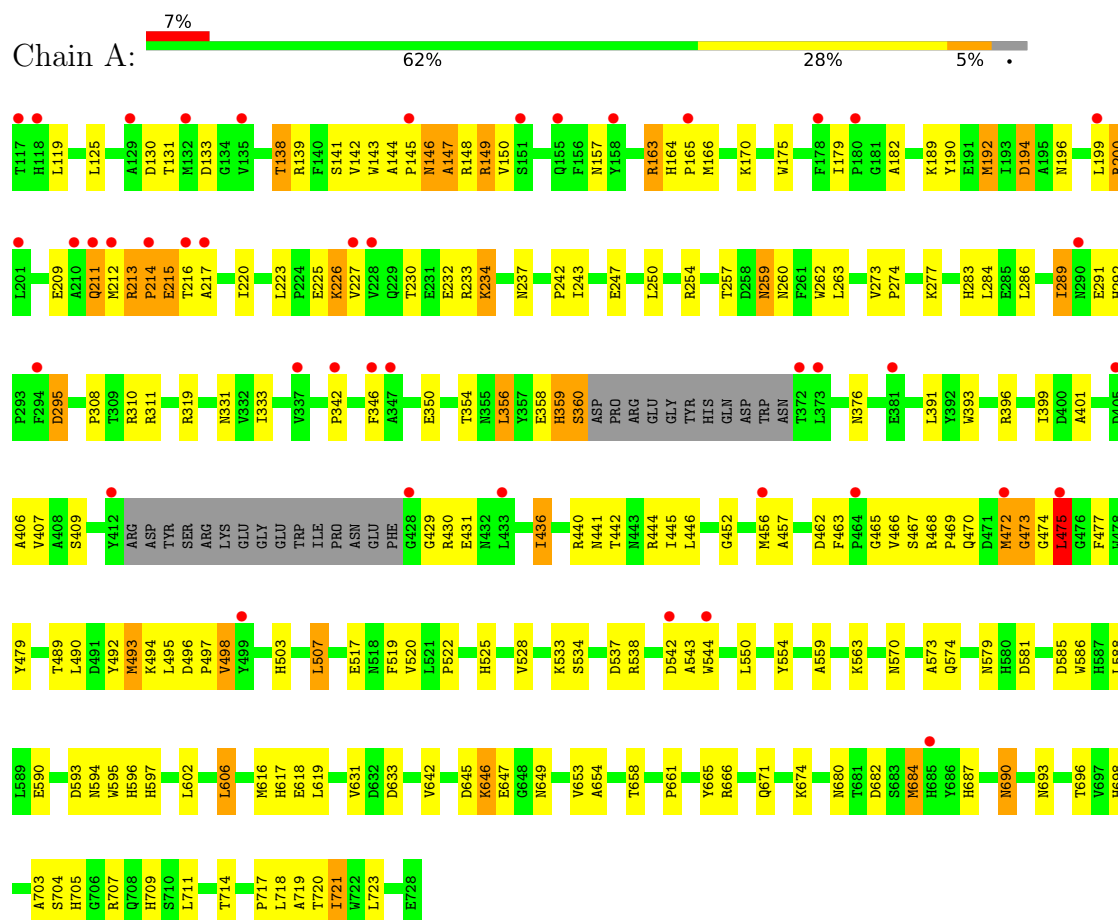
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	101	Total	O	0	0
			101	101		
5	C	159	Total	O	0	0
			159	159		
5	D	232	Total	O	0	0
			232	232		

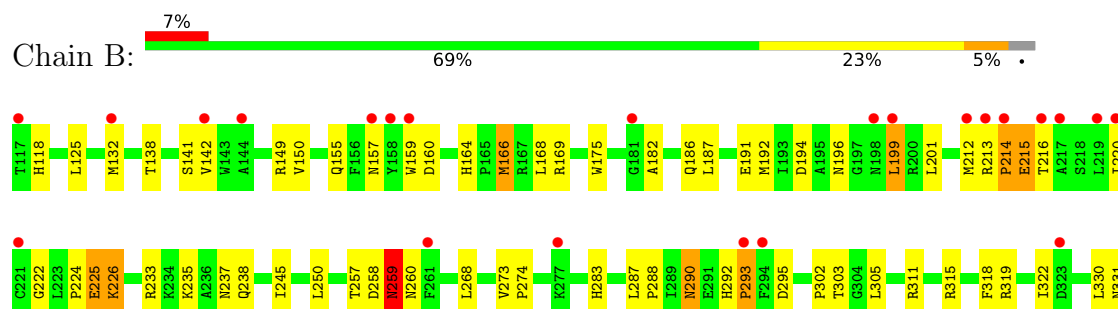
3 Residue-property plots

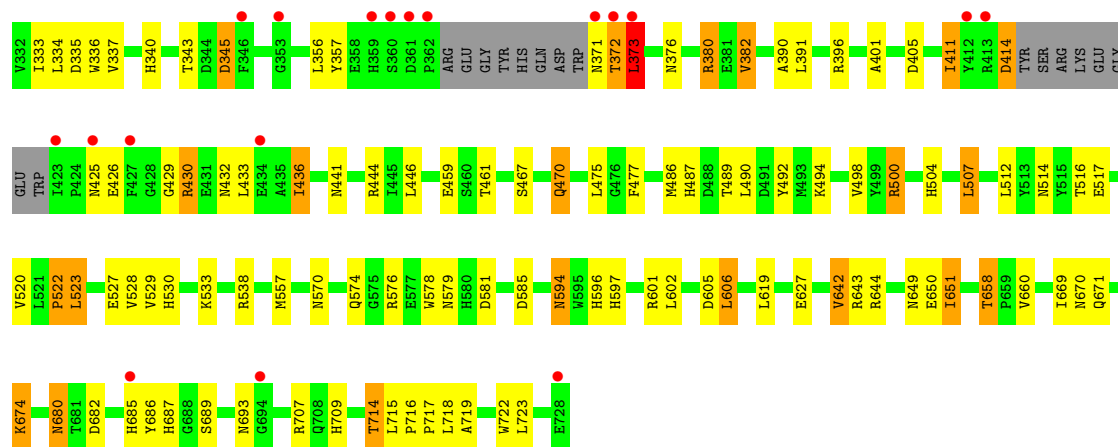
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

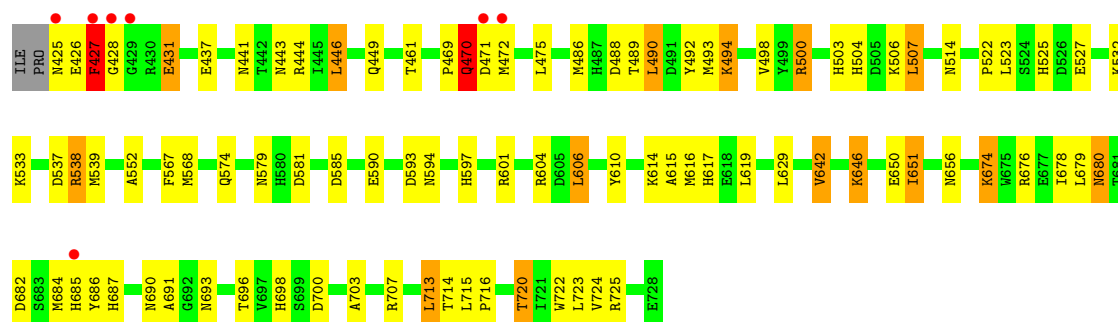
- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



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



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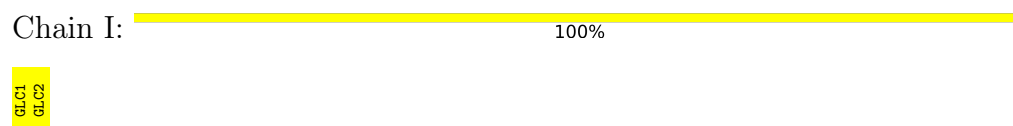
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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



- Molecule 2: 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	93.69Å 104.11Å 186.71Å 90.00° 91.85° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.55) 95.9 (50.00-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.224 0.181 , 0.228	Depositor DCC
R_{free} test set	11224 reflections (9.63%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20219	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, BGC, GOL

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	0.47	0/4970	0.78	3/6749 (0.0%)
1	B	0.53	0/5061	0.82	3/6874 (0.0%)
1	C	0.63	0/4993	0.87	3/6778 (0.0%)
1	D	0.76	0/5112	0.97	14/6937 (0.2%)
All	All	0.61	0/20136	0.86	23/27338 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	LEU	N-CA-C	-7.27	99.69	110.23
1	B	715	LEU	CA-C-N	6.99	124.76	119.66
1	B	715	LEU	C-N-CA	6.99	124.76	119.66
1	D	446	LEU	CA-C-N	-6.63	108.42	121.41
1	D	446	LEU	C-N-CA	-6.63	108.42	121.41
1	A	179	ILE	N-CA-C	6.26	113.26	107.56
1	D	461	THR	N-CA-C	-6.24	97.51	110.80
1	B	245	ILE	N-CA-C	6.24	117.28	108.36
1	C	432	ASN	N-CA-C	5.85	118.25	108.02
1	D	470	GLN	N-CA-C	5.75	118.28	111.33
1	D	215	GLU	CA-C-N	5.73	132.02	121.70
1	D	215	GLU	C-N-CA	5.73	132.02	121.70
1	D	257	THR	N-CA-C	5.67	117.54	111.36
1	D	713	LEU	N-CA-C	5.43	116.51	108.86
1	D	678	ILE	N-CA-C	-5.36	107.59	113.43
1	D	650	GLU	CA-C-N	-5.28	116.64	123.19
1	D	650	GLU	C-N-CA	-5.28	116.64	123.19
1	A	468	ARG	CA-C-N	5.22	125.22	119.90
1	A	468	ARG	C-N-CA	5.22	125.22	119.90
1	D	446	LEU	O-C-N	-5.18	116.50	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	678	ILE	N-CA-C	-5.17	108.46	113.53
1	C	519	PHE	N-CA-C	5.07	118.21	110.20
1	D	245	ILE	N-CA-C	5.06	115.25	108.17

