Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 02:33 PM EDT

PDB ID	:	2EXJ
Title	:	Structure of the family43 beta-Xylosidase D128G mutant from geobacillus stearothermophilus in complex with xylobiose
Authors	:	Brux, C.; Niefind, K.; Shallom-Shezifi, D.; Shoham, Y.; Schomburg, D.
Deposited on	:	2005-11-08
Resolution	:	2.20 Å(reported)

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

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

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

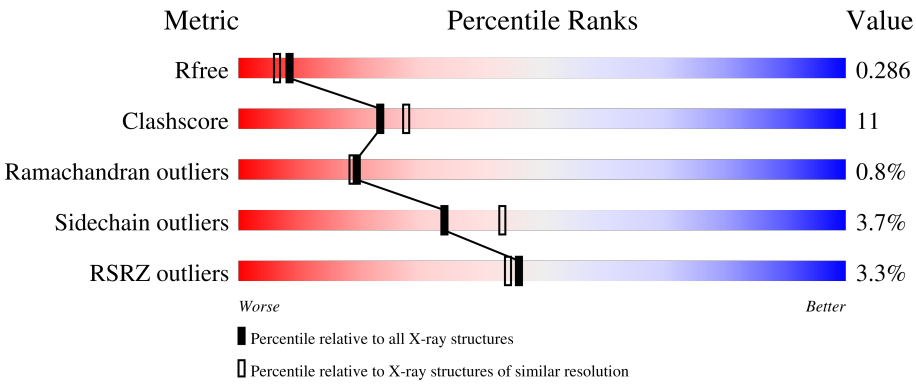
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	535	81% 16%
1	B	535	83% 15%
1	C	535	10% 63% 34%
1	D	535	78% 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%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XYS	E	1	X	-	-	-
2	XYS	E	2	X	-	-	-
2	XYS	F	1	X	-	-	-
2	XYS	F	2	X	-	-	-
2	XYS	G	1	X	-	-	X
2	XYS	G	2	X	-	-	-
2	XYS	H	1	X	-	-	-
2	XYS	H	2	X	-	-	-
4	MES	D	2015	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19279 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 beta-D-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	533	4372	2812	748	802	10	0	0	0
1	B	533	4372	2812	748	802	10	0	0	0
1	C	533	4372	2812	748	802	10	0	0	0
1	D	533	4372	2812	748	802	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP Q68HB3
A	128	GLY	ASP	engineered mutation	UNP Q68HB3
B	2	ALA	SER	engineered mutation	UNP Q68HB3
B	128	GLY	ASP	engineered mutation	UNP Q68HB3
C	2	ALA	SER	engineered mutation	UNP Q68HB3
C	128	GLY	ASP	engineered mutation	UNP Q68HB3
D	2	ALA	SER	engineered mutation	UNP Q68HB3
D	128	GLY	ASP	engineered mutation	UNP Q68HB3

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	2	19	10	9	0	0	0
2	F	2	19	10	9	0	0	0

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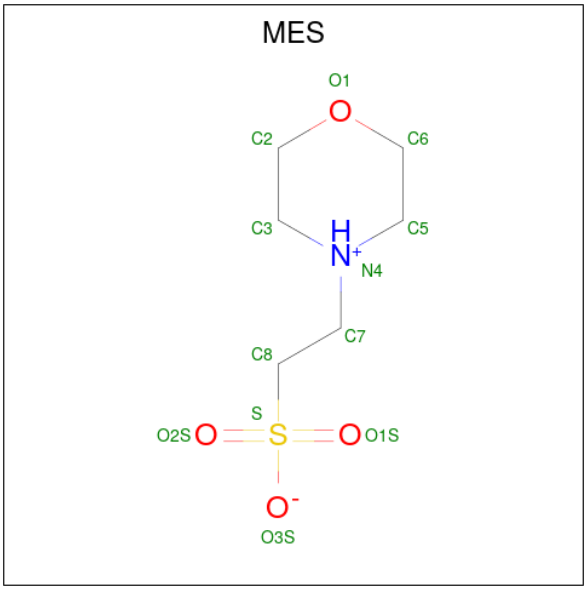
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	G	2	19	10	9	0	0	0
			Total	C	O			
2	H	2	19	10	9	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

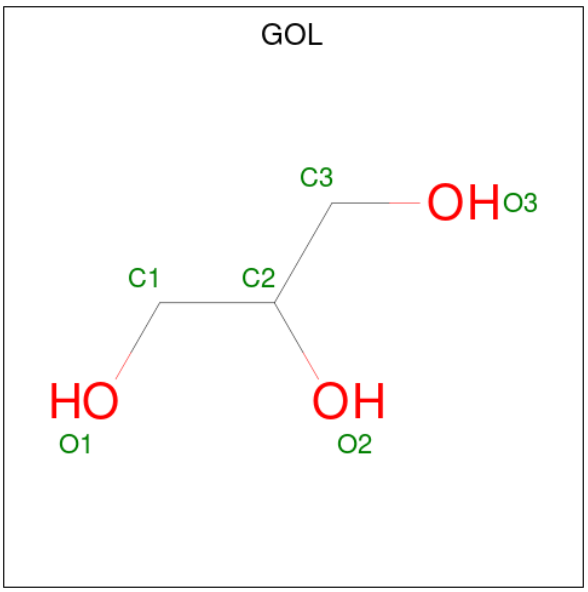
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	1	1	1	0	0
			Total	Ca		
3	C	1	1	1	0	0
			Total	Ca		
3	D	1	1	1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	D	1	12	6	1	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

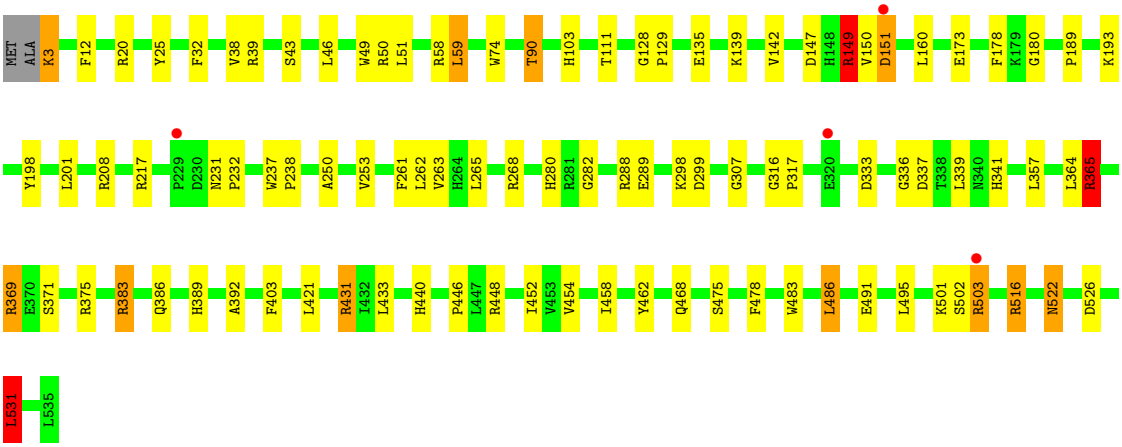
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	451	451	451	0	0
6	B	469	469	469	0	0
6	C	316	316	316	0	0
6	D	415	415	415	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

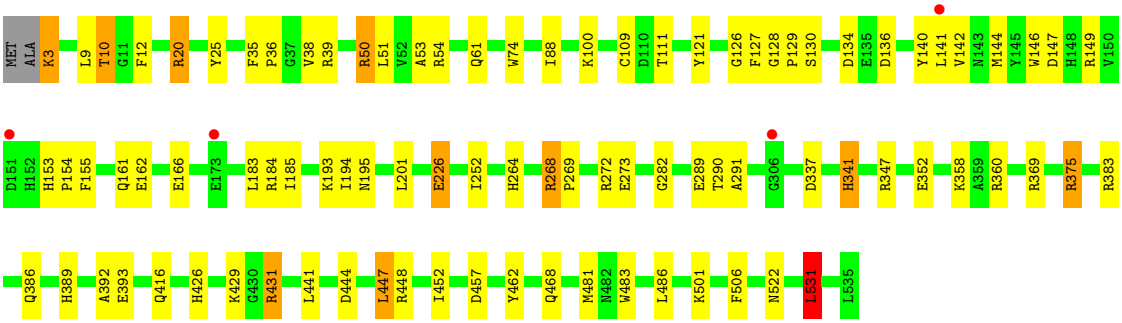
• Molecule 1: beta-D-xylosidase

Chain A:



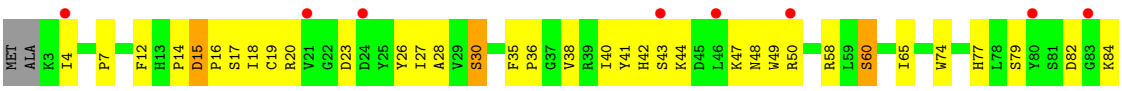
• Molecule 1: beta-D-xylosidase

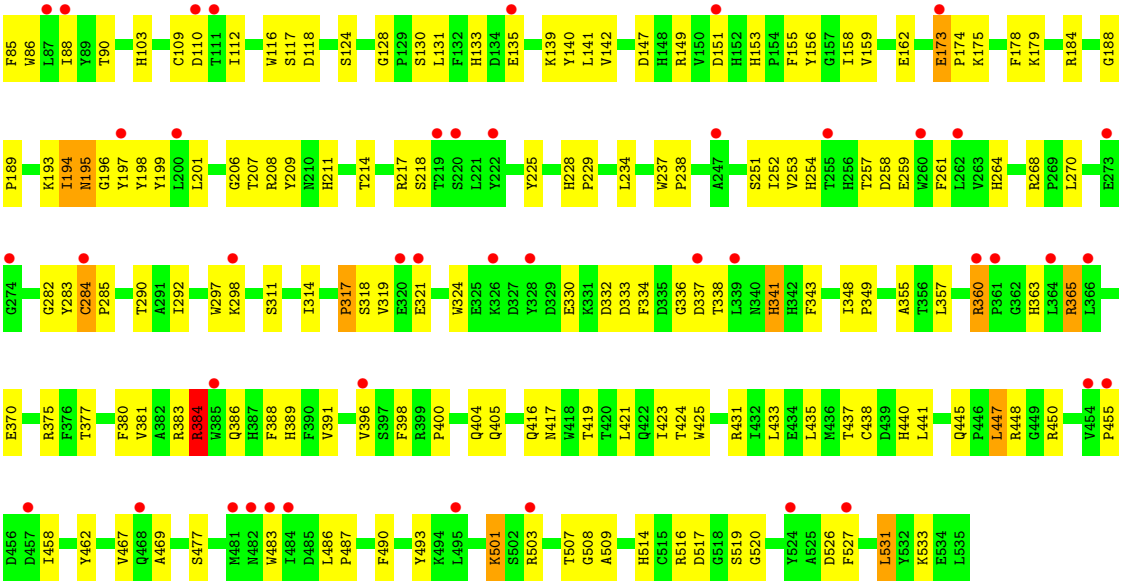
Chain B:



• Molecule 1: beta-D-xylosidase

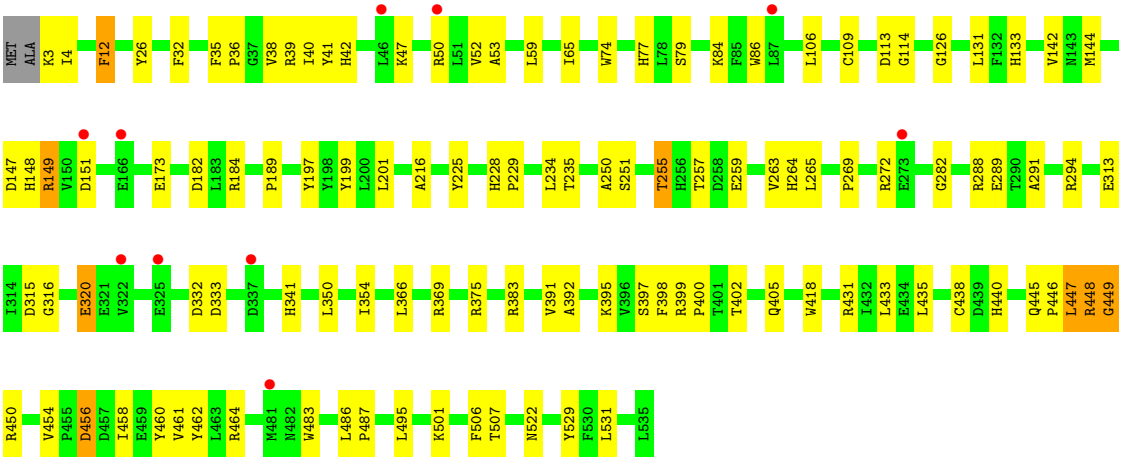
Chain C:





- Molecule 1: beta-D-xylosidase

Chain D:



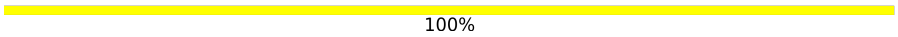
- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-xylopyranose

Chain E:

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

Chain F:

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

Chain G: 

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.38Å 140.38Å 232.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.20) 99.8 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.282 0.214 , 0.286	Depositor DCC
R_{free} test set	5923 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19279	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XYS, GOL, MES, CA

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	0.69	0/4516	0.80	10/6154 (0.2%)
1	B	0.72	0/4516	0.76	3/6154 (0.0%)
1	C	0.62	1/4516 (0.0%)	0.70	1/6154 (0.0%)
1	D	0.68	0/4516	0.73	3/6154 (0.0%)
All	All	0.68	1/18064 (0.0%)	0.75	17/24616 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	CYS	CB-SG	-7.56	1.69	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	531	LEU	CA-CB-CG	9.18	136.41	115.30
1	A	365	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	268	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	369	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	531	LEU	CA-CB-CG	7.11	131.65	115.30
1	A	58	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	383	ARG	NE-CZ-NH2	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	39	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	149	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	268	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	383	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	149	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	449	GLY	N-CA-C	-5.21	100.07	113.10
1	A	486	LEU	CA-CB-CG	-5.08	103.63	115.30
1	C	531	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	384	ARG	Peptide

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	4372	0	4162	75	0
1	B	4372	0	4162	75	0
1	C	4372	0	4162	160	0
1	D	4372	0	4162	78	0
2	E	19	0	17	2	0
2	F	19	0	17	2	0
2	G	19	0	17	0	0
2	H	19	0	17	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	5	0
4	D	12	0	12	6	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	451	0	0	20	0
6	B	469	0	0	29	0
6	C	316	0	0	34	0
6	D	415	0	0	17	0
All	All	19279	0	16784	387	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 11.