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	4817	0	4547	159	0
1	B	4904	0	4616	155	0
1	C	4840	0	4565	188	0
1	D	4954	0	4664	163	0
2	E	23	0	21	0	0
2	F	23	0	21	1	0
2	G	23	0	21	1	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
3	A	12	0	12	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0
5	A	61	0	0	7	0
5	B	101	0	0	9	0
5	C	159	0	0	10	0
5	D	232	0	0	24	0
All	All	20219	0	18541	664	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (664) 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:527:GLU:O	1:B:538:ARG:NH2	1.75	1.20
1:C:380:ARG:HG2	5:C:972:HOH:O	1.43	1.19
1:B:380:ARG:HG2	1:B:380:ARG:HH21	1.12	1.12
1:C:444:ARG:HG2	1:C:444:ARG:HH21	1.08	1.11
1:A:212:MET:HG2	1:A:213:ARG:H	1.12	1.10
1:D:214:PRO:HA	1:D:215:GLU:O	1.53	1.08
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.16	1.07
1:C:211:GLN:HA	1:C:212:MET:HB2	1.31	1.06
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.13	1.06
1:C:426:GLU:HG3	1:C:427:PHE:CD2	1.91	1.05
1:B:430:ARG:H	1:B:430:ARG:HD3	1.19	1.05
1:D:215:GLU:HB2	1:D:217:ALA:H	1.21	1.04
1:D:441:ASN:ND2	1:D:444:ARG:HH11	1.54	1.04
1:A:200:ARG:HH11	1:A:200:ARG:CG	1.70	1.04
1:B:292:HIS:O	1:B:311:ARG:NH1	1.89	1.03
1:D:373:LEU:HD22	1:D:373:LEU:H	1.22	1.03
1:C:470:GLN:HE21	1:C:470:GLN:N	1.60	1.00
1:C:426:GLU:HG3	1:C:427:PHE:HD2	1.26	0.99
1:C:470:GLN:H	1:C:470:GLN:NE2	1.60	0.99
1:D:215:GLU:HB3	1:D:216:THR:OG1	1.60	0.99
1:C:658:THR:HG22	1:C:660:VAL:H	1.23	0.97
1:D:171:GLU:HG3	5:D:1040:HOH:O	1.64	0.96
1:B:670:ASN:HD21	1:B:707:ARG:HE	1.11	0.95
1:D:441:ASN:HD21	1:D:444:ARG:NH1	1.63	0.95
1:A:232:GLU:HG2	5:A:934:HOH:O	1.68	0.94
1:D:693:ASN:HD21	1:D:713:LEU:HB2	1.32	0.94
1:D:164:HIS:HE1	5:D:1010:HOH:O	1.49	0.94
1:D:470:GLN:H	1:D:470:GLN:HE21	0.95	0.94
1:B:470:GLN:H	1:B:470:GLN:NE2	1.65	0.93
1:B:470:GLN:HE21	1:B:470:GLN:N	1.66	0.93
1:B:380:ARG:HH21	1:B:380:ARG:CG	1.80	0.93
1:C:444:ARG:HG2	1:C:444:ARG:NH2	1.76	0.93
1:D:337:VAL:HG23	1:D:337:VAL:O	1.67	0.92
1:C:225:GLU:O	1:C:226:LYS:CB	2.19	0.90
1:C:157:ASN:HD21	1:C:164:HIS:CD2	1.89	0.90
1:C:574:GLN:NE2	1:C:585:ASP:H	1.69	0.90
1:C:225:GLU:O	1:C:226:LYS:HB3	1.69	0.89
1:A:544:TRP:HE3	5:A:919:HOH:O	1.56	0.89
1:B:670:ASN:ND2	1:B:707:ARG:HE	1.71	0.88
1:B:594:ASN:H	1:B:597:HIS:HD2	1.21	0.88
1:D:215:GLU:HB2	1:D:217:ALA:N	1.89	0.88
1:C:693:ASN:HD21	1:C:714:THR:H	1.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HG2	1:C:310:ARG:HH11	1.38	0.87
1:C:211:GLN:CA	1:C:212:MET:HB2	2.04	0.86
1:C:310:ARG:HH11	1:C:310:ARG:CG	1.88	0.86
1:A:214:PRO:O	1:A:215:GLU:HB2	1.75	0.86
1:D:215:GLU:HB3	1:D:216:THR:HG1	1.41	0.86
1:A:212:MET:CG	1:A:213:ARG:H	1.85	0.85
1:C:213:ARG:HB3	1:C:214:PRO:HA	1.59	0.85
1:A:225:GLU:O	1:A:226:LYS:HB3	1.75	0.85
1:D:470:GLN:H	1:D:470:GLN:NE2	1.74	0.84
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.06	0.84
1:B:372:THR:O	1:B:373:LEU:HD23	1.78	0.83
1:C:429:GLY:HA2	1:C:430:ARG:HG3	1.59	0.83
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.76	0.83
1:C:590:GLU:HA	1:C:590:GLU:OE2	1.76	0.83
1:B:658:THR:CG2	1:B:660:VAL:H	1.92	0.83
1:B:225:GLU:O	1:B:226:LYS:HB2	1.79	0.82
1:B:658:THR:HG22	1:B:660:VAL:H	1.43	0.82
1:A:574:GLN:NE2	1:A:585:ASP:H	1.77	0.82
1:A:212:MET:HG2	1:A:213:ARG:N	1.88	0.81
1:D:616:MET:SD	1:D:651:ILE:HG12	2.19	0.81
1:B:237:ASN:ND2	1:B:283:HIS:HE1	1.78	0.81
1:B:470:GLN:H	1:B:470:GLN:HE21	0.84	0.81
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.62	0.81
1:A:200:ARG:HG2	1:A:200:ARG:NH1	1.87	0.81
1:D:693:ASN:ND2	1:D:713:LEU:HB2	1.94	0.81
1:C:651:ILE:CD1	1:C:722:TRP:HB3	2.11	0.81
1:B:191:GLU:HG2	1:B:201:LEU:HD23	1.63	0.80
1:B:430:ARG:HD3	1:B:430:ARG:N	1.96	0.80
1:D:441:ASN:HD21	1:D:444:ARG:HH11	0.84	0.79
1:C:162:ARG:HH11	1:C:162:ARG:CG	1.94	0.79
1:D:427:PHE:HB3	5:D:1007:HOH:O	1.81	0.79
1:D:713:LEU:HD12	1:D:713:LEU:C	2.06	0.78
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.66	0.78
1:D:426:GLU:O	1:D:427:PHE:HB3	1.82	0.78
1:C:412:TYR:CD2	1:C:431:GLU:HB3	2.18	0.78
1:A:474:GLY:O	1:A:475:LEU:HB2	1.84	0.77
1:C:532:LYS:C	1:C:533:LYS:HG2	2.08	0.77
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.48	0.77
1:D:302:PRO:HG3	1:D:337:VAL:HG21	1.64	0.76
1:C:340:HIS:HE1	1:C:405:ASP:OD2	1.69	0.76
1:A:709:HIS:HD2	5:A:924:HOH:O	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:HG2	1:B:380:ARG:NH2	1.92	0.76
1:D:371:ASN:ND2	1:D:372:THR:H	1.84	0.76
1:C:490:LEU:O	1:C:494:LYS:HG3	1.85	0.76
1:C:213:ARG:HB2	1:C:213:ARG:HH11	1.51	0.75
1:B:651:ILE:HD12	1:B:722:TRP:HB3	1.69	0.75
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.21	0.75
1:C:157:ASN:HD21	1:C:164:HIS:HD2	1.31	0.74
1:A:211:GLN:OE1	1:A:215:GLU:HB3	1.86	0.74
1:C:444:ARG:HH21	1:C:444:ARG:CG	1.91	0.74
1:D:187:LEU:HD23	1:D:219:LEU:HD12	1.69	0.74
1:C:594:ASN:H	1:C:597:HIS:HD2	1.35	0.74
1:B:376:ASN:O	1:B:382:VAL:HG11	1.88	0.74
1:C:429:GLY:CA	1:C:430:ARG:HG3	2.16	0.74
1:B:212:MET:C	1:B:214:PRO:HA	2.12	0.74
1:D:346:PHE:HD2	1:D:346:PHE:N	1.85	0.74
1:D:470:GLN:HE21	1:D:470:GLN:N	1.79	0.73
1:D:371:ASN:CG	1:D:372:THR:H	1.96	0.73
1:C:399:ILE:HD11	1:C:401:ALA:O	1.88	0.73
1:A:237:ASN:ND2	1:A:283:HIS:HE1	1.86	0.73
1:D:120:ARG:NH1	1:D:395:GLU:OE1	2.20	0.73
1:C:213:ARG:CB	1:C:214:PRO:HA	2.19	0.73
1:B:318:PHE:CZ	1:B:322:ILE:HD11	2.24	0.73
1:C:411:ILE:O	1:C:431:GLU:HB2	1.87	0.73
1:D:346:PHE:N	1:D:346:PHE:CD2	2.58	0.72
1:D:469:PRO:HD2	1:D:472:MET:HE2	1.71	0.72
1:A:138:THR:HG22	1:A:182:ALA:O	1.90	0.71
1:B:132:MET:HE2	1:B:132:MET:HA	1.71	0.71
1:C:399:ILE:HD12	1:C:401:ALA:H	1.55	0.71
1:B:257:THR:OG1	5:B:908:HOH:O	2.07	0.71
1:D:149[A]:ARG:HH11	1:D:149[A]:ARG:HB3	1.56	0.71
1:C:341:PHE:CZ	1:C:358:GLU:HB3	2.26	0.71
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.74	0.70
1:B:372:THR:O	1:B:373:LEU:CD2	2.40	0.69
1:D:214:PRO:CA	1:D:215:GLU:O	2.38	0.69
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.46	0.69
1:B:334:LEU:HD11	5:B:994:HOH:O	1.91	0.69
1:D:149[A]:ARG:HH21	1:D:165:PRO:HB3	1.58	0.68
1:C:469:PRO:HG2	1:C:472:MET:HE2	1.75	0.68
1:C:636:ARG:HG2	1:C:662:ARG:NH2	2.09	0.68
1:B:693:ASN:HD21	1:B:714:THR:H	1.40	0.68
1:C:213:ARG:HB2	1:C:213:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:HIS:O	1:A:311:ARG:NH1	2.27	0.68
1:A:472:MET:HG2	1:A:473:GLY:N	2.07	0.68
1:C:399:ILE:CD1	1:C:401:ALA:O	2.42	0.67
1:D:606:LEU:HD13	1:D:679:LEU:HD11	1.76	0.67
1:C:627:GLU:OE1	1:C:707:ARG:NH2	2.27	0.67
1:D:693:ASN:HD21	1:D:714:THR:H	1.43	0.67
1:A:359:HIS:O	1:A:360:SER:HB2	1.95	0.67
1:A:213:ARG:HB2	1:A:214:PRO:CD	2.26	0.66
1:C:157:ASN:ND2	1:C:164:HIS:HD2	1.93	0.66
1:D:493:MET:HB3	1:D:539:MET:HE1	1.78	0.66
1:B:430:ARG:H	1:B:430:ARG:CD	2.05	0.66
1:D:373:LEU:HD22	1:D:373:LEU:N	2.01	0.66
1:D:399:ILE:HD11	1:D:402:LEU:CD2	2.25	0.66
1:A:225:GLU:O	1:A:226:LYS:CB	2.44	0.66
1:B:486:MET:CE	1:B:487:HIS:CD2	2.79	0.66
1:A:618:GLU:OE2	1:A:646:LYS:HB2	1.95	0.66
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.42	0.66
1:C:684:MET:H	1:C:690:ASN:HD22	1.44	0.65
1:D:163:ARG:HD3	5:D:985:HOH:O	1.97	0.65
1:C:616:MET:SD	1:C:651:ILE:HG12	2.36	0.65
1:C:444:ARG:HD3	5:C:982:HOH:O	1.96	0.65
1:D:680:ASN:HD22	1:D:680:ASN:C	2.02	0.65
1:C:412:TYR:HD2	1:C:431:GLU:HB3	1.60	0.65
1:B:486:MET:CE	1:B:487:HIS:HD2	2.09	0.65
1:B:224:PRO:HG2	1:B:396:ARG:HB3	1.80	0.64
1:D:149[A]:ARG:HB3	1:D:149[A]:ARG:NH1	2.12	0.64
1:B:651:ILE:HD11	1:B:722:TRP:HB3	1.77	0.64
1:C:532:LYS:O	1:C:533:LYS:HG2	1.96	0.64
1:D:215:GLU:HB3	1:D:216:THR:CB	2.27	0.64
1:B:157:ASN:OD1	1:B:164:HIS:HD2	1.80	0.64
1:B:166:MET:CE	1:B:175:TRP:HB3	2.27	0.64
1:B:380:ARG:CG	1:B:380:ARG:NH2	2.50	0.64
1:C:277:LYS:HD3	1:C:328:ALA:HB1	1.79	0.64
1:C:492:TYR:CE2	1:C:507:LEU:HD21	2.33	0.64
1:C:693:ASN:ND2	1:C:714:THR:H	1.93	0.64
1:C:310:ARG:CG	1:C:310:ARG:NH1	2.57	0.64
1:A:671:GLN:OE1	5:A:930:HOH:O	2.15	0.63
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.80	0.63
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.80	0.63
1:D:258:ASP:O	1:D:259:ASN:ND2	2.31	0.63
1:A:146:ASN:O	1:A:147:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HB2	1:A:214:PRO:HD3	1.80	0.63
1:D:427:PHE:CG	1:D:427:PHE:O	2.51	0.63
1:B:459:GLU:OE2	1:B:461:THR:OG1	2.16	0.63
1:C:234:LYS:HG2	1:C:452:GLY:HA3	1.79	0.63
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.81	0.62
1:C:680:ASN:C	1:C:680:ASN:HD22	2.08	0.62
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.97	0.62
1:A:647:GLU:O	1:A:647:GLU:HG3	2.00	0.62
1:B:233:ARG:NH1	5:B:928:HOH:O	2.22	0.62
1:D:680:ASN:ND2	1:D:682:ASP:H	1.98	0.62
1:B:594:ASN:H	1:B:597:HIS:CD2	2.11	0.61
1:A:213:ARG:CB	1:A:214:PRO:CD	2.77	0.61
1:D:574:GLN:NE2	1:D:585:ASP:H	1.98	0.61
1:A:469:PRO:HG2	1:A:472:MET:SD	2.40	0.61
1:C:302:PRO:HG3	1:C:337:VAL:HG21	1.81	0.61
1:C:194:ASP:HB3	1:C:196:ASN:H	1.66	0.61
1:D:117:THR:HB	5:D:1002:HOH:O	2.00	0.61
1:D:539:MET:HE2	1:D:539:MET:HA	1.82	0.61
1:B:290:ASN:C	1:B:290:ASN:HD22	2.03	0.61
1:C:574:GLN:HE21	1:C:585:ASP:H	1.46	0.61
1:C:478:TRP:HZ3	5:C:1055:HOH:O	1.84	0.61
1:C:211:GLN:CA	1:C:212:MET:CB	2.77	0.61
1:C:680:ASN:ND2	1:C:682:ASP:H	1.99	0.61
1:D:537:ASP:O	5:D:1091:HOH:O	2.17	0.60
1:A:594:ASN:H	1:A:597:HIS:HD2	1.46	0.60
1:A:149:ARG:HA	1:A:175:TRP:CH2	2.36	0.60
1:D:486:MET:O	1:D:490:LEU:HB2	2.02	0.60
1:C:456:MET:HG3	1:C:479:TYR:HB2	1.82	0.60
1:B:680:ASN:HD22	1:B:682:ASP:H	1.48	0.60
1:C:290:ASN:HD21	1:C:337:VAL:CG2	2.14	0.60
1:C:162:ARG:HG3	1:C:162:ARG:NH1	1.95	0.60
1:C:590:GLU:OE2	1:C:590:GLU:CA	2.50	0.60
1:C:579:ASN:HD22	1:C:579:ASN:C	2.10	0.59
1:B:166:MET:CE	1:B:175:TRP:CB	2.79	0.59
1:C:213:ARG:HB3	1:C:214:PRO:CA	2.30	0.59
1:C:213:ARG:CB	1:C:214:PRO:CA	2.80	0.59
1:D:504:HIS:HD2	5:D:986:HOH:O	1.84	0.59
1:C:552:ALA:O	1:C:720:THR:HG21	2.03	0.59
1:C:634:LYS:HE2	5:C:945:HOH:O	2.01	0.59
1:A:574:GLN:HE21	1:A:585:ASP:H	1.47	0.59
1:B:214:PRO:O	1:B:215:GLU:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:HD21	1:A:283:HIS:HE1	1.49	0.58
1:C:335:ASP:OD1	1:C:403:ARG:HD3	2.02	0.58
1:D:674:LYS:HZ3	1:D:674:LYS:HB3	1.68	0.58
1:D:373:LEU:H	1:D:373:LEU:CD2	2.07	0.58
1:B:486:MET:HE1	1:B:487:HIS:CD2	2.38	0.58
1:C:290:ASN:HD21	1:C:337:VAL:HG21	1.68	0.58
1:B:138:THR:HG21	1:B:220:ILE:HG21	1.84	0.58
1:C:532:LYS:O	1:C:533:LYS:CG	2.51	0.58
1:B:191:GLU:HG2	1:B:201:LEU:CD2	2.33	0.58
1:C:680:ASN:HD22	1:C:682:ASP:H	1.48	0.58
1:D:258:ASP:O	1:D:259:ASN:CB	2.52	0.58
1:D:319:ARG:NH2	1:D:396:ARG:O	2.37	0.58
1:A:142:VAL:HG21	1:A:190:TYR:CE1	2.38	0.58
1:C:237:ASN:HD22	1:C:283:HIS:HE1	1.48	0.58
1:D:441:ASN:ND2	1:D:444:ARG:NH1	2.37	0.58
1:B:670:ASN:HD21	1:B:707:ARG:NE	1.91	0.58
1:C:350:GLU:HA	1:C:354:THR:O	2.04	0.58
1:D:337:VAL:O	1:D:337:VAL:CG2	2.42	0.58
1:D:601:ARG:HD2	1:D:685[A]:HIS:NE2	2.19	0.58
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.56	0.57
1:A:680:ASN:C	1:A:680:ASN:HD22	2.12	0.57
1:B:514:ASN:ND2	5:B:958:HOH:O	2.37	0.57
1:D:425:ASN:ND2	5:D:925:HOH:O	2.25	0.57
1:A:234:LYS:HD2	1:A:452:GLY:HA3	1.87	0.57
1:B:601:ARG:HD2	1:B:685[A]:HIS:CE1	2.40	0.57
1:C:337:VAL:HG23	1:C:337:VAL:O	2.04	0.57
1:C:693:ASN:O	1:C:695:GLY:N	2.37	0.57
1:C:225:GLU:OE2	1:C:225:GLU:HA	2.04	0.57
1:C:427:PHE:CG	1:C:427:PHE:O	2.57	0.57
1:B:258:ASP:O	1:B:260:ASN:N	2.38	0.57
1:D:693:ASN:HD21	1:D:713:LEU:CB	2.12	0.57
1:B:142:VAL:HG12	1:B:166:MET:HE1	1.86	0.57
1:D:494:LYS:HB2	1:D:494:LYS:HZ3	1.70	0.57
1:A:213:ARG:CB	1:A:214:PRO:HD3	2.35	0.57
1:D:120:ARG:NH1	1:D:395:GLU:CD	2.62	0.57
1:C:282:THR:OG1	1:C:283:HIS:HD2	1.87	0.56
1:D:259:ASN:HB3	1:D:261:PHE:H	1.68	0.56
1:A:472:MET:CG	1:A:473:GLY:H	2.19	0.56
1:B:224:PRO:HB2	1:B:319:ARG:NH2	2.20	0.56
1:B:260:ASN:ND2	1:B:260:ASN:O	2.38	0.56
1:D:494:LYS:HB2	1:D:494:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:HB3	1:A:696:THR:CG2	2.35	0.56
1:C:579:ASN:ND2	1:C:581:ASP:H	2.03	0.56
1:A:358:GLU:OE2	1:A:358:GLU:N	2.33	0.56
1:C:426:GLU:CA	1:C:426:GLU:OE1	2.53	0.56
1:D:157:ASN:HD22	1:D:157:ASN:C	2.14	0.56
1:D:215:GLU:CB	1:D:216:THR:CA	2.83	0.56
1:D:606:LEU:CD1	1:D:679:LEU:HD11	2.36	0.56
1:B:576:ARG:HH21	1:B:585:ASP:CG	2.14	0.55
1:D:691:ALA:HB3	1:D:716:PRO:HB3	1.87	0.55
1:A:528:VAL:HG12	1:A:534:SER:HA	1.87	0.55
1:C:194:ASP:OD1	1:C:198:ASN:HB2	2.07	0.55
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.88	0.55
1:B:336:TRP:CZ2	1:B:390:ALA:HB2	2.42	0.55
1:C:504:HIS:HD2	5:C:957:HOH:O	1.90	0.55
1:A:289:ILE:C	1:A:289:ILE:HD12	2.31	0.55
1:B:333:ILE:HG12	1:B:401:ALA:HB3	1.89	0.55
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.19	0.55
1:C:259:ASN:ND2	1:C:261:PHE:H	2.04	0.54
1:A:588:LEU:HD13	1:A:596:HIS:CE1	2.42	0.54
1:D:371:ASN:CG	1:D:372:THR:N	2.62	0.54
1:B:642:VAL:HG22	1:B:650:GLU:HB2	1.89	0.54
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.55	0.54
1:D:713:LEU:C	1:D:713:LEU:CD1	2.78	0.54
1:A:496:ASP:O	1:A:498:VAL:N	2.40	0.54
1:D:676:ARG:HD2	5:D:1038:HOH:O	2.05	0.54
1:A:472:MET:HG2	1:A:473:GLY:H	1.70	0.54
1:C:656:ASN:HD22	1:C:656:ASN:C	2.16	0.54
1:A:680:ASN:HD22	1:A:682:ASP:H	1.54	0.54
1:B:528:VAL:HG11	5:B:945:HOH:O	2.07	0.54
1:C:604:ARG:NH2	5:C:958:HOH:O	2.41	0.54
1:D:215:GLU:HB3	1:D:216:THR:CA	2.37	0.54
1:D:399:ILE:HD11	1:D:402:LEU:HD23	1.90	0.54
1:C:373:LEU:N	1:C:373:LEU:CD2	2.71	0.53
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.68	0.53
1:D:183:HIS:H	1:D:186:GLN:HE21	1.57	0.53
1:C:426:GLU:OE1	1:C:426:GLU:HA	2.08	0.53
1:D:214:PRO:HA	1:D:215:GLU:C	2.30	0.53
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.90	0.53
1:C:693:ASN:HD21	1:C:714:THR:N	2.00	0.53
1:D:724:VAL:HG22	1:D:725:ARG:N	2.24	0.53
1:B:125:LEU:HD23	1:B:141:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ASN:ND2	1:B:444:ARG:HH22	2.07	0.53
1:A:693:ASN:HD21	1:A:714:THR:H	1.57	0.53
1:C:213:ARG:HA	1:C:215:GLU:N	2.24	0.53
1:C:676:ARG:O	1:C:723:LEU:HA	2.09	0.53
1:A:200:ARG:CG	1:A:200:ARG:NH1	2.42	0.53
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.91	0.53
1:A:150:VAL:HG12	1:A:166:MET:SD	2.49	0.53
1:D:399:ILE:HD11	1:D:402:LEU:HD21	1.90	0.53
1:A:573:ALA:O	1:A:596:HIS:CE1	2.62	0.53
1:B:504:HIS:HD2	5:B:925:HOH:O	1.91	0.53
1:D:503:HIS:HB3	1:D:506:LYS:HD2	1.90	0.53
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.67	0.52
1:D:132:MET:SD	1:D:139[B]:ARG:NH1	2.76	0.52
1:D:594:ASN:H	1:D:597:HIS:HD2	1.57	0.52
1:A:406:ALA:HB1	1:A:409:SER:HB3	1.90	0.52
1:A:704:SER:OG	1:A:705:HIS:HD2	1.93	0.52
1:A:150:VAL:HG22	1:A:192:MET:HB2	1.91	0.52
1:A:570:ASN:ND2	5:A:907:HOH:O	2.43	0.52
1:C:148:ARG:HG3	1:C:194:ASP:O	2.09	0.52
1:D:120:ARG:NH2	1:D:449:GLN:OE1	2.42	0.52
1:A:472:MET:O	1:A:473:GLY:C	2.51	0.52
1:D:183:HIS:H	1:D:186:GLN:NE2	2.07	0.52
1:D:680:ASN:HD22	1:D:682:ASP:H	1.56	0.52
1:A:119:LEU:HD21	1:A:445:ILE:HD13	1.90	0.52
1:A:125:LEU:HD23	1:A:141:SER:HB3	1.92	0.52
1:A:233:ARG:HG2	1:A:331:ASN:ND2	2.25	0.52
1:B:716:PRO:HB2	1:B:719:ALA:HB3	1.92	0.52
1:A:359:HIS:O	1:A:360:SER:CB	2.57	0.52
1:C:676:ARG:NH1	1:C:726:GLU:OE2	2.43	0.52
1:B:594:ASN:N	1:B:597:HIS:HD2	2.00	0.52
1:D:289:ILE:HG13	1:D:334:LEU:HD11	1.91	0.52
1:A:674:LYS:HD2	1:A:696:THR:HG21	1.92	0.51
1:B:166:MET:HE3	1:B:175:TRP:HB3	1.91	0.51
1:B:295:ASP:OD2	1:B:311:ARG:NH2	2.43	0.51
1:D:117:THR:CA	5:D:1002:HOH:O	2.58	0.51
1:B:605:ASP:OD1	1:B:686:TYR:OH	2.24	0.51
1:A:436:ILE:O	1:A:440:ARG:HG3	2.10	0.51
1:A:594:ASN:H	1:A:597:HIS:CD2	2.27	0.51
1:D:489:THR:HG22	1:D:507:LEU:HD12	1.92	0.51
1:A:146:ASN:HD22	1:A:354:THR:CG2	2.23	0.51
1:A:292:HIS:CD2	1:A:311:ARG:NH1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:N	5:C:903:HOH:O	2.43	0.51
1:B:259:ASN:H	1:B:259:ASN:ND2	2.07	0.51
1:D:629:LEU:HD11	1:D:642:VAL:HG23	1.93	0.51
1:D:674:LYS:NZ	1:D:674:LYS:CB	2.73	0.51
1:C:514:ASN:ND2	5:C:1019:HOH:O	2.43	0.51
1:C:614:LYS:HB3	1:C:618:GLU:HG3	1.93	0.51
1:C:656:ASN:C	1:C:656:ASN:ND2	2.68	0.51
1:D:117:THR:CB	5:D:1002:HOH:O	2.59	0.51
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.93	0.50
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.46	0.50
1:C:285:GLU:OE1	1:C:403:ARG:HD2	2.11	0.50
1:D:614:LYS:NZ	5:D:1024:HOH:O	2.39	0.50
1:D:693:ASN:ND2	1:D:713:LEU:CB	2.72	0.50
1:A:146:ASN:ND2	1:A:354:THR:HG21	2.26	0.50
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.47	0.50
1:A:717:PRO:O	1:A:718:LEU:C	2.54	0.50
1:C:290:ASN:ND2	1:C:337:VAL:HG22	2.26	0.50
1:C:656:ASN:ND2	1:C:658:THR:H	2.08	0.50
1:D:693:ASN:ND2	1:D:714:THR:H	2.09	0.50
1:A:289:ILE:C	1:A:289:ILE:CD1	2.84	0.50
1:A:647:GLU:O	1:A:647:GLU:CG	2.60	0.50
1:C:583:SER:HB3	2:G:1:GLC:H62	1.93	0.50
1:C:588:LEU:HD13	1:C:596:HIS:CE1	2.47	0.50
1:B:302:PRO:HG3	1:B:337:VAL:HG21	1.93	0.50
1:A:163:ARG:O	1:A:165:PRO:HD3	2.11	0.50
1:B:149:ARG:O	1:B:192:MET:HA	2.11	0.50
1:A:133:ASP:OD1	1:A:133:ASP:C	2.55	0.50
1:B:441:ASN:HD21	1:B:444:ARG:HH22	1.58	0.50
1:C:256:HIS:HB2	1:C:259:ASN:HD21	1.77	0.50
1:B:166:MET:CE	1:B:175:TRP:HB2	2.42	0.50
1:C:194:ASP:HB2	1:C:198:ASN:N	2.27	0.50
1:B:166:MET:HE2	1:B:175:TRP:HB3	1.92	0.49
1:B:293:PRO:HD3	1:B:303:THR:HG23	1.93	0.49
1:C:497:PRO:HA	1:C:500:ARG:HD2	1.92	0.49
1:A:543:ALA:HB1	1:A:595:TRP:HZ3	1.77	0.49
1:B:340:HIS:HE1	1:B:405:ASP:OD2	1.94	0.49
1:B:670:ASN:ND2	1:B:707:ARG:NE	2.52	0.49
1:C:429:GLY:CA	1:C:430:ARG:CG	2.88	0.49
1:C:685:HIS:CE1	1:D:685[A]:HIS:HD2	2.30	0.49
1:D:425:ASN:OD1	1:D:425:ASN:O	2.30	0.49
1:A:474:GLY:O	1:A:475:LEU:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:HA	1:B:238:GLN:OE1	2.12	0.49
1:B:643:ARG:O	1:B:650:GLU:HA	2.12	0.49
1:B:150:VAL:O	1:B:166:MET:HG3	2.12	0.49
1:A:295:ASP:OD2	1:A:295:ASP:N	2.45	0.49
1:B:376:ASN:O	1:B:382:VAL:CG1	2.58	0.49
1:C:426:GLU:CG	1:C:427:PHE:CD2	2.80	0.49
1:B:343:THR:HG22	1:B:373:LEU:HD21	1.95	0.49
1:C:532:LYS:C	1:C:533:LYS:CG	2.83	0.49
1:B:224:PRO:HB2	1:B:319:ARG:HH22	1.78	0.49
1:B:470:GLN:NE2	1:B:470:GLN:N	2.42	0.49
1:D:437:GLU:OE2	1:D:437:GLU:HA	2.12	0.49
1:A:472:MET:HE3	1:A:472:MET:HB3	1.74	0.49
1:C:170:LYS:NZ	5:C:990:HOH:O	2.45	0.49
1:D:278:TRP:O	1:D:604:ARG:HD2	2.13	0.49
1:C:249:HIS:ND1	1:C:252:SER:OG	2.38	0.48
1:D:724:VAL:HG22	1:D:725:ARG:H	1.78	0.48
1:B:345:ASP:OD2	1:B:345:ASP:N	2.47	0.48
1:C:157:ASN:ND2	1:C:164:HIS:CD2	2.67	0.48
1:A:645:ASP:OD1	1:A:649:ASN:ND2	2.36	0.48
1:C:256:HIS:CE1	1:C:267:GLU:OE1	2.66	0.48
1:D:258:ASP:O	1:D:259:ASN:CG	2.55	0.48
1:A:215:GLU:HG3	1:A:216:THR:H	1.78	0.48
1:A:633:ASP:OD2	1:A:665:TYR:OH	2.22	0.48
1:B:237:ASN:ND2	1:B:283:HIS:CE1	2.70	0.48
1:B:259:ASN:ND2	1:B:259:ASN:N	2.61	0.48
1:D:674:LYS:HZ3	1:D:674:LYS:CB	2.26	0.48
1:A:216:THR:O	1:A:217:ALA:HB2	2.13	0.48
1:B:336:TRP:CH2	1:B:390:ALA:HB2	2.49	0.48
1:A:680:ASN:ND2	1:A:682:ASP:H	2.12	0.48
1:A:212:MET:HE2	1:A:213:ARG:HG2	1.96	0.48
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.97	0.48
1:B:529:VAL:CG1	1:B:578:TRP:HE3	2.27	0.48
1:B:579:ASN:ND2	1:B:581:ASP:H	2.10	0.48
1:D:215:GLU:CB	1:D:217:ALA:N	2.70	0.48
1:D:258:ASP:O	1:D:259:ASN:HB2	2.14	0.48
1:C:290:ASN:ND2	1:C:337:VAL:CG2	2.76	0.48
1:C:450:VAL:HG23	1:C:450:VAL:O	2.14	0.48
1:C:560:PHE:CD2	1:C:561:PRO:HD2	2.48	0.48
1:A:259:ASN:C	1:A:259:ASN:HD22	2.21	0.48
1:B:570:ASN:ND2	5:B:945:HOH:O	2.45	0.48
1:C:182:ALA:HA	1:C:186:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:TYR:O	1:C:687:HIS:HB2	2.13	0.48
1:B:528:VAL:HA	1:B:533:LYS:O	2.14	0.47
1:C:234:LYS:HE2	1:C:451:SER:O	2.14	0.47
1:D:651:ILE:CD1	1:D:722:TRP:HB3	2.44	0.47
1:D:651:ILE:HD13	1:D:722:TRP:HB3	1.95	0.47
1:C:552:ALA:O	1:C:720:THR:CG2	2.62	0.47
1:C:684:MET:H	1:C:690:ASN:ND2	2.11	0.47
1:A:542:ASP:OD1	1:A:544:TRP:NE1	2.47	0.47
1:B:194:ASP:C	1:B:196:ASN:H	2.22	0.47
1:B:411:ILE:HB	1:B:436:ILE:HD11	1.96	0.47
1:A:579:ASN:ND2	1:A:581:ASP:H	2.13	0.47
1:B:290:ASN:C	1:B:290:ASN:ND2	2.72	0.47
1:B:492:TYR:CZ	1:B:507:LEU:HD22	2.49	0.47
1:C:237:ASN:HD22	1:C:283:HIS:CE1	2.31	0.47
1:D:117:THR:HA	5:D:1002:HOH:O	2.15	0.47
1:D:646:LYS:NZ	1:D:646:LYS:HB2	2.29	0.47
1:D:167:ARG:NH1	5:D:1122:HOH:O	2.47	0.47
1:D:211:GLN:NE2	1:D:217:ALA:HB3	2.29	0.47
1:A:142:VAL:CG2	1:A:190:TYR:CE1	2.97	0.47
1:A:146:ASN:O	1:A:147:ALA:CB	2.63	0.47
1:A:496:ASP:C	1:A:498:VAL:H	2.21	0.47
1:A:654:ALA:HB3	1:A:721:ILE:HD13	1.97	0.47
1:B:658:THR:CG2	1:B:660:VAL:HB	2.45	0.47
1:B:644:ARG:HG3	1:B:650:GLU:HB3	1.97	0.47
1:A:243:ILE:HB	1:A:563:LYS:HD2	1.97	0.47
1:A:494:LYS:HB3	1:A:494:LYS:HE2	1.78	0.47
1:B:411:ILE:O	1:B:432:ASN:N	2.47	0.47
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.97	0.47
1:C:579:ASN:C	1:C:579:ASN:ND2	2.72	0.47
1:D:646:LYS:NZ	1:D:646:LYS:CB	2.77	0.47
1:A:259:ASN:HD22	1:A:260:ASN:N	2.13	0.46