All (387) 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:251:SER:HA	6:C:2142:HOH:O	1.20	1.31
4:D:2015:MES:S	4:D:2015:MES:O3S	1.92	1.26
1:B:3:LYS:HB3	6:B:2325:HOH:O	1.08	1.25
1:A:369:ARG:HH22	1:A:522:ASN:ND2	1.34	1.24
1:B:144:MET:SD	6:B:2468:HOH:O	1.92	1.23
1:C:419:THR:HG22	1:C:437:THR:HG22	1.34	1.04
1:A:3:LYS:HB3	6:A:2330:HOH:O	1.61	1.00
1:A:369:ARG:NH2	1:A:522:ASN:ND2	2.11	0.96
1:C:324:TRP:HA	6:C:2200:HOH:O	1.65	0.96
1:A:336:GLY:HA3	6:A:2242:HOH:O	1.65	0.95
1:D:53:ALA:HA	4:D:2015:MES:H82	1.50	0.94
1:B:134:ASP:OD1	6:B:2358:HOH:O	1.88	0.91
1:C:284:CYS:SG	6:C:2143:HOH:O	2.14	0.90
1:C:297:TRP:HB3	6:C:2092:HOH:O	1.71	0.90
1:A:369:ARG:NH2	1:A:522:ASN:HD22	1.70	0.90
1:A:369:ARG:HH22	1:A:522:ASN:HD21	1.17	0.87
1:B:431:ARG:NH1	6:B:2435:HOH:O	2.08	0.86
1:C:517:ASP:OD1	1:C:519:SER:OG	1.93	0.86
1:C:270:LEU:HD22	6:C:2121:HOH:O	1.73	0.85
1:A:369:ARG:HH22	1:A:522:ASN:HD22	1.21	0.85
1:C:455:PRO:HA	6:C:2285:HOH:O	1.77	0.84
1:D:431:ARG:NH1	6:D:2348:HOH:O	2.10	0.83
4:D:2015:MES:O3S	4:D:2015:MES:O2S	1.95	0.83
1:B:389:HIS:HB3	6:B:2278:HOH:O	1.77	0.82
1:C:7:PRO:HG3	1:C:268:ARG:HH11	1.44	0.82
1:A:389:HIS:HB3	6:A:2174:HOH:O	1.80	0.81
1:C:135:GLU:HG2	6:C:2173:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ARG:NH2	1:C:116:TRP:O	2.14	0.81
1:C:147:ASP:OD1	1:C:149:ARG:HD3	1.85	0.77
1:D:288:ARG:HH12	2:H:2:XYS:H52	1.50	0.76
1:B:166:GLU:HB2	6:B:2440:HOH:O	1.84	0.76
1:D:440:HIS:NE2	1:D:501:LYS:HG2	2.00	0.76
1:D:182:ASP:HB3	6:D:2308:HOH:O	1.86	0.75
1:C:7:PRO:CG	1:C:268:ARG:HH11	2.01	0.74
1:A:365:ARG:CG	1:A:526:ASP:OD1	2.36	0.74
1:C:77:HIS:CD2	1:C:131:LEU:H	2.05	0.73
1:A:250:ALA:HB1	1:A:262:LEU:HD11	1.71	0.73
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.69	0.73
1:D:53:ALA:CA	4:D:2015:MES:H82	2.18	0.72
1:C:15:ASP:OD2	1:C:30:SER:OG	2.07	0.72
1:C:365:ARG:HH11	1:C:365:ARG:CG	2.01	0.72
1:D:42:HIS:ND1	6:D:2380:HOH:O	2.22	0.72
1:C:261:PHE:CZ	1:C:317:PRO:HG3	2.25	0.72
1:C:334:PHE:HB3	1:C:357:LEU:CD1	2.20	0.71
1:C:77:HIS:HD2	1:C:131:LEU:H	1.36	0.71
1:B:54:ARG:HE	4:B:2014:MES:H82	1.55	0.70
1:C:17:SER:HB3	1:C:28:ALA:HB3	1.73	0.70
1:D:53:ALA:HA	4:D:2015:MES:C8	2.20	0.70
1:D:255:THR:HG23	1:D:257:THR:H	1.56	0.70
1:C:184:ARG:HD3	6:C:2112:HOH:O	1.90	0.70
1:C:254:HIS:HE1	1:C:258:ASP:HA	1.57	0.69
1:D:501:LYS:HE3	6:D:2273:HOH:O	1.90	0.69
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.27	0.69
1:B:50:ARG:HH11	1:B:50:ARG:HB3	1.56	0.69
1:B:53:ALA:HA	4:B:2014:MES:H51	1.73	0.69
1:C:509:ALA:O	6:C:2106:HOH:O	2.11	0.68
1:D:255:THR:HG22	1:D:259:GLU:H	1.57	0.68
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.75	0.68
1:A:365:ARG:HG3	1:A:526:ASP:OD1	1.92	0.68
1:C:334:PHE:CD2	1:C:527:PHE:O	2.47	0.68
1:A:440:HIS:NE2	1:A:501:LYS:HG2	2.09	0.67
1:C:30:SER:HB3	1:C:74:TRP:O	1.93	0.67
1:C:35:PHE:CE1	1:C:349:PRO:HG3	2.29	0.67
1:A:208:ARG:NH2	1:A:503:ARG:HG3	2.08	0.67
1:A:173:GLU:O	6:A:2459:HOH:O	2.13	0.66
1:B:146:TRP:HB2	6:B:2468:HOH:O	1.93	0.66
1:C:334:PHE:HB3	1:C:357:LEU:HD11	1.76	0.66
1:C:462:TYR:HB2	1:C:477:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:ARG:NH2	1:D:458:ILE:O	2.28	0.66
1:B:369:ARG:NH2	1:B:522:ASN:OD1	2.28	0.66
1:C:384:ARG:HH11	1:C:384:ARG:CG	2.08	0.66
1:A:458:ILE:HD12	1:A:478:PHE:HB3	1.76	0.66
1:B:10:THR:CG2	1:B:386:GLN:HB3	2.25	0.66
1:C:109:CYS:HB3	6:C:2045:HOH:O	1.94	0.66
1:C:507:THR:O	6:C:2147:HOH:O	2.14	0.66
1:A:111:THR:HG22	6:A:2328:HOH:O	1.96	0.65
1:B:426:HIS:ND1	1:B:429:LYS:HG3	2.11	0.65
1:C:355:ALA:O	6:C:2189:HOH:O	2.14	0.65
1:D:272:ARG:HD2	6:D:2374:HOH:O	1.96	0.64
1:A:365:ARG:HG2	1:A:526:ASP:OD1	1.97	0.64
1:C:384:ARG:HH11	1:C:384:ARG:HG3	1.63	0.64
1:C:334:PHE:HD2	1:C:527:PHE:O	1.81	0.64
1:D:375:ARG:NH2	6:D:2130:HOH:O	2.31	0.64
1:C:12:PHE:CD1	1:C:14:PRO:HD3	2.32	0.63
1:C:23:ASP:O	1:C:44:LYS:HD3	1.97	0.63
1:C:270:LEU:HG	1:C:283:TYR:O	1.99	0.63
1:C:341:HIS:HD2	6:C:2162:HOH:O	1.82	0.63
1:D:320:GLU:HG3	6:D:2298:HOH:O	1.97	0.63
1:C:110:ASP:C	6:C:2211:HOH:O	2.36	0.63
1:A:3:LYS:N	6:A:2309:HOH:O	2.32	0.62
1:C:43:SER:HB2	1:C:49:TRP:CE3	2.34	0.62
1:D:288:ARG:HH12	2:H:2:XYS:C5	2.12	0.62
1:C:319:VAL:HG22	6:C:2202:HOH:O	2.00	0.62
1:B:147:ASP:OD1	1:B:149:ARG:HD3	2.00	0.62
1:C:503:ARG:HB3	6:C:2253:HOH:O	1.99	0.62
1:B:448:ARG:HD3	6:B:2485:HOH:O	1.99	0.61
1:C:158:ILE:HD12	1:C:189:PRO:HB3	1.83	0.61
1:D:288:ARG:NH1	2:H:2:XYS:H52	2.14	0.61
1:A:316:GLY:N	6:A:2330:HOH:O	2.29	0.61
1:C:7:PRO:CG	1:C:268:ARG:NH1	2.63	0.61
1:C:20:ARG:HD3	1:C:254:HIS:O	2.01	0.60
1:B:50:ARG:HD2	6:B:2359:HOH:O	2.00	0.60
1:A:20:ARG:HG3	1:A:25:TYR:CE1	2.36	0.60
1:C:462:TYR:HB3	1:C:483:TRP:CH2	2.36	0.60
1:C:16:PRO:HG3	1:C:290:THR:HG23	1.83	0.60
1:A:522:ASN:HA	6:A:2388:HOH:O	2.01	0.59
1:C:435:LEU:HD12	1:C:447:LEU:HD22	1.83	0.59
1:D:147:ASP:OD1	1:D:149:ARG:HD2	2.02	0.59
1:C:398:PHE:CD2	1:C:400:PRO:HD3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:HG2	1:C:526:ASP:OD1	2.03	0.59
1:D:397:SER:HA	6:D:2402:HOH:O	2.01	0.59
1:A:250:ALA:HB1	1:A:262:LEU:CD1	2.32	0.59
1:A:403:PHE:O	1:D:148:HIS:HE1	1.86	0.59
1:C:26:TYR:HA	1:C:41:TYR:O	2.03	0.59
1:C:156:TYR:O	1:C:179:LYS:NZ	2.31	0.58
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.18	0.58
1:C:85:PHE:HD2	6:C:2045:HOH:O	1.85	0.58
1:C:389:HIS:HA	1:C:467:VAL:O	2.03	0.58
1:C:380:PHE:HB2	1:C:514:HIS:CD2	2.38	0.58
1:D:332:ASP:O	1:D:529:TYR:HB2	2.03	0.58
1:C:330:GLU:HG3	6:C:2100:HOH:O	2.03	0.58
1:C:197:TYR:HB2	1:C:199:TYR:HE1	1.69	0.58
1:D:50:ARG:NE	6:D:2380:HOH:O	2.35	0.58
1:D:447:LEU:HD21	1:D:486:LEU:HD22	1.86	0.57
1:A:502:SER:O	1:A:503:ARG:HB2	2.03	0.57
1:C:228:HIS:ND1	1:C:229:PRO:HD2	2.19	0.57
1:D:391:VAL:HG21	1:D:464:ARG:HD2	1.87	0.57
1:C:365:ARG:HH11	1:C:365:ARG:HG2	1.69	0.57
1:A:151:ASP:OD1	1:A:151:ASP:N	2.36	0.56
1:B:272:ARG:HD2	6:B:2102:HOH:O	2.05	0.56
1:A:208:ARG:CZ	6:A:2447:HOH:O	2.53	0.56
1:C:193:LYS:C	1:C:194:ILE:HG12	2.24	0.56
1:C:197:TYR:HB2	1:C:199:TYR:CE1	2.40	0.56
1:C:398:PHE:CE2	1:C:400:PRO:HB3	2.40	0.56
1:C:424:THR:HG23	1:C:425:TRP:N	2.19	0.56
1:B:201:LEU:HD22	1:B:252:ILE:HG13	1.88	0.56
1:C:365:ARG:CG	1:C:365:ARG:NH1	2.63	0.56
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.53	0.56
1:C:174:PRO:O	1:C:175:LYS:HG3	2.05	0.56
1:D:77:HIS:CD2	1:D:131:LEU:H	2.23	0.56
1:D:391:VAL:CG2	1:D:464:ARG:HD2	2.36	0.56
1:B:128:GLY:N	1:B:129:PRO:CD	2.68	0.56
1:B:88:ILE:HG21	1:B:129:PRO:HB2	1.87	0.55
1:A:50:ARG:HG3	6:A:2177:HOH:O	2.05	0.55
1:C:336:GLY:HA3	6:C:2309:HOH:O	2.06	0.55
1:B:10:THR:HG23	1:B:386:GLN:O	2.07	0.55
1:C:421:LEU:HD13	1:C:486:LEU:HD13	1.88	0.55
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.89	0.55
1:A:316:GLY:HA3	6:A:2330:HOH:O	2.06	0.55
1:C:153:HIS:NE2	1:C:184:ARG:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:THR:HG23	1:D:405:GLN:HG3	1.89	0.55
1:A:365:ARG:HG3	1:A:365:ARG:HH11	1.72	0.54
1:C:261:PHE:HB3	1:C:292:ILE:HD11	1.89	0.54
1:C:404:GLN:NE2	1:C:519:SER:HA	2.22	0.54
1:C:252:ILE:HG22	6:C:2150:HOH:O	2.07	0.54
1:C:440:HIS:NE2	1:C:501:LYS:HD3	2.23	0.54
1:C:337:ASP:HA	6:C:2216:HOH:O	2.08	0.54
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.08	0.54
1:C:60:SER:HB2	1:C:118:ASP:OD1	2.08	0.54
1:A:250:ALA:CB	1:A:262:LEU:HD11	2.37	0.53
1:A:431:ARG:HD2	6:A:2075:HOH:O	2.08	0.53
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.89	0.53
1:D:126:GLY:HA3	1:D:144:MET:O	2.08	0.53
1:B:50:ARG:HG3	6:B:2142:HOH:O	2.07	0.53
1:C:330:GLU:O	1:C:531:LEU:HA	2.09	0.53
1:D:398:PHE:CD2	1:D:400:PRO:HD3	2.43	0.53
1:D:3:LYS:HG3	6:D:2214:HOH:O	2.09	0.53
1:B:20:ARG:HG3	1:B:25:TYR:CE1	2.43	0.53
1:C:261:PHE:CE2	1:C:317:PRO:HG3	2.44	0.53
1:D:440:HIS:CD2	1:D:501:LYS:HG2	2.43	0.53
1:C:58:ARG:NH1	1:C:118:ASP:OD1	2.42	0.53
1:C:365:ARG:NH1	1:C:365:ARG:HG3	2.23	0.53
1:B:126:GLY:HA2	6:B:2468:HOH:O	2.09	0.53
1:C:18:ILE:HG12	1:C:253:VAL:HB	1.90	0.52
1:C:380:PHE:HB2	1:C:514:HIS:HD2	1.74	0.52
1:B:39:ARG:NH2	6:B:2167:HOH:O	2.24	0.52
6:B:2242:HOH:O	1:C:375:ARG:CZ	2.57	0.52
1:D:431:ARG:HH12	1:D:456:ASP:HA	1.74	0.52
1:B:184:ARG:HD2	6:B:2143:HOH:O	2.09	0.52
1:B:74:TRP:CE3	2:F:2:XYS:H2	2.45	0.52
1:B:126:GLY:HA3	1:B:144:MET:O	2.10	0.52
1:B:3:LYS:HD3	6:B:2325:HOH:O	2.10	0.51
1:C:58:ARG:HH12	1:C:118:ASP:CG	2.13	0.51
1:A:43:SER:HB2	1:A:49:TRP:CE3	2.45	0.51
1:A:231:ASN:CG	1:A:232:PRO:HA	2.31	0.51
1:B:54:ARG:HE	4:B:2014:MES:C8	2.24	0.51
1:C:360:ARG:HG2	1:C:363:HIS:CG	2.45	0.51
1:C:419:THR:CG2	1:C:437:THR:HG22	2.24	0.51
1:C:254:HIS:CE1	1:C:258:ASP:HA	2.42	0.51
1:C:365:ARG:NH2	6:C:2167:HOH:O	2.43	0.51
1:C:370:GLU:HB2	1:C:377:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLY:C	1:C:208:ARG:H	2.14	0.51
1:D:294:ARG:NH1	1:D:315:ASP:O	2.36	0.51
1:A:288:ARG:NH2	2:E:2:XYS:O4	2.41	0.50
1:A:316:GLY:CA	6:A:2330:HOH:O	2.59	0.50
1:B:273:GLU:O	6:B:2345:HOH:O	2.20	0.50
1:C:17:SER:O	1:C:27:ILE:HA	2.11	0.50
1:C:338:THR:C	6:C:2064:HOH:O	2.49	0.50
1:A:150:VAL:HG23	1:D:445:GLN:OE1	2.11	0.50
1:A:339:LEU:HD21	1:A:364:LEU:HD13	1.92	0.50
1:A:39:ARG:NH2	1:A:51:LEU:HD22	2.27	0.50
1:A:383:ARG:HD2	6:A:2120:HOH:O	2.11	0.50
4:D:2015:MES:O3S	4:D:2015:MES:C8	2.59	0.50
1:A:189:PRO:HA	1:A:201:LEU:O	2.12	0.49
1:B:468:GLN:CD	6:B:2278:HOH:O	2.49	0.49
1:A:371:SER:HA	1:A:516:ARG:HD3	1.94	0.49
1:B:416:GLN:HG2	1:B:441:LEU:HD13	1.94	0.49
1:A:74:TRP:O	6:A:2028:HOH:O	2.18	0.49
1:B:10:THR:HG22	1:B:386:GLN:HB3	1.92	0.49
1:B:39:ARG:NE	6:B:2167:HOH:O	2.34	0.49
1:B:51:LEU:HD23	1:B:341:HIS:ND1	2.27	0.49
1:C:435:LEU:HD12	1:C:447:LEU:CD2	2.43	0.49
1:B:264:HIS:CE1	1:B:291:ALA:HB3	2.48	0.49
1:B:347:ARG:HD3	1:B:375:ARG:O	2.13	0.49
1:C:334:PHE:N	6:C:2170:HOH:O	2.46	0.49
1:D:369:ARG:NH1	6:D:2223:HOH:O	2.46	0.49
1:C:285:PRO:HD2	6:C:2033:HOH:O	2.13	0.48
1:C:234:LEU:HD21	1:C:264:HIS:CD2	2.48	0.48
1:D:313:GLU:HB2	6:D:2141:HOH:O	2.12	0.48
1:B:121:TYR:OH	1:C:520:GLY:HA3	2.14	0.48
1:A:502:SER:O	1:A:503:ARG:NH1	2.47	0.48
1:B:9:LEU:HB2	1:B:290:THR:HB	1.95	0.48
1:D:26:TYR:HA	1:D:41:TYR:O	2.13	0.48
1:A:193:LYS:HD3	1:A:198:TYR:CE1	2.49	0.48
1:C:455:PRO:HB2	1:C:458:ILE:HG12	1.95	0.48
1:C:357:LEU:HD23	6:C:2064:HOH:O	2.13	0.48
1:A:90:THR:HA	1:A:103:HIS:O	2.14	0.47
1:D:433:LEU:HD21	1:D:461:VAL:HG11	1.96	0.47
1:A:421:LEU:HD13	1:A:486:LEU:HD13	1.96	0.47
1:C:405:GLN:HA	1:C:516:ARG:O	2.15	0.47
1:B:136:ASP:HB3	6:B:2227:HOH:O	2.13	0.47
1:B:452:ILE:N	1:B:452:ILE:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HG3	1:A:365:ARG:NH1	2.29	0.47
1:B:183:LEU:HD11	6:D:2364:HOH:O	2.14	0.47
1:C:209:TYR:OH	1:C:282:GLY:O	2.33	0.47
1:D:216:ALA:HB1	1:D:225:TYR:HB3	1.96	0.47
1:C:386:GLN:NE2	6:C:2295:HOH:O	2.46	0.47
1:B:184:ARG:CD	6:B:2143:HOH:O	2.61	0.47
1:B:226:GLU:HB2	6:B:2403:HOH:O	2.15	0.47
1:C:445:GLN:O	1:C:448:ARG:HG3	2.14	0.47
1:C:283:TYR:CB	1:C:493:TYR:HB2	2.45	0.47
1:A:299:ASP:CG	6:A:2147:HOH:O	2.53	0.47
1:A:198:TYR:O	1:A:217:ARG:HA	2.15	0.46
1:A:446:PRO:HA	1:A:448:ARG:HH21	1.79	0.46
1:B:88:ILE:CG2	1:B:129:PRO:HB2	2.45	0.46
1:C:343:PHE:HB3	1:C:381:VAL:HG12	1.96	0.46
1:C:416:GLN:NE2	1:C:441:LEU:HD13	2.30	0.46
1:B:54:ARG:HH21	4:B:2014:MES:H82	1.81	0.46
1:B:109:CYS:SG	1:B:111:THR:O	2.73	0.46
1:D:228:HIS:ND1	1:D:229:PRO:HD2	2.31	0.46
1:B:444:ASP:OD1	6:B:2402:HOH:O	2.20	0.46
1:C:139:LYS:O	1:C:162:GLU:HG3	2.16	0.46
1:B:141:LEU:N	1:B:161:GLN:O	2.46	0.46
1:B:393:GLU:HB3	1:B:531:LEU:HG	1.97	0.46
1:D:447:LEU:CD2	1:D:486:LEU:HD22	2.46	0.46
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.51	0.45
1:B:375:ARG:NH2	6:B:2242:HOH:O	2.49	0.45
1:C:40:ILE:HG21	1:C:112:ILE:HD11	1.98	0.45
1:D:52:VAL:O	1:D:113:ASP:HB3	2.16	0.45
1:A:383:ARG:NH2	1:A:386:GLN:OE1	2.50	0.45
1:D:447:LEU:HD21	1:D:486:LEU:CD2	2.45	0.45
1:D:462:TYR:HB3	1:D:483:TRP:CH2	2.51	0.45
1:B:35:PHE:CG	1:B:36:PRO:HA	2.51	0.45
1:C:4:ILE:HB	1:C:314:ILE:HG13	1.98	0.45
1:C:208:ARG:O	1:C:211:HIS:HB2	2.17	0.45
1:C:43:SER:OG	1:C:48:ASN:O	2.08	0.45
1:D:506:PHE:CD1	2:H:2:XYS:H51	2.52	0.45
1:C:42:HIS:O	1:C:49:TRP:HA	2.17	0.45
1:D:418:TRP:CZ2	1:D:438:CYS:HB2	2.52	0.45
1:B:54:ARG:NE	4:B:2014:MES:H82	2.29	0.45
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.64	0.45
1:B:447:LEU:HD21	1:B:486:LEU:HD22	1.99	0.45
1:A:280:HIS:CD2	1:A:282:GLY:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TRP:CD1	1:C:86:TRP:N	2.85	0.45
1:C:234:LEU:CD2	1:C:264:HIS:CD2	3.00	0.45
1:D:109:CYS:SG	1:D:114:GLY:HA3	2.57	0.45
1:D:265:LEU:HA	1:D:289:GLU:O	2.16	0.45
1:C:109:CYS:HB2	1:C:116:TRP:CD2	2.52	0.44
1:C:142:VAL:HA	1:C:159:VAL:O	2.17	0.44
1:B:462:TYR:HB3	1:B:483:TRP:CH2	2.52	0.44
1:C:128:GLY:O	1:C:189:PRO:HD2	2.17	0.44
1:A:491:GLU:HG2	6:A:2301:HOH:O	2.16	0.44
1:A:142:VAL:CG1	1:A:160:LEU:HD12	2.48	0.44
1:C:201:LEU:HD12	1:C:214:THR:O	2.18	0.44
1:C:388:PHE:O	1:C:467:VAL:HG12	2.17	0.44
1:A:375:ARG:HE	1:A:375:ARG:HB2	1.59	0.44
1:C:195:ASN:HB3	1:C:196:GLY:H	1.68	0.44
1:A:392:ALA:HA	1:A:531:LEU:O	2.18	0.44
1:B:3:LYS:CD	6:B:2325:HOH:O	2.65	0.44
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.98	0.44
1:B:352:GLU:OE1	1:B:358:LYS:HD2	2.17	0.44
1:C:103:HIS:ND1	1:C:124:SER:OG	2.39	0.44
1:A:59:LEU:HD22	6:A:2406:HOH:O	2.18	0.44
1:D:250:ALA:HA	1:D:263:VAL:O	2.18	0.44
1:D:431:ARG:HG2	1:D:454:VAL:HB	1.99	0.44
1:B:3:LYS:CB	6:B:2325:HOH:O	1.96	0.44
1:B:153:HIS:HA	1:B:154:PRO:HD3	1.84	0.44
1:D:269:PRO:HB3	1:D:282:GLY:HA3	2.00	0.44
1:A:462:TYR:HB3	1:A:483:TRP:CH2	2.52	0.43
6:B:2401:HOH:O	1:C:173:GLU:HG2	2.17	0.43
1:C:153:HIS:O	6:C:2037:HOH:O	2.21	0.43
1:C:450:ARG:NH1	1:C:487:PRO:HG2	2.32	0.43
1:B:140:TYR:HA	1:B:162:GLU:HA	2.00	0.43
1:D:86:TRP:HE3	1:D:106:LEU:HD11	1.83	0.43
1:D:184:ARG:NH1	6:D:2119:HOH:O	2.51	0.43
1:D:79:SER:CB	1:D:133:HIS:HE2	2.32	0.43
1:C:234:LEU:HD21	1:C:264:HIS:CG	2.54	0.43
1:D:392:ALA:HA	1:D:531:LEU:O	2.19	0.43
1:A:265:LEU:HA	1:A:289:GLU:O	2.18	0.43
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.72	0.43
1:C:360:ARG:HG2	1:C:363:HIS:HB2	2.00	0.43
1:C:435:LEU:HD22	1:C:490:PHE:HZ	1.84	0.43
1:A:43:SER:HB2	1:A:49:TRP:CD2	2.54	0.43
1:C:88:ILE:HG21	1:C:141:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LYS:HE2	6:A:2453:HOH:O	2.18	0.43
1:D:197:TYR:HB2	1:D:199:TYR:CE1	2.54	0.43
1:B:166:GLU:CB	6:B:2440:HOH:O	2.56	0.43
1:C:155:PHE:N	1:C:155:PHE:CD2	2.85	0.43
1:C:341:HIS:CD2	6:C:2162:HOH:O	2.65	0.43
1:D:369:ARG:NH2	1:D:522:ASN:OD1	2.51	0.43
1:C:7:PRO:HG2	1:C:268:ARG:NH1	2.34	0.43
1:A:32:PHE:HZ	2:E:2:XYS:H4	1.83	0.42
1:C:19:CYS:SG	6:C:2073:HOH:O	2.54	0.42
1:C:42:HIS:HB3	1:C:50:ARG:HG3	2.01	0.42
1:A:147:ASP:OD1	1:A:149:ARG:HD2	2.19	0.42
1:C:4:ILE:HG12	1:C:47:LYS:HB2	2.01	0.42
1:C:268:ARG:HH21	1:C:388:PHE:HE2	1.67	0.42
1:C:435:LEU:HD22	1:C:490:PHE:CZ	2.54	0.42
1:B:468:GLN:NE2	6:B:2278:HOH:O	2.52	0.42
1:C:17:SER:O	1:C:28:ALA:N	2.44	0.42
1:C:259:GLU:OE2	1:C:317:PRO:HB3	2.19	0.42
1:C:375:ARG:NH2	6:C:2028:HOH:O	2.51	0.42
1:A:433:LEU:HB2	1:A:452:ILE:HB	2.00	0.42
1:B:506:PHE:CD1	2:F:2:XYS:H52	2.55	0.42
1:D:35:PHE:CG	1:D:36:PRO:HA	2.55	0.42
1:D:435:LEU:HB2	1:D:446:PRO:HG2	2.02	0.42
1:C:79:SER:OG	1:C:133:HIS:NE2	2.43	0.42
1:D:399:ARG:CD	6:D:2258:HOH:O	2.67	0.42
1:D:12:PHE:CE1	1:D:507:THR:HA	2.54	0.42
1:C:391:VAL:HG13	1:C:533:LYS:HB3	2.02	0.42
1:D:3:LYS:HB2	1:D:316:GLY:H	1.85	0.42
1:D:40:ILE:HB	1:D:53:ALA:HB3	2.01	0.42
1:A:421:LEU:HD13	1:A:486:LEU:CD1	2.50	0.42
1:B:121:TYR:OH	1:C:520:GLY:CA	2.68	0.42
1:C:469:ALA:C	6:C:2121:HOH:O	2.58	0.42
1:D:234:LEU:O	1:D:235:THR:HB	2.19	0.41
1:D:264:HIS:CE1	1:D:291:ALA:HB3	2.55	0.41
1:D:447:LEU:HD11	1:D:487:PRO:HD2	2.01	0.41
1:C:324:TRP:HE3	6:C:2200:HOH:O	2.04	0.41
1:A:253:VAL:CG1	1:A:261:PHE:HB2	2.50	0.41
1:B:100:LYS:HG2	1:B:127:PHE:CE2	2.56	0.41
1:B:392:ALA:HA	1:B:531:LEU:O	2.20	0.41
1:C:417:ASN:HA	1:C:438:CYS:O	2.21	0.41
1:D:448:ARG:HA	1:D:449:GLY:HA2	1.84	0.41
1:C:35:PHE:HE1	1:C:349:PRO:HG3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ILE:HD12	1:C:348:ILE:HG21	2.02	0.41
1:A:298:LYS:O	1:A:299:ASP:HB2	2.20	0.41
1:C:90:THR:HA	1:C:103:HIS:O	2.21	0.41
1:C:218:SER:HB2	1:C:225:TYR:HA	2.03	0.41
1:D:251:SER:HB2	6:D:2294:HOH:O	2.20	0.41
1:C:131:LEU:HA	1:C:140:TYR:O	2.21	0.41
1:C:365:ARG:HH11	1:C:365:ARG:HG3	1.77	0.41
1:A:337:ASP:HB2	6:A:2178:HOH:O	2.20	0.41
1:B:130:SER:HB3	1:B:142:VAL:HG23	2.03	0.41
1:D:402:THR:CG2	1:D:405:GLN:HG3	2.50	0.41
1:B:153:HIS:NE2	1:B:184:ARG:HB3	2.36	0.41
1:B:155:PHE:CG	1:B:185:ILE:HA	2.56	0.41
1:C:16:PRO:HB3	1:C:290:THR:CG2	2.51	0.41
1:C:237:TRP:HB3	1:C:238:PRO:HD3	2.01	0.41
1:C:421:LEU:HD13	1:C:486:LEU:CD1	2.49	0.41
1:D:84:LYS:HE2	6:D:2337:HOH:O	2.21	0.41
1:D:189:PRO:HA	1:D:201:LEU:O	2.21	0.41
1:A:250:ALA:HA	1:A:263:VAL:O	2.21	0.41
1:B:193:LYS:C	1:B:194:ILE:HG13	2.41	0.41
1:C:321:GLU:HB2	6:C:2227:HOH:O	2.20	0.41
1:D:350:LEU:HD22	1:D:354:ILE:HG21	2.02	0.41
1:C:396:VAL:HG13	1:C:423:ILE:HD11	2.03	0.40
1:D:32:PHE:CE2	1:D:74:TRP:CD1	3.09	0.40
1:A:128:GLY:N	1:A:129:PRO:CD	2.84	0.40
1:B:61:GLN:O	5:B:2017:GOL:H12	2.21	0.40
1:C:198:TYR:O	1:C:217:ARG:HA	2.22	0.40
1:D:395:LYS:HD2	1:D:462:TYR:CE1	2.56	0.40
1:D:395:LYS:HG3	1:D:460:TYR:HB3	2.03	0.40
1:A:237:TRP:HB3	1:A:238:PRO:HD3	2.04	0.40
1:C:35:PHE:CG	1:C:36:PRO:HA	2.56	0.40
1:C:58:ARG:HH22	1:C:117:SER:C	2.25	0.40
1:C:12:PHE:HB2	1:C:508:GLY:HA3	2.02	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	531/535 (99%)	493 (93%)	35 (7%)	3 (1%)	25	26
1	B	531/535 (99%)	492 (93%)	36 (7%)	3 (1%)	25	26
1	C	531/535 (99%)	479 (90%)	44 (8%)	8 (2%)	10	8
1	D	531/535 (99%)	495 (93%)	32 (6%)	4 (1%)	19	19
All	All	2124/2140 (99%)	1959 (92%)	147 (7%)	18 (1%)	19	19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	VAL
1	A	38	VAL
1	B	12	PHE
1	B	38	VAL
1	C	188	GLY
1	C	318	SER
1	D	38	VAL
1	D	456	ASP
1	A	12	PHE
1	A	307	GLY
1	C	178	PHE
1	D	12	PHE
1	D	450	ARG
1	C	207	THR
1	C	298	LYS
1	B	195	ASN
1	C	195	ASN
1	C	317	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/469 (100%)	449 (96%)	19 (4%)	30	39
1	B	468/469 (100%)	452 (97%)	16 (3%)	37	47
1	C	468/469 (100%)	447 (96%)	21 (4%)	27	34
1	D	468/469 (100%)	454 (97%)	14 (3%)	41	53
All	All	1872/1876 (100%)	1802 (96%)	70 (4%)	34	43