1:B:191:GLU:CG	1:B:201:LEU:CD2	2.93	0.46
1:B:213:ARG:HD2	1:B:215:GLU:HB2	1.96	0.46
1:B:671:GLN:HB3	1:D:498:VAL:HG11	1.97	0.46
1:C:259:ASN:ND2	1:C:259:ASN:H	2.13	0.46
1:D:532:LYS:O	1:D:533:LYS:HB2	2.15	0.46
1:B:250:LEU:HD22	1:B:268:LEU:HD13	1.96	0.46
1:C:651:ILE:HD11	1:C:722:TRP:HB3	1.96	0.46
1:D:538:ARG:HD3	5:D:981:HOH:O	2.14	0.46
1:A:130:ASP:OD2	1:A:131:THR:N	2.46	0.46
1:A:146:ASN:HD22	1:A:354:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:CG	1:A:213:ARG:N	2.59	0.46
1:B:520:VAL:O	1:B:522:PRO:HD3	2.14	0.46
1:B:523:LEU:HD22	1:B:557:MET:SD	2.55	0.46
1:C:256:HIS:HE1	1:C:267:GLU:OE1	1.98	0.46
1:D:552:ALA:HA	1:D:720:THR:HG23	1.97	0.46
1:A:273:VAL:HB	1:A:274:PRO:HD3	1.97	0.46
1:C:429:GLY:HA3	1:C:430:ARG:HG3	1.96	0.46
1:D:215:GLU:HA	1:D:216:THR:HG23	1.96	0.46
1:D:431:GLU:H	1:D:431:GLU:HG2	1.39	0.46
1:D:590:GLU:HA	5:D:990:HOH:O	2.14	0.46
1:A:684:MET:H	1:A:690:ASN:ND2	2.14	0.46
1:C:551:ARG:NH1	1:C:681:THR:O	2.45	0.46
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.45	0.46
1:D:646:LYS:HB2	1:D:646:LYS:HZ1	1.81	0.46
1:B:644:ARG:HA	1:B:649:ASN:O	2.16	0.46
1:C:658:THR:HG22	1:C:660:VAL:N	2.08	0.46
1:B:237:ASN:HD22	1:B:283:HIS:CE1	2.28	0.46
1:B:426:GLU:OE2	1:B:433:LEU:HD12	2.16	0.46
1:C:431:GLU:OE1	1:C:431:GLU:C	2.59	0.46
1:A:645:ASP:OD2	1:A:649:ASN:N	2.48	0.46
1:D:118[A]:HIS:N	5:D:1002:HOH:O	2.49	0.46
1:A:359:HIS:CD2	1:A:376:ASN:HA	2.51	0.46
1:D:232:GLU:H	1:D:232:GLU:CD	2.24	0.46
1:B:166:MET:HE2	1:B:175:TRP:CB	2.45	0.45
1:A:213:ARG:O	1:A:215:GLU:N	2.49	0.45
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.23	0.45
1:D:118[B]:HIS:N	5:D:1002:HOH:O	2.49	0.45
1:D:187:LEU:CD2	1:D:219:LEU:HD12	2.43	0.45
1:A:661:PRO:HB3	1:A:717:PRO:HD3	1.99	0.45
1:B:182:ALA:HA	1:B:186:GLN:OE1	2.15	0.45
1:C:247:GLU:OE1	1:C:525:HIS:HD2	1.99	0.45
1:C:593:ASP:OD2	1:C:687:HIS:HE1	1.99	0.45
1:A:138:THR:HG21	1:A:220:ILE:HD13	1.96	0.45
1:A:209:GLU:OE2	1:A:310:ARG:NH1	2.49	0.45
1:B:425:ASN:OD1	1:B:429:GLY:N	2.50	0.45
1:B:494:LYS:HB3	1:B:494:LYS:HE2	1.74	0.45
1:B:658:THR:HG23	1:B:660:VAL:H	1.74	0.45
1:C:492:TYR:CE2	1:C:507:LEU:CD2	3.00	0.45
1:C:331:ASN:ND2	5:C:928:HOH:O	2.49	0.45
1:C:426:GLU:OE1	1:C:426:GLU:C	2.60	0.45
1:C:626:PHE:C	1:C:626:PHE:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASP:C	1:D:160:ASP:OD1	2.60	0.45
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.99	0.45
1:D:713:LEU:HD11	1:D:715:LEU:HD21	1.97	0.45
1:D:247:GLU:CD	1:D:525:HIS:HD2	2.25	0.45
1:A:430:ARG:O	1:A:431:GLU:C	2.59	0.45
1:A:574:GLN:HG3	1:A:585:ASP:HB2	1.98	0.45
1:B:674:LYS:HB2	1:B:674:LYS:HE2	1.55	0.45
1:C:194:ASP:HB2	1:C:198:ASN:H	1.81	0.45
1:C:278:TRP:O	1:C:604:ARG:HD2	2.17	0.45
1:A:254:ARG:HG2	1:A:586:TRP:NE1	2.32	0.45
1:C:211:GLN:HB3	1:C:212:MET:HB3	1.99	0.45
1:C:552:ALA:HA	1:C:720:THR:CG2	2.47	0.45
1:D:136:THR:HG22	5:D:997:HOH:O	2.16	0.45
1:A:441:ASN:OD1	1:A:444:ARG:NH1	2.46	0.45
1:A:631:VAL:O	1:A:631:VAL:HG22	2.17	0.45
1:B:594:ASN:HD22	1:B:594:ASN:C	2.25	0.45
1:C:456:MET:HE3	1:C:456:MET:HB2	1.61	0.45
1:D:399:ILE:HD12	1:D:401:ALA:H	1.82	0.45
1:A:550:LEU:HD11	1:A:554:TYR:CZ	2.51	0.45
1:C:528:VAL:O	1:C:577:GLU:HB2	2.17	0.45
1:C:533:LYS:O	1:C:538:ARG:NH2	2.49	0.44
1:A:472:MET:CG	1:A:473:GLY:N	2.71	0.44
1:B:467:SER:HA	1:B:477:PHE:O	2.17	0.44
1:B:574:GLN:NE2	1:B:585:ASP:H	2.14	0.44
1:C:211:GLN:HB3	1:C:212:MET:CB	2.47	0.44
1:D:674:LYS:HD2	1:D:698[B]:HIS:CD2	2.53	0.44
1:A:242:PRO:HD3	1:A:617:HIS:CE1	2.52	0.44
1:A:496:ASP:C	1:A:498:VAL:N	2.72	0.44
1:A:543:ALA:CB	1:A:595:TRP:HZ3	2.31	0.44
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.58	0.44
1:D:340:HIS:CE1	1:D:405:ASP:OD2	2.63	0.44
1:A:213:ARG:C	1:A:215:GLU:H	2.25	0.44
1:A:467:SER:OG	1:A:517:GLU:OE2	2.35	0.44
1:B:669:ILE:O	1:B:707:ARG:HD3	2.17	0.44
1:C:399:ILE:CD1	1:C:401:ALA:H	2.28	0.44
1:A:593:ASP:OD2	1:A:687:HIS:CE1	2.69	0.44
1:B:155:GLN:O	5:B:961:HOH:O	2.21	0.44
1:C:426:GLU:CG	1:C:427:PHE:N	2.78	0.44
1:D:656:ASN:ND2	5:D:1043:HOH:O	2.46	0.44
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.52	0.44
1:C:225:GLU:O	1:C:226:LYS:HB2	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:GLU:OE1	1:B:707:ARG:NH2	2.49	0.44
1:C:289:ILE:HD12	1:C:289:ILE:C	2.42	0.44
1:A:148:ARG:H	1:A:148:ARG:HG2	1.54	0.44
1:A:684:MET:HG2	1:A:690:ASN:CG	2.43	0.44
1:D:703:ALA:HA	1:D:707:ARG:O	2.18	0.44
1:A:142:VAL:CG2	1:A:190:TYR:CZ	3.01	0.44
1:C:194:ASP:HB3	1:C:196:ASN:N	2.33	0.44
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.53	0.44
1:D:414:ASP:O	1:D:415:TYR:CG	2.71	0.44
1:D:615:ALA:HB3	1:D:651:ILE:HG23	1.98	0.44
1:B:658:THR:HG22	1:B:660:VAL:N	2.22	0.43
1:C:655:SER:OG	1:C:720:THR:HB	2.18	0.43
1:C:559:ALA:HB1	1:C:653:VAL:HG21	2.00	0.43
1:C:593:ASP:HA	1:C:597:HIS:CD2	2.52	0.43
1:C:610:TYR:O	1:C:617:HIS:HD2	2.01	0.43
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.52	0.43
1:A:533:LYS:O	1:A:538:ARG:NH2	2.52	0.43
1:C:130:ASP:HB3	1:C:178:PHE:CE2	2.53	0.43
1:A:289:ILE:O	1:A:308:PRO:HA	2.18	0.43
1:A:489:THR:O	1:A:493:MET:HB2	2.18	0.43
1:D:399:ILE:CD1	1:D:402:LEU:HD23	2.48	0.43
1:A:237:ASN:ND2	1:A:283:HIS:CE1	2.76	0.43
1:B:191:GLU:CG	1:B:201:LEU:HD23	2.42	0.43
1:C:472:MET:SD	1:C:472:MET:N	2.91	0.43
1:A:393:TRP:HB3	1:A:399:ILE:HG13	2.00	0.43
1:A:463:PHE:O	1:A:466:VAL:HG23	2.19	0.43
1:B:212:MET:O	1:B:214:PRO:HA	2.18	0.43
1:D:118[A]:HIS:CD2	1:D:118[A]:HIS:H	2.31	0.43
1:A:194:ASP:CG	1:A:196:ASN:H	2.26	0.43
1:A:682:ASP:HB2	1:A:719:ALA:HB2	2.01	0.43
1:B:594:ASN:HD21	1:B:596:HIS:HB2	1.83	0.43
1:C:302:PRO:HG3	1:C:337:VAL:CG2	2.49	0.43
1:A:467:SER:HA	1:A:477:PHE:O	2.18	0.43
1:C:429:GLY:HA3	1:C:430:ARG:CG	2.49	0.43
1:D:427:PHE:N	1:D:428:GLY:HA2	2.33	0.43
1:A:407:VAL:HG21	1:A:457:ALA:HB1	2.01	0.43
1:B:213:ARG:N	1:B:214:PRO:CA	2.82	0.43
1:C:492:TYR:CD2	1:C:507:LEU:HD21	2.54	0.43
1:D:610:TYR:O	1:D:617:HIS:HD2	2.01	0.43
1:A:465:GLY:O	1:A:474:GLY:O	2.37	0.42
1:A:495:LEU:HD13	1:A:503:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLU:HB2	1:A:519:PHE:CZ	2.53	0.42
1:C:490:LEU:HD13	1:C:490:LEU:HA	1.86	0.42
1:D:656:ASN:C	1:D:656:ASN:HD22	2.27	0.42
2:F:1:GLC:H62	2:F:2:GLC:O5	2.19	0.42
1:A:333:ILE:HG12	1:A:401:ALA:HB3	2.01	0.42
1:B:658:THR:HG21	1:B:660:VAL:HB	2.01	0.42
1:C:259:ASN:HD22	1:C:261:PHE:H	1.67	0.42
1:A:223:LEU:HD23	1:A:396:ARG:CZ	2.50	0.42
1:A:590:GLU:OE1	1:A:590:GLU:HA	2.19	0.42
1:B:579:ASN:ND2	1:B:579:ASN:C	2.77	0.42
1:C:171:GLU:CD	1:C:171:GLU:H	2.27	0.42
1:D:579:ASN:ND2	1:D:581:ASP:H	2.18	0.42
1:C:426:GLU:HG3	1:C:427:PHE:N	2.34	0.42
1:C:542:ASP:OD2	1:C:542:ASP:C	2.62	0.42
1:C:560:PHE:O	1:C:564:LYS:NZ	2.53	0.42
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.91	0.42
1:B:213:ARG:HD3	1:B:215:GLU:HG3	2.02	0.42
1:D:302:PRO:HG3	1:D:337:VAL:CG2	2.41	0.42
1:A:666:ARG:HA	1:A:711:LEU:O	2.20	0.42
1:C:211:GLN:CB	1:C:212:MET:CB	2.97	0.42
1:B:287:LEU:O	1:B:288:PRO:C	2.62	0.42
1:C:310:ARG:HD2	1:C:310:ARG:O	2.20	0.42
1:C:444:ARG:O	1:C:448:GLU:HG3	2.20	0.42
1:D:171:GLU:CG	5:D:1040:HOH:O	2.43	0.42
1:D:552:ALA:O	1:D:720:THR:CG2	2.68	0.42
1:B:414:ASP:OD2	1:B:414:ASP:N	2.53	0.42
1:D:674:LYS:HZ3	1:D:696:THR:HG21	1.84	0.42
1:C:259:ASN:HD22	1:C:260:ASN:N	2.17	0.41
1:A:250:LEU:HD21	1:A:286:LEU:HD22	2.02	0.41
1:B:213:ARG:CD	1:B:215:GLU:HG3	2.50	0.41
1:B:686:TYR:O	1:B:687:HIS:HB2	2.20	0.41
1:C:682:ASP:HB2	1:C:719:ALA:HB2	2.02	0.41
1:D:514:ASN:ND2	5:D:938:HOH:O	2.52	0.41
1:A:157:ASN:OD1	1:A:164:HIS:CD2	2.74	0.41
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.92	0.41
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.55	0.41
1:B:199:LEU:HD13	1:B:199:LEU:H	1.84	0.41
1:B:594:ASN:HD22	1:B:596:HIS:H	1.67	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.92	0.41
1:B:194:ASP:C	1:B:196:ASN:N	2.77	0.41
1:B:529:VAL:CG1	1:B:578:TRP:CE3	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:HD3	5:D:1046:HOH:O	2.20	0.41
1:B:222:GLY:O	1:B:315:ARG:NH1	2.41	0.41
1:B:318:PHE:CE2	1:B:322:ILE:HD11	2.53	0.41
1:C:704:SER:OG	1:C:705:HIS:HD2	2.03	0.41
1:A:157:ASN:OD1	1:A:164:HIS:HD2	2.03	0.41
1:B:357:TYR:CD1	1:B:382:VAL:HG23	2.56	0.41
1:B:516:THR:C	1:B:517:GLU:HG2	2.45	0.41
1:C:425:ASN:ND2	1:C:425:ASN:N	2.69	0.41
1:D:567:PHE:O	1:D:568:MET:C	2.64	0.41
1:A:230:THR:O	1:A:234:LYS:HG2	2.20	0.41
1:D:212[A]:MET:HG2	1:D:310:ARG:HG2	2.03	0.41
1:D:443:ASN:O	1:D:446:LEU:O	2.39	0.41
1:D:533:LYS:O	1:D:538:ARG:NH2	2.53	0.41
1:D:684:MET:H	1:D:690:ASN:ND2	2.19	0.41
1:A:442:THR:O	1:A:446:LEU:HG	2.21	0.41
1:B:717:PRO:O	1:B:718:LEU:C	2.63	0.41
1:C:160:ASP:OD2	1:C:160:ASP:C	2.64	0.41
1:D:488:ASP:OD2	5:D:1041:HOH:O	2.22	0.41
1:D:493:MET:CB	1:D:539:MET:HE1	2.46	0.41
1:A:456:MET:HG2	1:A:479:TYR:HB2	2.03	0.41
1:A:709:HIS:CD2	5:A:924:HOH:O	2.54	0.41
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.79	0.41
1:B:213:ARG:HB2	1:B:215:GLU:HB2	2.03	0.41
1:B:489:THR:HG22	1:B:507:LEU:HD12	2.02	0.41
1:C:289:ILE:C	1:C:289:ILE:CD1	2.94	0.41
1:D:214:PRO:C	1:D:215:GLU:O	2.62	0.41
1:D:486:MET:CE	1:D:527:GLU:CD	2.94	0.41
1:D:686:TYR:O	1:D:687:HIS:HB2	2.21	0.41
1:B:213:ARG:N	1:B:214:PRO:HA	2.35	0.41
1:C:486:MET:HE3	1:C:486:MET:HB3	1.86	0.41
1:A:703:ALA:HA	1:A:707:ARG:O	2.20	0.40
1:D:656:ASN:ND2	1:D:656:ASN:C	2.78	0.40
1:A:227:VAL:HG22	1:A:319:ARG:NH2	2.36	0.40
1:B:693:ASN:ND2	1:B:714:THR:H	2.15	0.40
1:B:709:HIS:HD2	5:B:910:HOH:O	2.02	0.40
1:D:399:ILE:HD12	1:D:399:ILE:C	2.46	0.40
1:A:520:VAL:HG22	1:A:563:LYS:HB2	2.04	0.40
1:C:130:ASP:HB3	1:C:178:PHE:HE2	1.86	0.40
1:D:215:GLU:CB	1:D:216:THR:HG1	2.22	0.40
1:A:189:LYS:HE2	1:A:216:THR:O	2.21	0.40
1:B:602:LEU:HG	1:B:606:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:HA	1:C:342:PRO:HD3	1.92	0.40
1:C:412:TYR:C	1:C:414:ASP:N	2.78	0.40
1:C:551:ARG:HB3	1:C:681:THR:HB	2.03	0.40
1:A:654:ALA:HB3	1:A:721:ILE:CD1	2.51	0.40
1:A:698:HIS:HB3	5:A:902:HOH:O	2.22	0.40
1:B:233:ARG:HG2	1:B:331:ASN:HD21	1.86	0.40
1:C:119:LEU:HA	1:C:119:LEU:HD12	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	581/612 (95%)	529 (91%)	41 (7%)	11 (2%)	6 7
1	B	591/612 (97%)	544 (92%)	35 (6%)	12 (2%)	6 6
1	C	583/612 (95%)	550 (94%)	25 (4%)	8 (1%)	9 11
1	D	595/612 (97%)	568 (96%)	21 (4%)	6 (1%)	12 17
All	All	2350/2448 (96%)	2191 (93%)	122 (5%)	37 (2%)	7 9