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	59	LEU
1	A	90	THR
1	A	135	GLU
1	A	139	LYS
1	A	149	ARG
1	A	151	ASP
1	A	268	ARG
1	A	333	ASP
1	A	341	HIS
1	A	365	ARG
1	A	431	ARG
1	A	468	GLN
1	A	475	SER
1	A	495	LEU
1	A	503	ARG
1	A	516	ARG
1	A	522	ASN
1	A	531	LEU
1	B	3	LYS
1	B	10	THR
1	B	20	ARG
1	B	50	ARG
1	B	226	GLU
1	B	337	ASP
1	B	341	HIS
1	B	360	ARG
1	B	375	ARG
1	B	383	ARG
1	B	431	ARG
1	B	447	LEU
1	B	457	ASP
1	B	481	MET

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Mol	Chain	Res	Type
1	B	501	LYS
1	B	531	LEU
1	C	15	ASP
1	C	30	SER
1	C	60	SER
1	C	82	ASP
1	C	84	LYS
1	C	130	SER
1	C	151	ASP
1	C	173	GLU
1	C	194	ILE
1	C	257	THR
1	C	311	SER
1	C	332	ASP
1	C	333	ASP
1	C	341	HIS
1	C	360	ARG
1	C	365	ARG
1	C	383	ARG
1	C	384	ARG
1	C	433	LEU
1	C	447	LEU
1	C	501	LYS
1	D	59	LEU
1	D	65	ILE
1	D	142	VAL
1	D	151	ASP
1	D	173	GLU
1	D	255	THR
1	D	320	GLU
1	D	333	ASP
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	447	LEU
1	D	448	ARG
1	D	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS