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ARG
1	A	215	GLU
1	A	226	LYS
1	A	475	LEU
1	B	215	GLU
1	B	225	GLU
1	B	226	LYS
1	B	530	HIS

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Mol	Chain	Res	Type
1	C	194	ASP
1	C	226	LYS
1	C	426	GLU
1	C	430	ARG
1	D	215	GLU
1	D	345	ASP
1	D	427	PHE
1	B	259	ASN
1	C	212	MET
1	C	694	GLY
1	D	259	ASN
1	A	522	PRO
1	B	159	TRP
1	B	160	ASP
1	B	373	LEU
1	B	522	PRO
1	C	215	GLU
1	D	216	THR
1	D	522	PRO
1	B	372	THR
1	C	522	PRO
1	A	147	ALA
1	A	342	PRO
1	A	214	PRO
1	A	497	PRO
1	A	429	GLY
1	B	293	PRO
1	A	473	GLY
1	B	214	PRO

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	497/521 (95%)	452 (91%)	45 (9%)	9	11
1	B	507/521 (97%)	465 (92%)	42 (8%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	499/521 (96%)	445 (89%)	54 (11%)	6	7
1	D	511/521 (98%)	471 (92%)	40 (8%)	11	16
All	All	2014/2084 (97%)	1833 (91%)	181 (9%)	9	11

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	139	ARG
1	A	146	ASN
1	A	149	ARG
1	A	163	ARG
1	A	170	LYS
1	A	192	MET
1	A	194	ASP
1	A	199	LEU
1	A	200	ARG
1	A	211	GLN
1	A	234	LYS
1	A	257	THR
1	A	259	ASN
1	A	263	LEU
1	A	277	LYS
1	A	289	ILE
1	A	291	GLU
1	A	295	ASP
1	A	346	PHE
1	A	350	GLU
1	A	356	LEU
1	A	359	HIS
1	A	360	SER
1	A	391	LEU
1	A	436	ILE
1	A	462	ASP
1	A	472	MET
1	A	475	LEU
1	A	490	LEU
1	A	493	MET
1	A	498	VAL
1	A	507	LEU
1	A	537	ASP

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Mol	Chain	Res	Type
1	A	606	LEU
1	A	616	MET
1	A	619	LEU
1	A	642	VAL
1	A	646	LYS
1	A	658	THR
1	A	684	MET
1	A	690	ASN
1	A	720	THR
1	A	721	ILE
1	A	723	LEU
1	B	118	HIS
1	B	166	MET
1	B	168	LEU
1	B	187	LEU
1	B	199	LEU
1	B	216	THR
1	B	259	ASN
1	B	290	ASN
1	B	305	LEU
1	B	330	LEU
1	B	335	ASP
1	B	345	ASP
1	B	356	LEU
1	B	371	ASN
1	B	373	LEU
1	B	380	ARG
1	B	382	VAL
1	B	391	LEU
1	B	411	ILE
1	B	414	ASP
1	B	430	ARG
1	B	436	ILE
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	498	VAL
1	B	500	ARG
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU

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Mol	Chain	Res	Type
1	B	594	ASN
1	B	606	LEU
1	B	619	LEU
1	B	642	VAL
1	B	651	ILE
1	B	658	THR
1	B	674	LYS
1	B	680	ASN
1	B	689	SER
1	B	714	THR
1	B	723	LEU
1	C	119	LEU
1	C	131	THR
1	C	149	ARG
1	C	162	ARG
1	C	168	LEU
1	C	169	ARG
1	C	171	GLU
1	C	202	LYS
1	C	212	MET
1	C	213	ARG
1	C	219	LEU
1	C	223	LEU
1	C	258	ASP
1	C	259	ASN
1	C	289	ILE
1	C	297	SER
1	C	305	LEU
1	C	310	ARG
1	C	356	LEU
1	C	359	HIS
1	C	373	LEU
1	C	374	ILE
1	C	391	LEU
1	C	399	ILE
1	C	409	SER
1	C	425	ASN
1	C	426	GLU
1	C	427	PHE
1	C	430	ARG
1	C	431	GLU
1	C	444	ARG

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Mol	Chain	Res	Type
1	C	446	LEU
1	C	456	MET
1	C	470	GLN
1	C	471	ASP
1	C	472	MET
1	C	478	TRP
1	C	490	LEU
1	C	498	VAL
1	C	507	LEU
1	C	523	LEU
1	C	524	SER
1	C	590	GLU
1	C	604	ARG
1	C	619	LEU
1	C	642	VAL
1	C	647	GLU
1	C	651	ILE
1	C	656	ASN
1	C	658	THR
1	C	680	ASN
1	C	720	THR
1	C	723	LEU
1	C	726	GLU
1	D	118[A]	HIS
1	D	118[B]	HIS
1	D	119	LEU
1	D	131	THR
1	D	136	THR
1	D	148	ARG
1	D	149[A]	ARG
1	D	149[B]	ARG
1	D	157	ASN
1	D	171	GLU
1	D	216	THR
1	D	223	LEU
1	D	232	GLU
1	D	319	ARG
1	D	346	PHE
1	D	356	LEU
1	D	373	LEU
1	D	391	LEU
1	D	399	ILE

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Mol	Chain	Res	Type
1	D	427	PHE
1	D	431	GLU
1	D	470	GLN
1	D	471	ASP
1	D	475	LEU
1	D	490	LEU
1	D	494	LYS
1	D	500	ARG
1	D	507	LEU
1	D	523	LEU
1	D	538	ARG
1	D	606	LEU
1	D	619	LEU
1	D	642	VAL
1	D	646	LYS
1	D	651	ILE
1	D	674	LYS
1	D	680	ASN
1	D	700	ASP
1	D	720	THR
1	D	723	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	155	GLN
1	A	164	HIS
1	A	196	ASN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	260	ASN
1	A	283	HIS
1	A	326	HIS
1	A	331	ASN
1	A	355	ASN
1	A	359	HIS
1	A	376	ASN
1	A	384	ASN
1	A	501	GLN
1	A	503	HIS