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Mol	Chain	Res	Type
1	A	254	HIS
1	A	256	HIS
1	A	280	HIS
1	A	422	GLN
1	A	522	ASN
1	B	195	ASN
1	B	254	HIS
1	B	275	GLN
1	C	77	HIS
1	C	190	HIS
1	C	341	HIS
1	C	387	HIS
1	C	404	GLN
1	C	416	GLN
1	C	422	GLN
1	C	514	HIS
1	D	77	HIS
1	D	422	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	XYS	E	1	2	10,10,10	1.94	3 (30%)	14,14,14	2.51	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	XYS	E	2	2	9,9,10	1.02	1 (11%)	10,12,14	2.82	5 (50%)
2	XYS	F	1	2	10,10,10	1.90	3 (30%)	14,14,14	2.67	5 (35%)
2	XYS	F	2	2	9,9,10	1.55	2 (22%)	10,12,14	1.73	4 (40%)
2	XYS	G	1	2	10,10,10	2.54	6 (60%)	14,14,14	2.11	4 (28%)
2	XYS	G	2	2	9,9,10	1.23	1 (11%)	10,12,14	1.29	1 (10%)
2	XYS	H	1	2	10,10,10	2.26	5 (50%)	14,14,14	2.16	2 (14%)
2	XYS	H	2	2	9,9,10	0.73	0	10,12,14	1.87	1 (10%)

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	XYS	E	1	2	1/1/4/4	-	0/1/1/1
2	XYS	E	2	2	1/1/3/4	-	0/1/1/1
2	XYS	F	1	2	1/1/4/4	-	0/1/1/1
2	XYS	F	2	2	1/1/3/4	-	0/1/1/1
2	XYS	G	1	2	1/1/4/4	-	0/1/1/1
2	XYS	G	2	2	1/1/3/4	-	1/1/1/1
2	XYS	H	1	2	1/1/4/4	-	0/1/1/1
2	XYS	H	2	2	1/1/3/4	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	XYS	O5-C1	4.69	1.49	1.43
2	E	1	XYS	O4-C4	3.84	1.51	1.43
2	G	1	XYS	O4-C4	3.80	1.51	1.43
2	H	1	XYS	C4-C3	3.63	1.57	1.52
2	F	1	XYS	O5-C1	3.47	1.47	1.43
2	H	1	XYS	O5-C1	3.35	1.47	1.43
2	H	1	XYS	O4-C4	3.23	1.50	1.43
2	F	1	XYS	O4-C4	2.98	1.49	1.43
2	G	1	XYS	C4-C3	2.88	1.56	1.52
2	F	2	XYS	C2-C3	2.64	1.56	1.52
2	E	1	XYS	O5-C1	2.53	1.46	1.43
2	F	1	XYS	C4-C3	2.41	1.56	1.52
2	F	2	XYS	O5-C5	2.40	1.47	1.42
2	H	1	XYS	C1-C2	2.37	1.57	1.52
2	G	1	XYS	C5-C4	2.35	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	XYS	O5-C1	2.27	1.47	1.42
2	G	1	XYS	O5-C5	2.19	1.47	1.43
2	H	1	XYS	O1-C1	2.15	1.46	1.39
2	E	1	XYS	C4-C3	2.11	1.55	1.52
2	E	2	XYS	C1-C2	2.09	1.57	1.52
2	G	1	XYS	C1-C2	2.05	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	XYS	O5-C1-C2	6.93	119.72	109.43
2	F	1	XYS	O4-C4-C3	6.42	123.00	110.14
2	H	1	XYS	O4-C4-C3	5.82	121.80	110.14
2	F	1	XYS	O4-C4-C5	-5.63	97.63	109.15
2	E	2	XYS	C1-C2-C3	5.24	116.11	109.67
2	G	1	XYS	O4-C4-C3	4.88	119.92	110.14
2	G	1	XYS	O5-C1-C2	4.82	116.59	109.43
2	H	2	XYS	C1-C2-C3	4.66	115.39	109.67
2	E	1	XYS	O4-C4-C3	4.64	119.43	110.14
2	E	2	XYS	C4-C3-C2	4.62	116.41	110.92
2	H	1	XYS	O5-C1-C2	3.66	114.87	109.43
2	E	2	XYS	C5-C4-C3	3.56	114.04	109.67
2	G	2	XYS	C5-O5-C1	3.54	116.97	111.52
2	F	1	XYS	O5-C5-C4	3.18	115.68	110.77
2	E	2	XYS	C5-O5-C1	-3.11	106.75	111.52
2	F	2	XYS	C1-C2-C3	2.92	113.25	109.67
2	E	1	XYS	O1-C1-O5	-2.55	103.07	109.72
2	F	2	XYS	O3-C3-C2	2.48	114.74	109.99
2	G	1	XYS	O5-C5-C4	2.29	114.30	110.77
2	E	2	XYS	O2-C2-C3	-2.22	105.70	110.14
2	F	1	XYS	O5-C1-C2	2.21	112.72	109.43
2	F	2	XYS	O4-C4-C3	-2.21	105.72	110.14
2	F	2	XYS	O3-C3-C4	-2.13	105.92	109.99
2	F	1	XYS	C5-C4-C3	2.06	112.20	109.67
2	G	1	XYS	C5-C4-C3	2.05	112.19	109.67

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	XYS	C1
2	E	2	XYS	C1
2	F	1	XYS	C1

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Mol	Chain	Res	Type	Atom
2	F	2	XYS	C1
2	G	1	XYS	C1
2	G	2	XYS	C1
2	H	1	XYS	C1
2	H	2	XYS	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

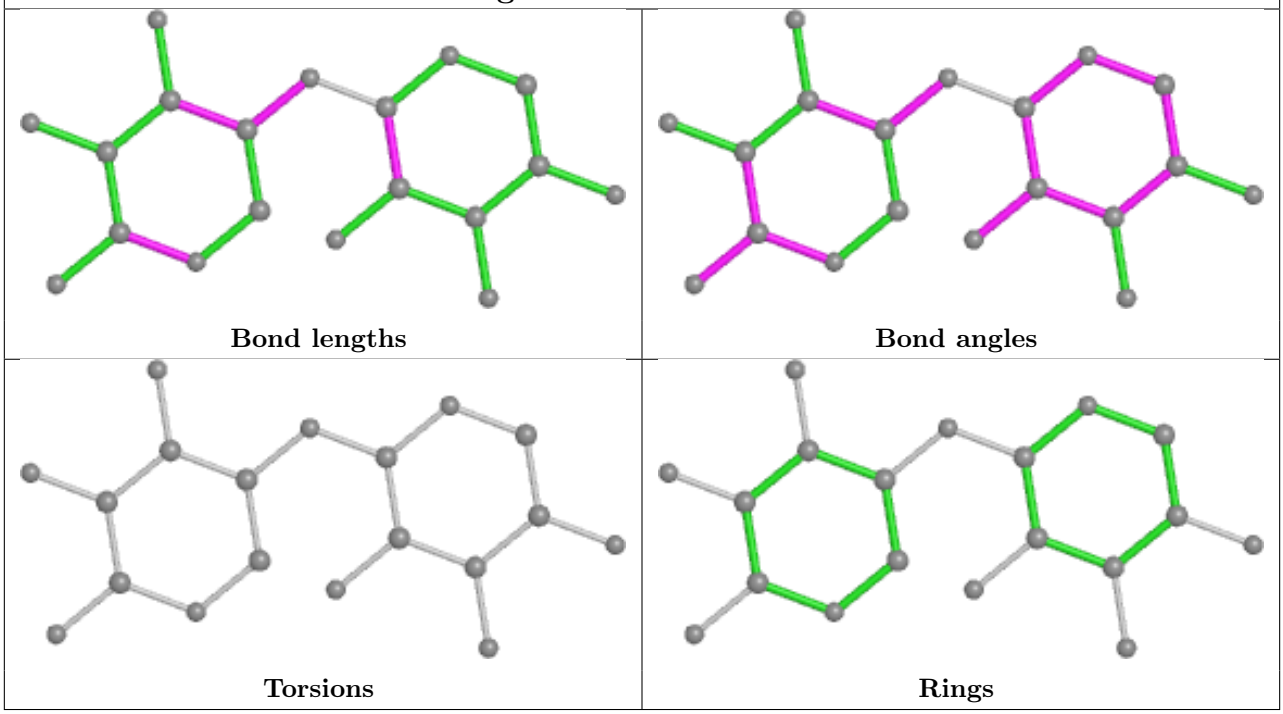
Mol	Chain	Res	Type	Atoms
2	G	2	XYS	C1-C2-C3-C4-C5-O5

3 monomers are involved in 8 short contacts:

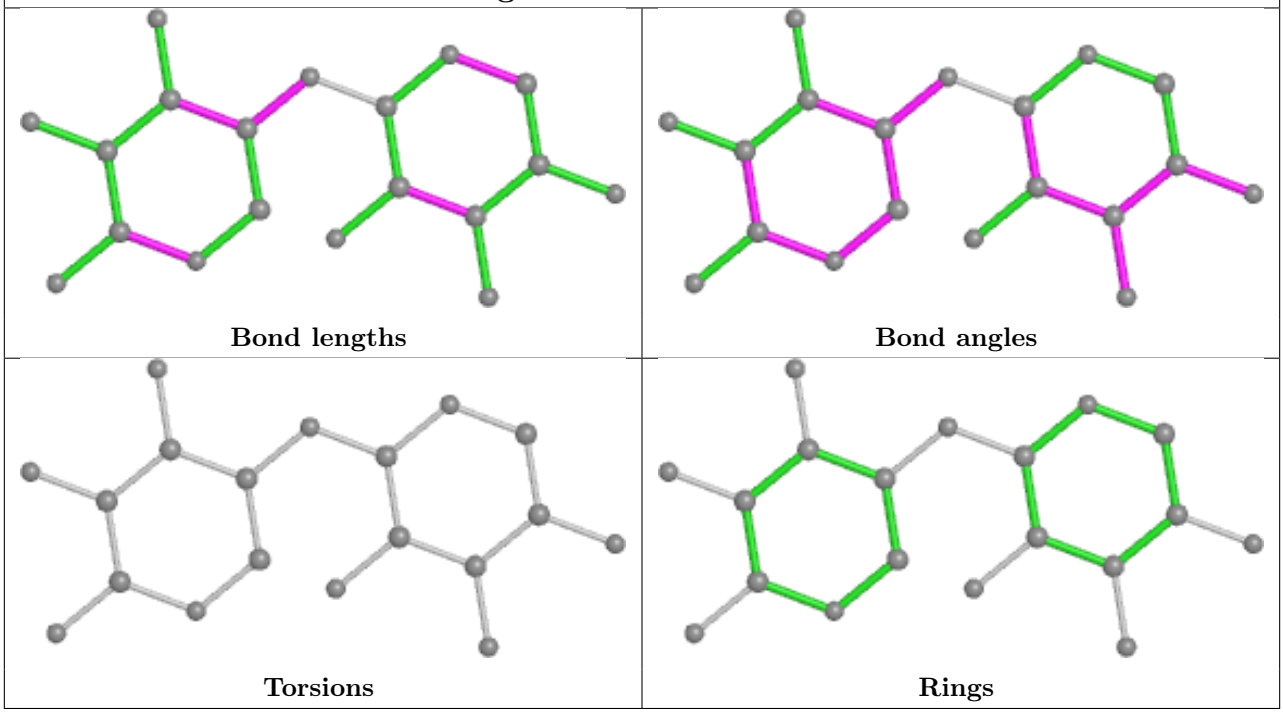
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	XYS	4	0
2	E	2	XYS	2	0
2	F	2	XYS	2	0

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

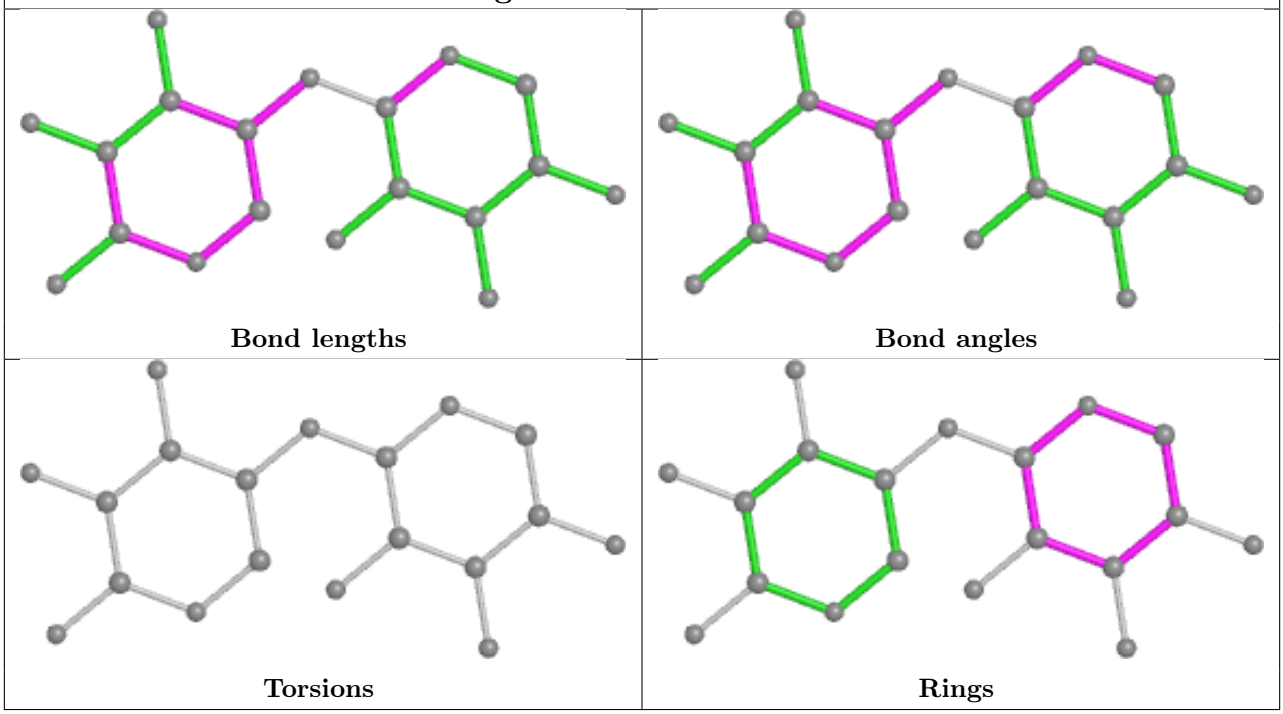
Oligosaccharide Chain E



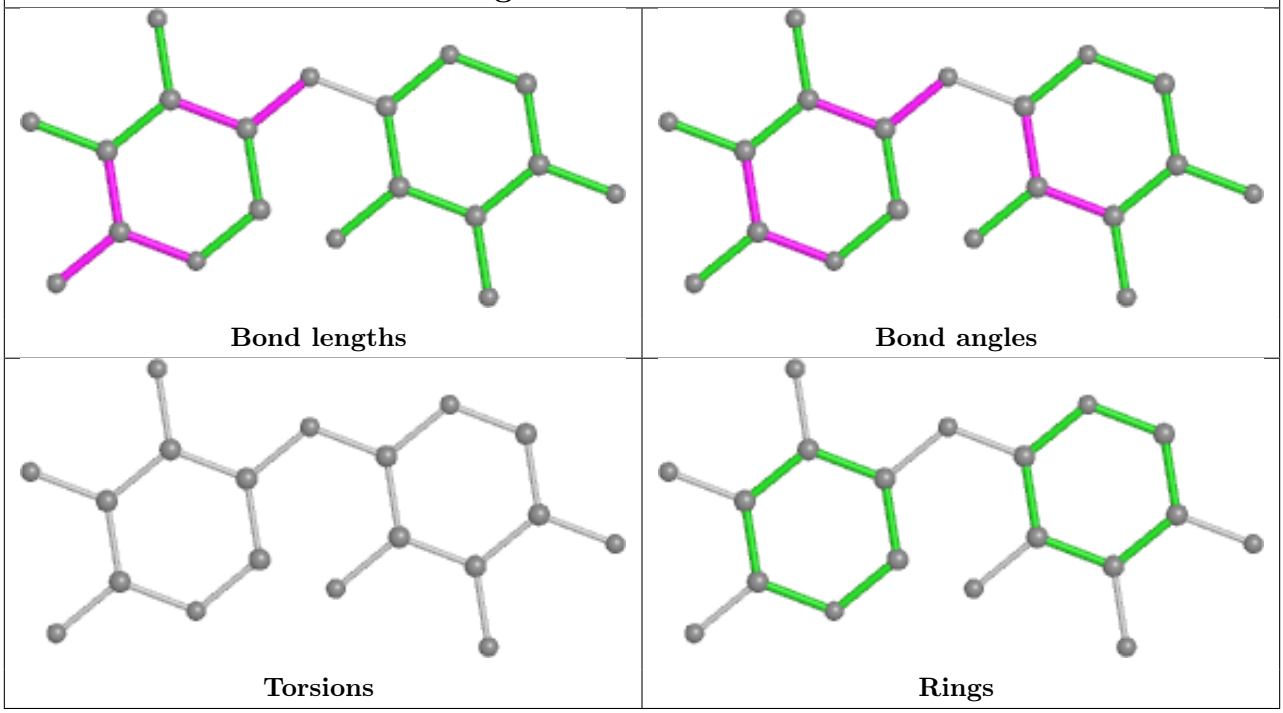
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
5	GOL	D	2019	-	5,5,5	0.57	0	5,5,5	0.48	0
5	GOL	C	2018	-	5,5,5	0.37	0	5,5,5	0.35	0
4	MES	B	2014	-	12,12,12	2.06	3 (25%)	14,16,16	7.17	9 (64%)
4	MES	D	2015	-	12,12,12	6.27	4 (33%)	14,16,16	7.75	7 (50%)
4	MES	A	2013	-	12,12,12	1.81	2 (16%)	14,16,16	6.60	9 (64%)
5	GOL	A	2016	-	5,5,5	0.46	0	5,5,5	0.80	0
5	GOL	B	2017	-	5,5,5	0.46	0	5,5,5	0.18	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
5	GOL	D	2019	-	-	0/4/4/4	-
5	GOL	C	2018	-	-	0/4/4/4	-
4	MES	B	2014	-	-	4/6/14/14	0/1/1/1
4	MES	D	2015	-	-	3/6/14/14	0/1/1/1
4	MES	A	2013	-	-	3/6/14/14	0/1/1/1
5	GOL	A	2016	-	-	4/4/4/4	-
5	GOL	B	2017	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2015	MES	O3S-S	12.74	1.92	1.47
4	D	2015	MES	O1S-S	12.20	1.81	1.45
4	D	2015	MES	O2S-S	10.52	1.76	1.45
4	D	2015	MES	C8-S	6.52	1.86	1.77
4	B	2014	MES	C8-S	5.65	1.85	1.77
4	A	2013	MES	C8-S	4.55	1.84	1.77
4	A	2013	MES	O1S-S	3.18	1.54	1.45
4	B	2014	MES	O1S-S	2.83	1.53	1.45
4	B	2014	MES	O2S-S	2.05	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2015	MES	O3S-S-O2S	-19.41	63.84	111.27
4	B	2014	MES	O3S-S-C8	-13.75	83.52	105.77
4	D	2015	MES	O2S-S-C8	13.44	123.10	106.92
4	A	2013	MES	O3S-S-O2S	-13.19	79.05	111.27
4	A	2013	MES	O3S-S-C8	-12.46	85.61	105.77
4	D	2015	MES	O3S-S-C8	-12.04	86.30	105.77
4	B	2014	MES	O1S-S-C8	11.15	120.34	106.92
4	B	2014	MES	O3S-S-O1S	-10.86	84.74	111.27
4	B	2014	MES	O3S-S-O2S	-10.75	85.01	111.27
4	B	2014	MES	O2S-S-C8	10.68	119.78	106.92
4	A	2013	MES	O3S-S-O1S	-9.02	89.24	111.27
4	A	2013	MES	O2S-S-C8	8.93	117.66	106.92
4	D	2015	MES	O3S-S-O1S	-8.85	89.66	111.27
4	A	2013	MES	C5-N4-C3	6.90	124.37	108.83
4	A	2013	MES	O1S-S-C8	6.48	114.72	106.92
4	D	2015	MES	C5-N4-C3	5.88	122.06	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2014	MES	C5-N4-C3	5.01	120.11	108.83
4	B	2014	MES	C7-N4-C5	3.64	120.53	111.23
4	D	2015	MES	C7-N4-C3	3.52	120.23	111.23
4	A	2013	MES	O2S-S-O1S	3.17	124.92	113.95
4	B	2014	MES	C7-N4-C3	3.17	119.34	111.23
4	A	2013	MES	C7-N4-C5	3.10	119.15	111.23
4	D	2015	MES	C7-N4-C5	2.53	117.71	111.23
4	B	2014	MES	O1-C6-C5	2.16	116.56	111.80
4	A	2013	MES	C7-N4-C3	2.05	116.48	111.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2013	MES	C8-C7-N4-C3
4	A	2013	MES	C7-C8-S-O1S
4	A	2013	MES	C7-C8-S-O3S
4	B	2014	MES	C8-C7-N4-C3
4	B	2014	MES	N4-C7-C8-S
4	D	2015	MES	N4-C7-C8-S
4	D	2015	MES	C7-C8-S-O2S
5	A	2016	GOL	O1-C1-C2-C3
5	B	2017	GOL	C1-C2-C3-O3
5	A	2016	GOL	O1-C1-C2-O2
5	B	2017	GOL	O2-C2-C3-O3
5	A	2016	GOL	O2-C2-C3-O3
4	D	2015	MES	C8-C7-N4-C5
4	B	2014	MES	C7-C8-S-O3S
4	B	2014	MES	C7-C8-S-O1S
5	A	2016	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2014	MES	5	0
4	D	2015	MES	6	0
5	B	2017	GOL	1	0