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Mol	Chain	Res	Type
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	613	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	687	HIS
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	A	709	HIS
1	B	155	GLN
1	B	164	HIS
1	B	198	ASN
1	B	237	ASN
1	B	259	ASN
1	B	260	ASN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	355	ASN
1	B	371	ASN
1	B	376	ASN
1	B	441	ASN
1	B	470	GLN
1	B	482	ASN
1	B	487	HIS
1	B	501	GLN
1	B	514	ASN
1	B	525	HIS
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	580	HIS
1	B	594	ASN
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	670	ASN

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Mol	Chain	Res	Type
1	B	680	ASN
1	B	690	ASN
1	B	693	ASN
1	B	705	HIS
1	B	709	HIS
1	C	157	ASN
1	C	164	HIS
1	C	183	HIS
1	C	186	GLN
1	C	229	GLN
1	C	237	ASN
1	C	238	GLN
1	C	256	HIS
1	C	259	ASN
1	C	283	HIS
1	C	290	ASN
1	C	301	GLN
1	C	340	HIS
1	C	359	HIS
1	C	425	ASN
1	C	470	GLN
1	C	501	GLN
1	C	504	HIS
1	C	514	ASN
1	C	525	HIS
1	C	570	ASN
1	C	574	GLN
1	C	579	ASN
1	C	597	HIS
1	C	617	HIS
1	C	656	ASN
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	705	HIS
1	D	157	ASN
1	D	164	HIS
1	D	186	GLN
1	D	237	ASN
1	D	256	HIS
1	D	259	ASN

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Mol	Chain	Res	Type
1	D	283	HIS
1	D	340	HIS
1	D	371	ASN
1	D	425	ASN
1	D	441	ASN
1	D	443	ASN
1	D	470	GLN
1	D	487	HIS
1	D	504	HIS
1	D	514	ASN
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	579	ASN
1	D	597	HIS
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	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 ⓘ

10 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	0.55	0	17,17,17	0.89	0
2	GLC	E	2	2	11,11,12	0.65	0	15,15,17	1.21	2 (13%)
2	GLC	F	1	2	12,12,12	0.55	0	17,17,17	0.87	0
2	GLC	F	2	2	11,11,12	0.58	0	15,15,17	1.04	1 (6%)
2	GLC	G	1	2	12,12,12	0.59	0	17,17,17	0.69	0
2	GLC	G	2	2	11,11,12	0.67	0	15,15,17	1.23	3 (20%)
2	GLC	H	1	2	12,12,12	0.51	0	17,17,17	0.62	0
2	GLC	H	2	2	11,11,12	0.44	0	15,15,17	2.62	2 (13%)
2	GLC	I	1	2	12,12,12	0.61	0	17,17,17	0.82	1 (5%)
2	GLC	I	2	2	11,11,12	0.72	0	15,15,17	1.42	2 (13%)

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
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	1/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	1/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	GLC	C1-O5-C5	8.46	123.53	112.19
2	H	2	GLC	C2-C3-C4	-4.14	103.58	110.86
2	I	2	GLC	C1-O5-C5	3.51	116.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-O5-C5	3.08	116.32	112.19
2	E	2	GLC	C3-C4-C5	2.63	115.01	110.23
2	I	2	GLC	C1-C2-C3	2.60	113.44	109.64
2	E	2	GLC	C1-O5-C5	2.24	115.18	112.19
2	G	2	GLC	C2-C3-C4	-2.20	106.99	110.86
2	I	1	GLC	O2-C2-C3	-2.10	105.43	110.38
2	G	2	GLC	C3-C4-C5	-2.08	106.47	110.23
2	G	2	GLC	O4-C4-C5	2.02	114.30	109.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

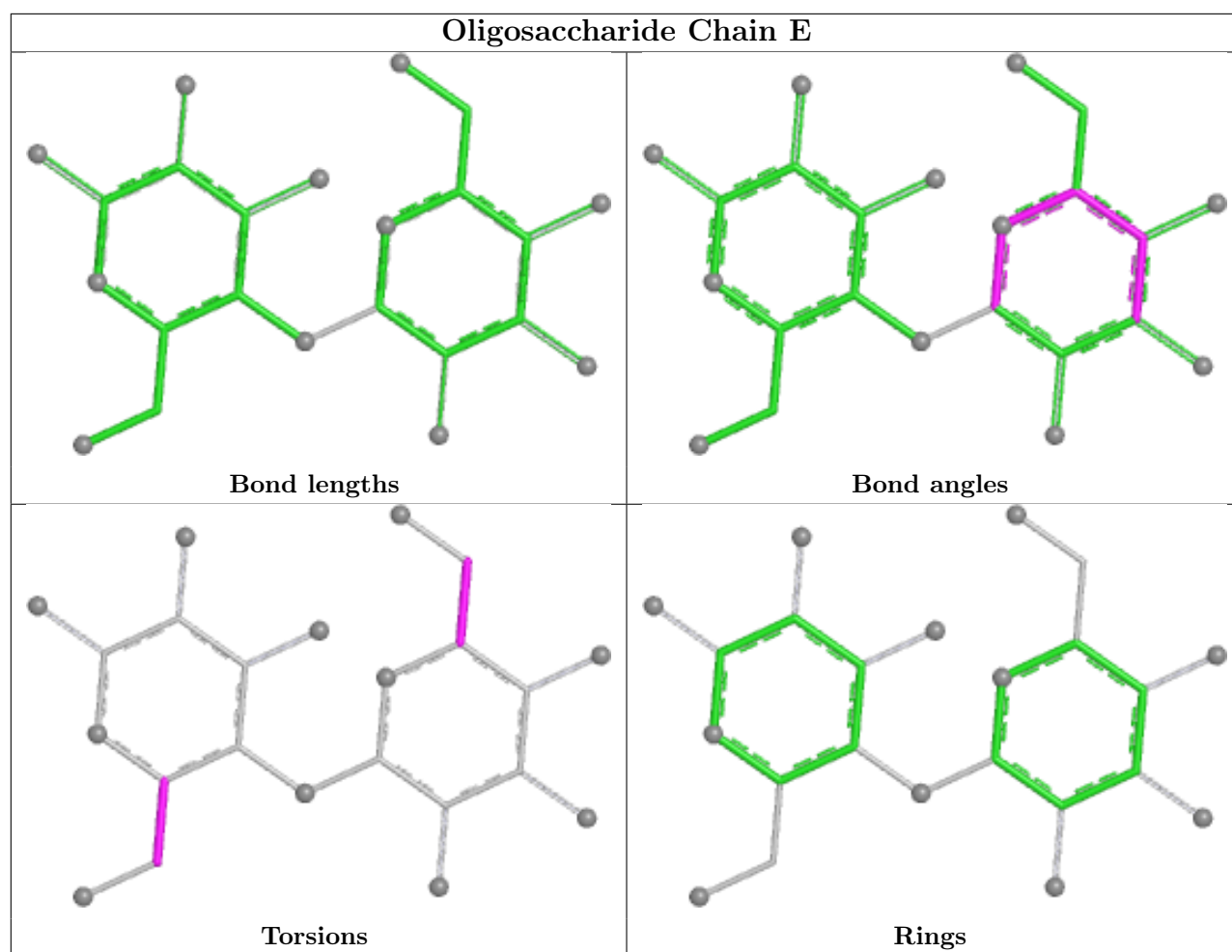
Mol	Chain	Res	Type	Atoms
2	H	1	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6

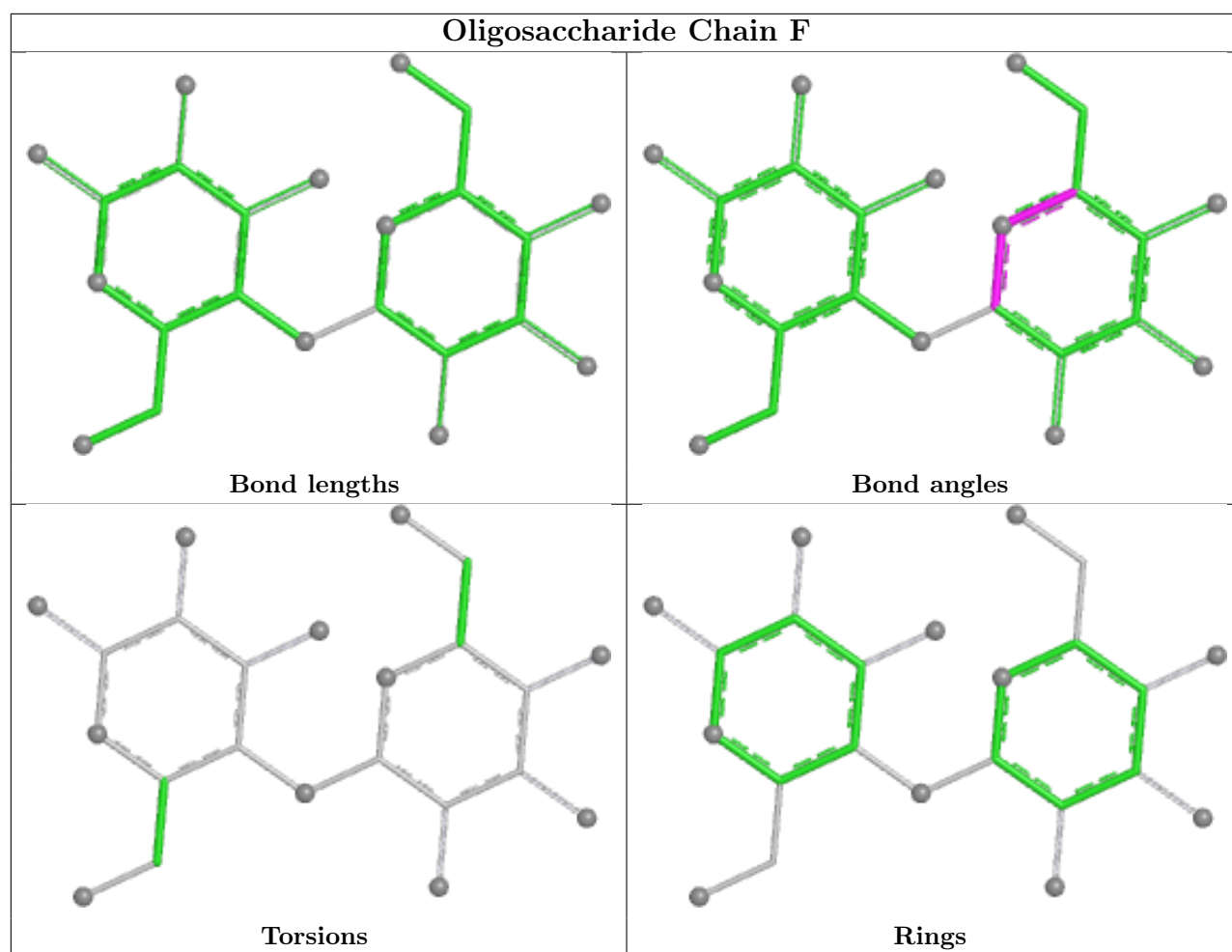
There are no ring outliers.

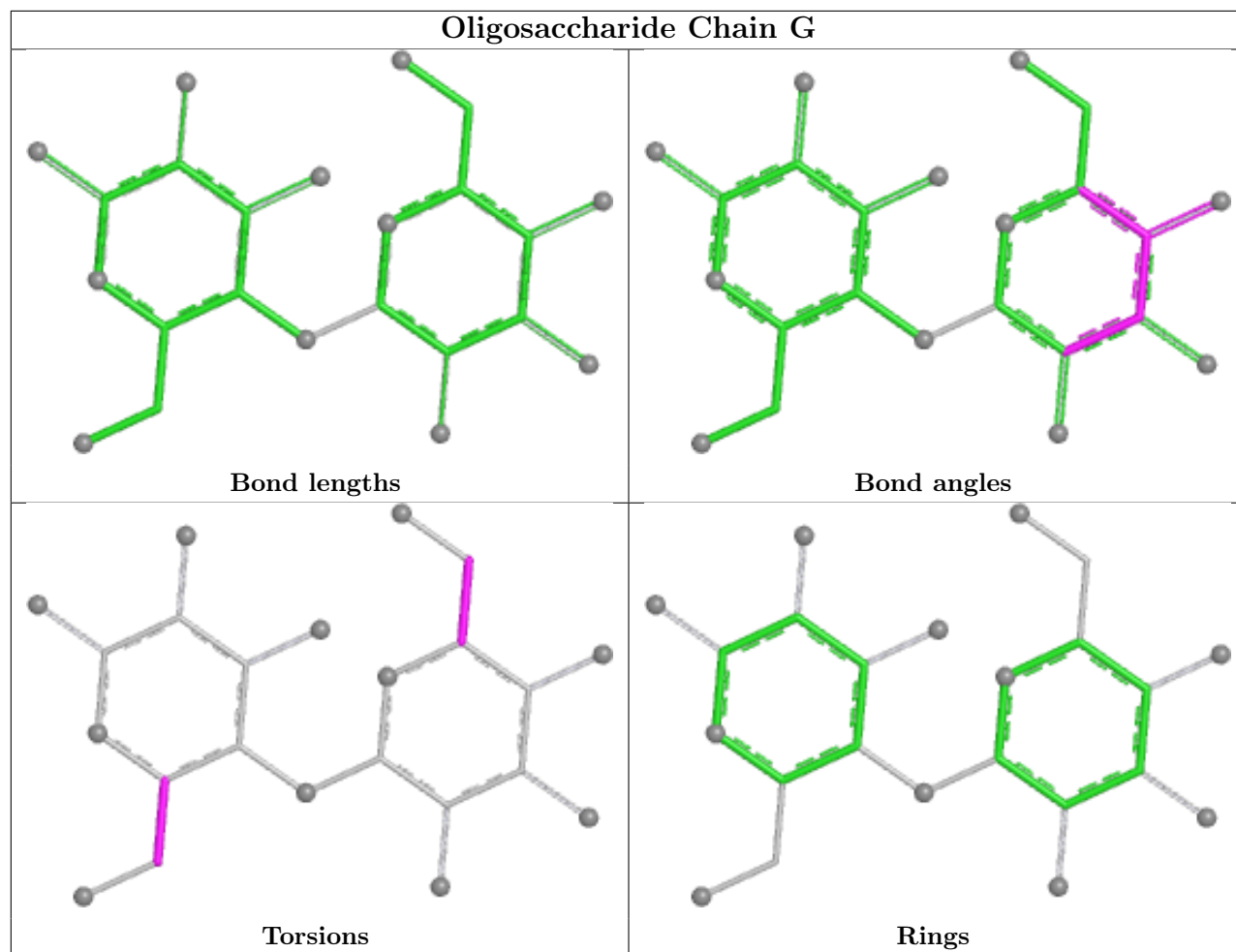
3 monomers are involved in 2 short contacts:

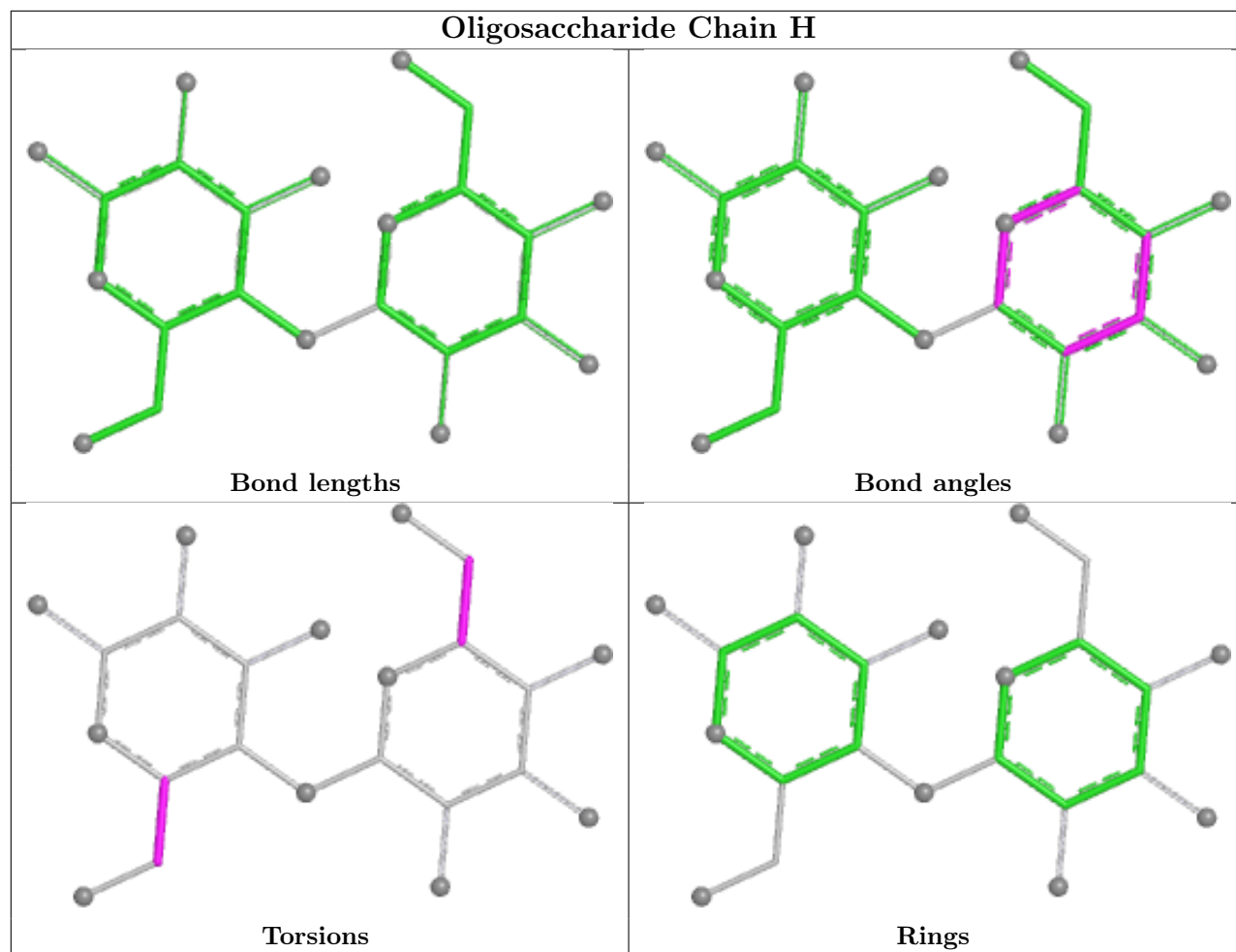
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0
2	F	2	GLC	1	0
2	G	1	GLC	1	0

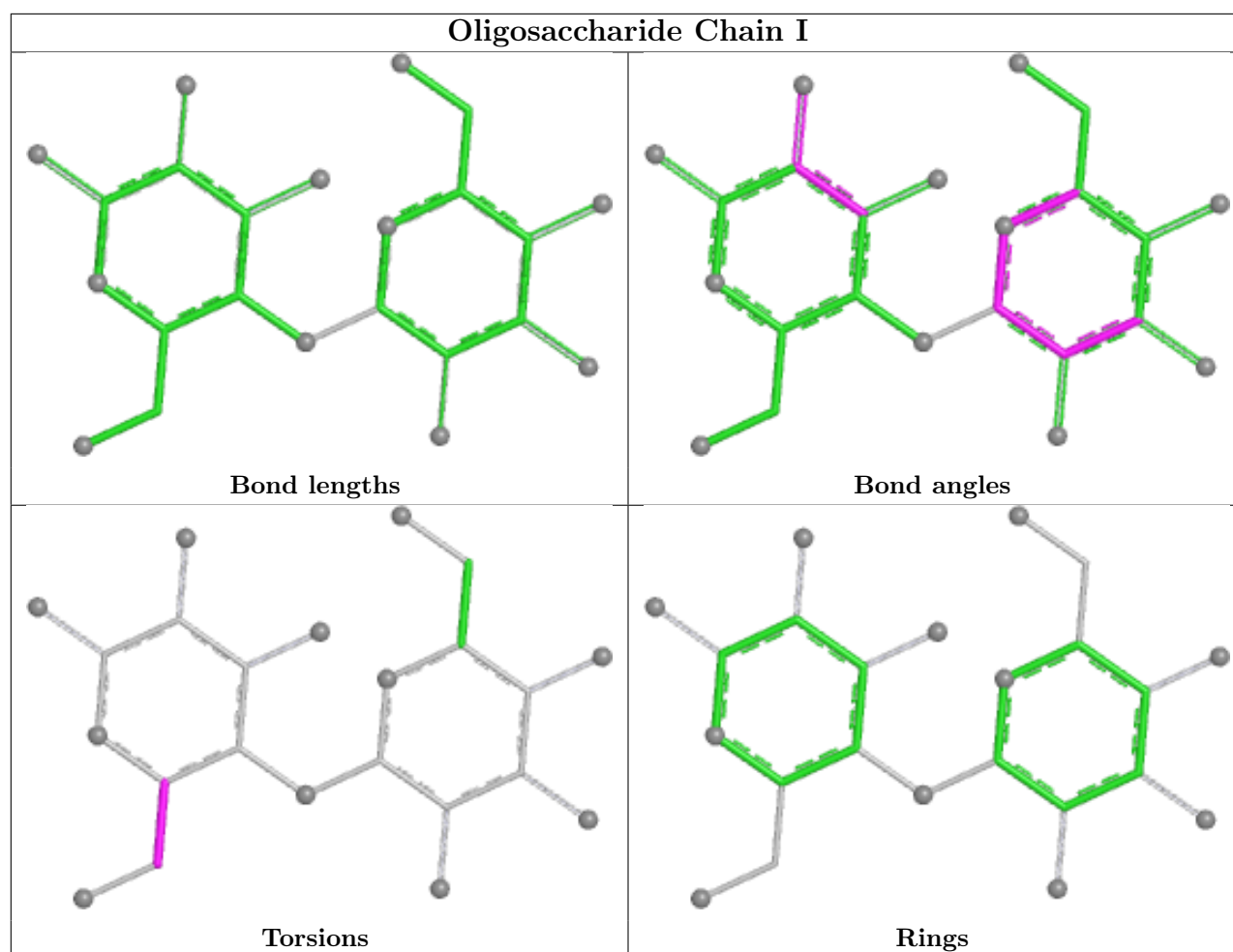
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BGC	A	801	-	12,12,12	0.47	0	17,17,17	0.93	1 (5%)
4	GOL	C	805	-	5,5,5	0.61	0	5,5,5	1.40	0
4	GOL	D	806	-	5,5,5	0.32	0	5,5,5	0.47	0
4	GOL	D	805	-	5,5,5	0.45	0	5,5,5	0.64	0
4	GOL	B	803	-	5,5,5	0.40	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	A	801	-	-	2/2/22/22	0/1/1/1
4	GOL	C	805	-	-	2/4/4/4	-
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	D	805	-	-	4/4/4/4	-
4	GOL	B	803	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	801	BGC	C4-C3-C2	-2.12	107.11	110.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	805	GOL	O1-C1-C2-C3
4	D	805	GOL	O1-C1-C2-C3
4	D	805	GOL	C1-C2-C3-O3
3	A	801	BGC	O5-C5-C6-O6
4	D	806	GOL	O1-C1-C2-C3
4	C	805	GOL	O1-C1-C2-O2
3	A	801	BGC	C4-C5-C6-O6
4	D	805	GOL	O1-C1-C2-O2
4	D	806	GOL	O1-C1-C2-O2
4	B	803	GOL	O1-C1-C2-O2
4	D	805	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	586/612 (95%)	0.78	43 (7%)	21	20	37, 87, 129, 153	5 (0%)
1	B	596/612 (97%)	0.74	41 (6%)	23	22	32, 82, 123, 153	9 (1%)
1	C	589/612 (96%)	0.22	16 (2%)	56	57	48, 69, 89, 109	6 (1%)
1	D	593/612 (96%)	0.02	19 (3%)	50	51	25, 53, 74, 100	17 (2%)
All	All	2364/2448 (96%)	0.44	119 (5%)	34	33	25, 73, 119, 153	37 (1%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ASN	8.8
1	D	685[A]	HIS	7.8
1	B	277	LYS	7.6
1	B	353	GLY	6.0
1	B	216	THR	5.9
1	B	362	PRO	4.9
1	B	423	ILE	4.6
1	C	431	GLU	4.5
1	B	214	PRO	4.4
1	A	118	HIS	4.1
1	A	117	THR	4.1
1	A	212	MET	4.1
1	A	372	THR	3.8
1	D	214	PRO	3.8
1	B	360	SER	3.7
1	D	212[A]	MET	3.6
1	A	214	PRO	3.6
1	A	217	ALA	3.6
1	B	294	PHE	3.6
1	D	429	GLY	3.5
1	D	117	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	158	TYR	3.4
1	D	371	ASN	3.4
1	A	211	GLN	3.4
1	C	425	ASN	3.3
1	B	199	LEU	3.3
1	A	346	PHE	3.3
1	C	428	GLY	3.3
1	A	685[A]	HIS	3.3
1	A	151	SER	3.3
1	B	159	TRP	3.2
1	B	117	THR	3.2
1	D	428	GLY	3.2
1	B	212	MET	3.1
1	C	430	ARG	3.1
1	A	132	MET	3.1
1	B	359	HIS	3.1
1	B	219	LEU	3.1
1	D	345	ASP	3.0
1	D	427	PHE	3.0
1	A	228	VAL	3.0
1	B	412	TYR	3.0
1	A	199	LEU	2.9
1	A	499	TYR	2.9
1	A	129	ALA	2.9
1	A	201	LEU	2.9
1	D	258	ASP	2.9
1	A	373	LEU	2.9
1	C	346	PHE	2.9
1	B	213	ARG	2.8
1	B	132	MET	2.8
1	B	372	THR	2.8
1	B	694	GLY	2.8
1	C	429	GLY	2.8
1	A	178	PHE	2.8
1	A	472	MET	2.8
1	A	475	LEU	2.7
1	B	427	PHE	2.7
1	A	433	LEU	2.7
1	B	157	ASN	2.7
1	D	346	PHE	2.7
1	A	412	TYR	2.7
1	A	155	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	405	ASP	2.6
1	A	294	PHE	2.6
1	B	346	PHE	2.6
1	C	595	TRP	2.6
1	B	685[A]	HIS	2.6
1	B	261	PHE	2.6
1	A	428	GLY	2.5
1	A	347	ALA	2.5
1	B	425	ASN	2.5
1	A	145	PRO	2.5
1	D	414	ASP	2.5
1	B	181	GLY	2.5
1	A	456	MET	2.5
1	D	472	MET	2.5
1	A	135	VAL	2.4
1	A	464	PRO	2.4
1	D	360	SER	2.4
1	B	220	ILE	2.4
1	B	371	ASN	2.4
1	C	118	HIS	2.3
1	C	413	ARG	2.3
1	B	144	ALA	2.3
1	B	373	LEU	2.3
1	A	542	ASP	2.3
1	C	728	GLU	2.3
1	A	158	TYR	2.3
1	D	425	ASN	2.3
1	C	427	PHE	2.3
1	D	215	GLU	2.3
1	B	142	VAL	2.3
1	B	198	ASN	2.2
1	B	217	ALA	2.2
1	D	415	TYR	2.3
1	C	216	THR	2.2
1	C	433	LEU	2.2
1	C	212	MET	2.2
1	D	471	ASP	2.2
1	A	544	TRP	2.2
1	C	132	MET	2.2
1	B	728	GLU	2.2
1	C	359	HIS	2.1
1	A	216	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	413	ARG	2.1
1	A	165	PRO	2.1
1	D	259	ASN	2.1
1	B	323	ASP	2.1
1	B	221	CYS	2.1
1	B	434	GLU	2.1
1	B	361	ASP	2.1
1	A	342	PRO	2.1
1	B	293	PRO	2.1
1	A	381	GLU	2.0
1	A	227	VAL	2.0
1	A	337	VAL	2.0
1	A	210	ALA	2.0
1	A	180	PRO	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](#)

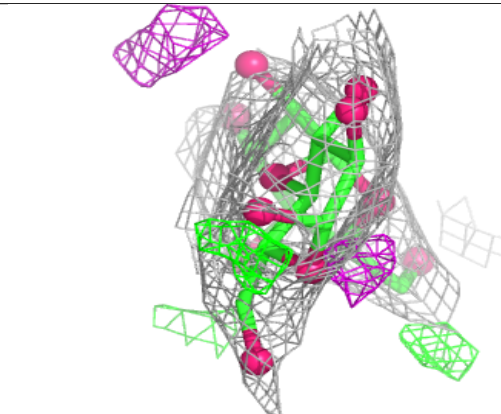
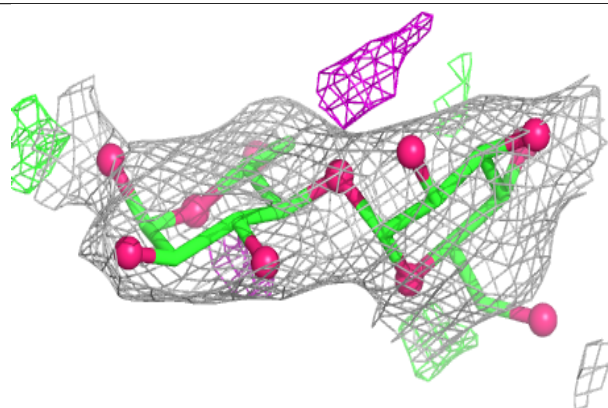
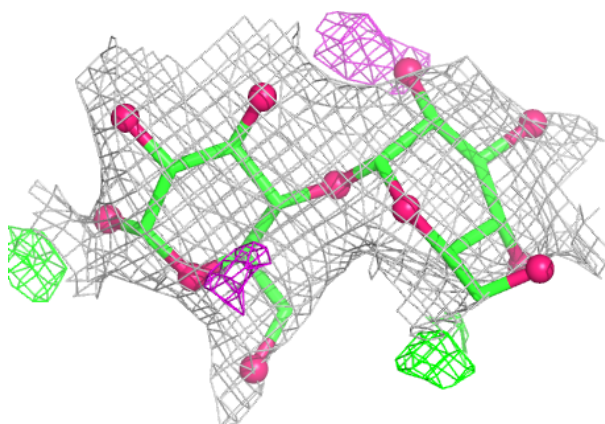
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	1	12/12	0.74	0.16	114,114,115,115	0
2	GLC	H	2	11/12	0.76	0.17	96,97,98,98	0
2	GLC	E	2	11/12	0.79	0.15	115,115,115,115	0
2	GLC	G	2	11/12	0.87	0.12	85,87,88,88	0
2	GLC	F	2	11/12	0.87	0.13	93,93,94,94	0
2	GLC	G	1	12/12	0.88	0.12	88,89,90,90	0
2	GLC	H	1	12/12	0.90	0.12	97,98,98,98	0
2	GLC	I	2	11/12	0.90	0.12	72,75,76,77	0
2	GLC	I	1	12/12	0.91	0.11	73,74,75,75	0
2	GLC	F	1	12/12	0.91	0.10	93,93,94,94	0

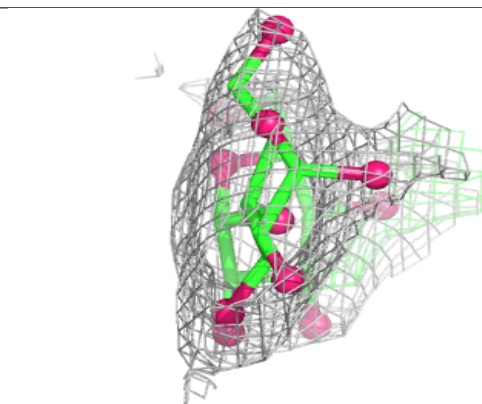
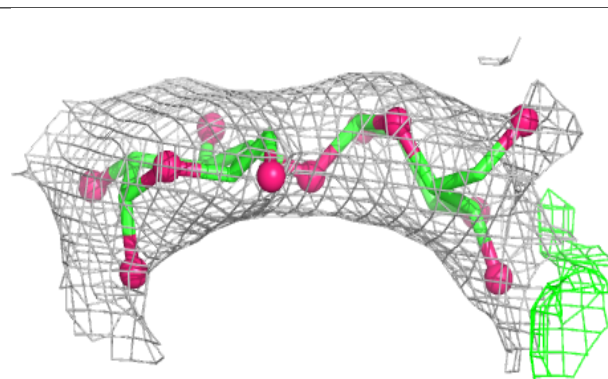
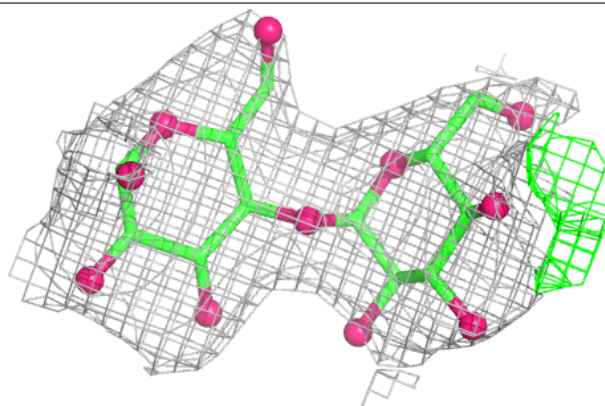
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

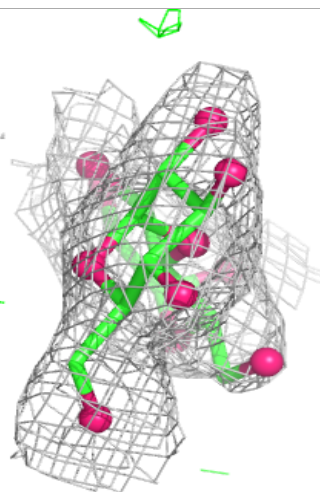
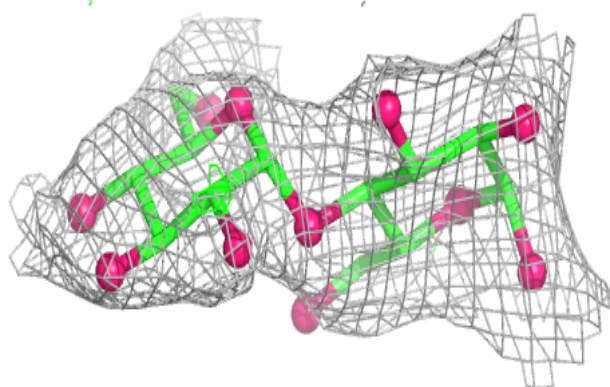
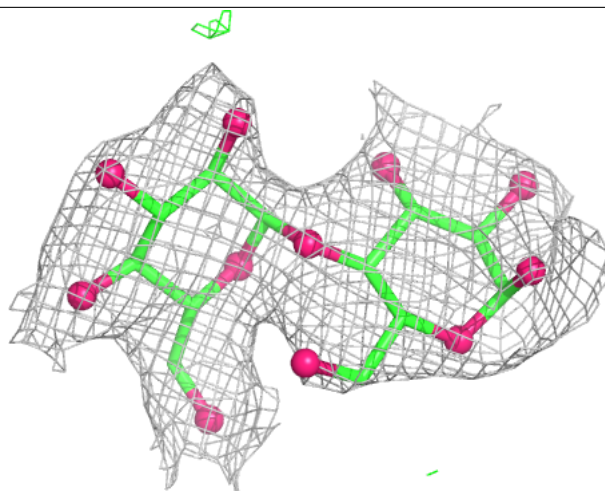
**Electron density around Chain F:**

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



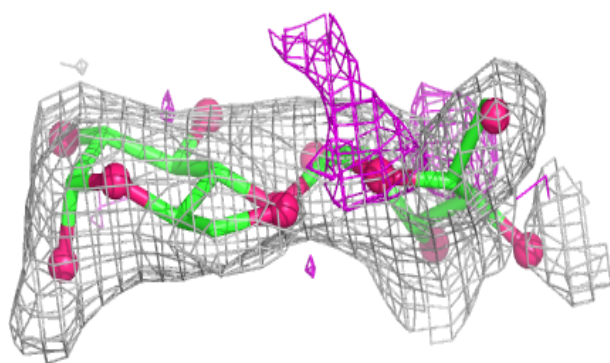
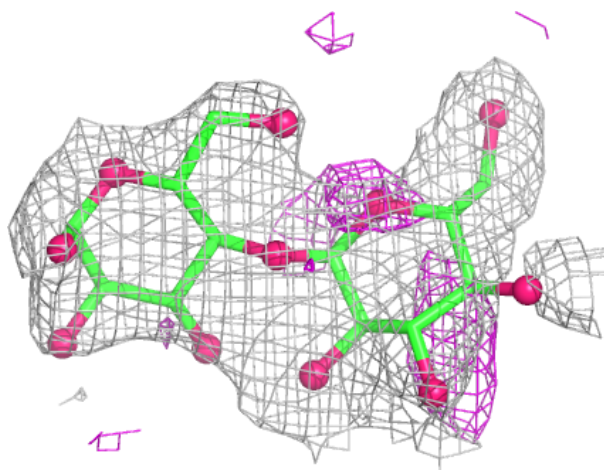
Electron density around Chain G:

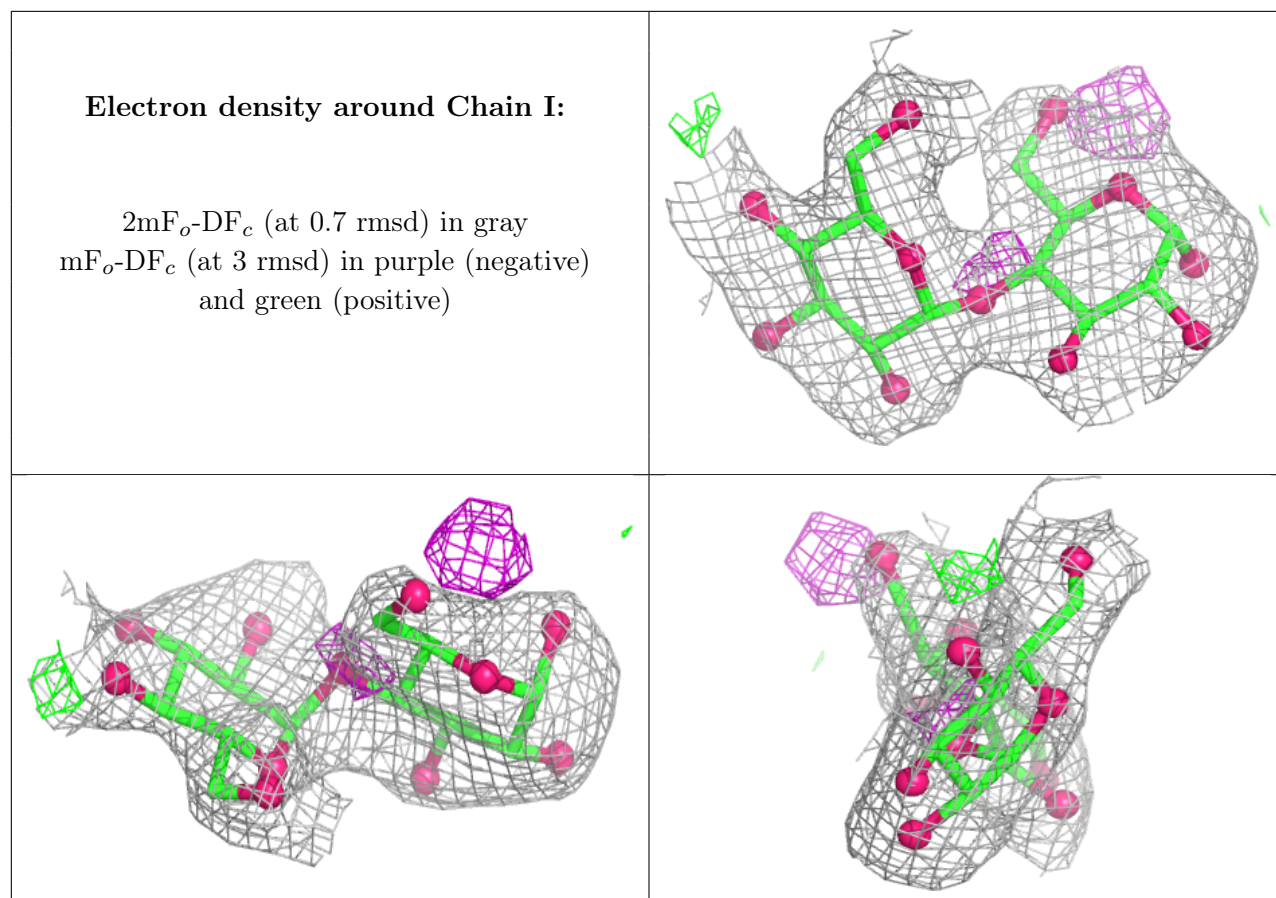
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	BGC	A	801	12/12	0.80	0.17	99,99,99,100	0
4	GOL	C	805	6/6	0.82	0.18	70,71,71,71	0
4	GOL	D	805	6/6	0.92	0.15	56,60,61,62	0
4	GOL	D	806	6/6	0.94	0.11	60,61,62,63	0
4	GOL	B	803	6/6	0.95	0.12	66,68,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.