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	533/535 (99%)	-0.25	4 (0%)	86	85	13, 31, 47, 59	0
1	B	533/535 (99%)	-0.20	4 (0%)	86	85	15, 30, 46, 52	0
1	C	533/535 (99%)	0.69	52 (9%)	7	6	23, 49, 65, 73	0
1	D	533/535 (99%)	-0.10	10 (1%)	66	65	16, 33, 49, 56	0
All	All	2132/2140 (99%)	0.04	70 (3%)	46	44	13, 35, 58, 73	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	VAL	4.9
1	B	151	ASP	4.1
1	C	482	ASN	4.0
1	C	364	LEU	3.8
1	C	326	LYS	3.5
1	C	481	MET	3.2
1	C	46	LEU	3.1
1	C	87	LEU	3.1
1	A	151	ASP	3.0
1	C	483	TRP	3.0
1	C	247	ALA	3.0
1	C	455	PRO	2.8
1	C	255	THR	2.8
1	C	527	PHE	2.8
1	C	284	CYS	2.8
1	C	524	TYR	2.8
1	C	298	LYS	2.6
1	C	328	TYR	2.6
1	C	83	GLY	2.6
1	C	80	TYR	2.6
1	C	457	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	273	GLU	2.6
1	C	135	GLU	2.5
1	C	173	GLU	2.5
1	C	454	VAL	2.5
1	C	220	SER	2.5
1	C	468	GLN	2.5
1	D	273	GLU	2.4
1	D	481	MET	2.4
1	C	4	ILE	2.4
1	C	337	ASP	2.3
1	C	274	GLY	2.3
1	C	262	LEU	2.3
1	A	503	ARG	2.3
1	C	361	PRO	2.3
1	C	260	TRP	2.3
1	B	141	LEU	2.3
1	C	197	TYR	2.3
1	A	320	GLU	2.3
1	C	110	ASP	2.3
1	C	503	ARG	2.2
1	D	166	GLU	2.2
1	D	151	ASP	2.2
1	C	396	VAL	2.2
1	C	88	ILE	2.2
1	C	43	SER	2.2
1	C	50	ARG	2.2
1	C	111	THR	2.2
1	D	87	LEU	2.2
1	C	320	GLU	2.1
1	C	495	LEU	2.1
1	D	46	LEU	2.1
1	B	173	GLU	2.1
1	C	366	LEU	2.1
1	D	50	ARG	2.1
1	C	321	GLU	2.1
1	C	222	TYR	2.1
1	C	360	ARG	2.1
1	C	484	ILE	2.1
1	C	24	ASP	2.1
1	A	229	PRO	2.1
1	D	325	GLU	2.1
1	C	219	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	322	VAL	2.1
1	C	151	ASP	2.1
1	D	337	ASP	2.0
1	C	339	LEU	2.0
1	C	385	TRP	2.0
1	C	200	LEU	2.0
1	B	306	GLY	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)

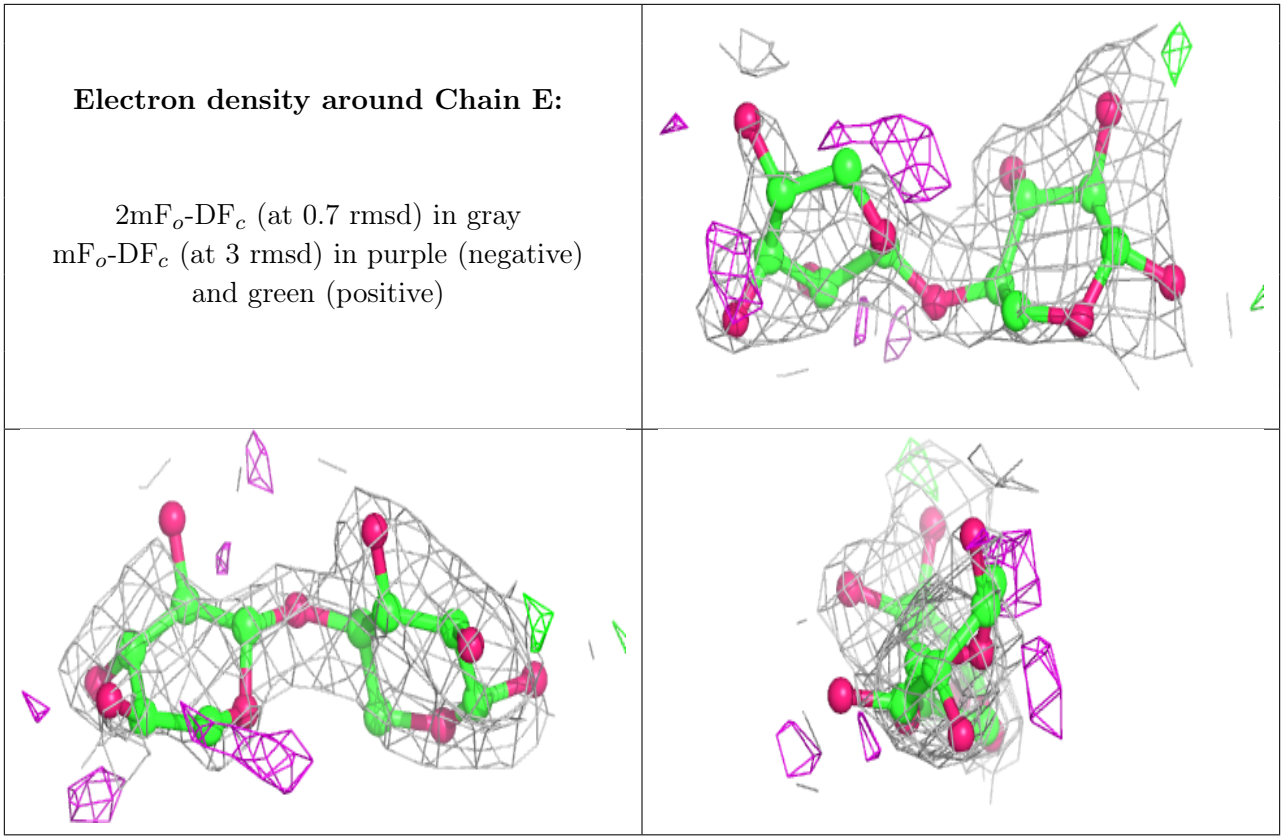
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYS	G	1	10/10	0.21	0.46	67,70,71,72	0
2	XYS	H	1	10/10	0.68	0.25	46,52,53,54	0
2	XYS	F	1	10/10	0.70	0.22	47,54,57,58	0
2	XYS	G	2	9/10	0.73	0.40	66,68,69,69	1
2	XYS	E	1	10/10	0.73	0.23	54,56,58,61	0
2	XYS	F	2	9/10	0.79	0.29	51,54,55,56	1
2	XYS	H	2	9/10	0.83	0.38	55,56,57,59	1
2	XYS	E	2	9/10	0.86	0.32	55,57,58,58	1

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.

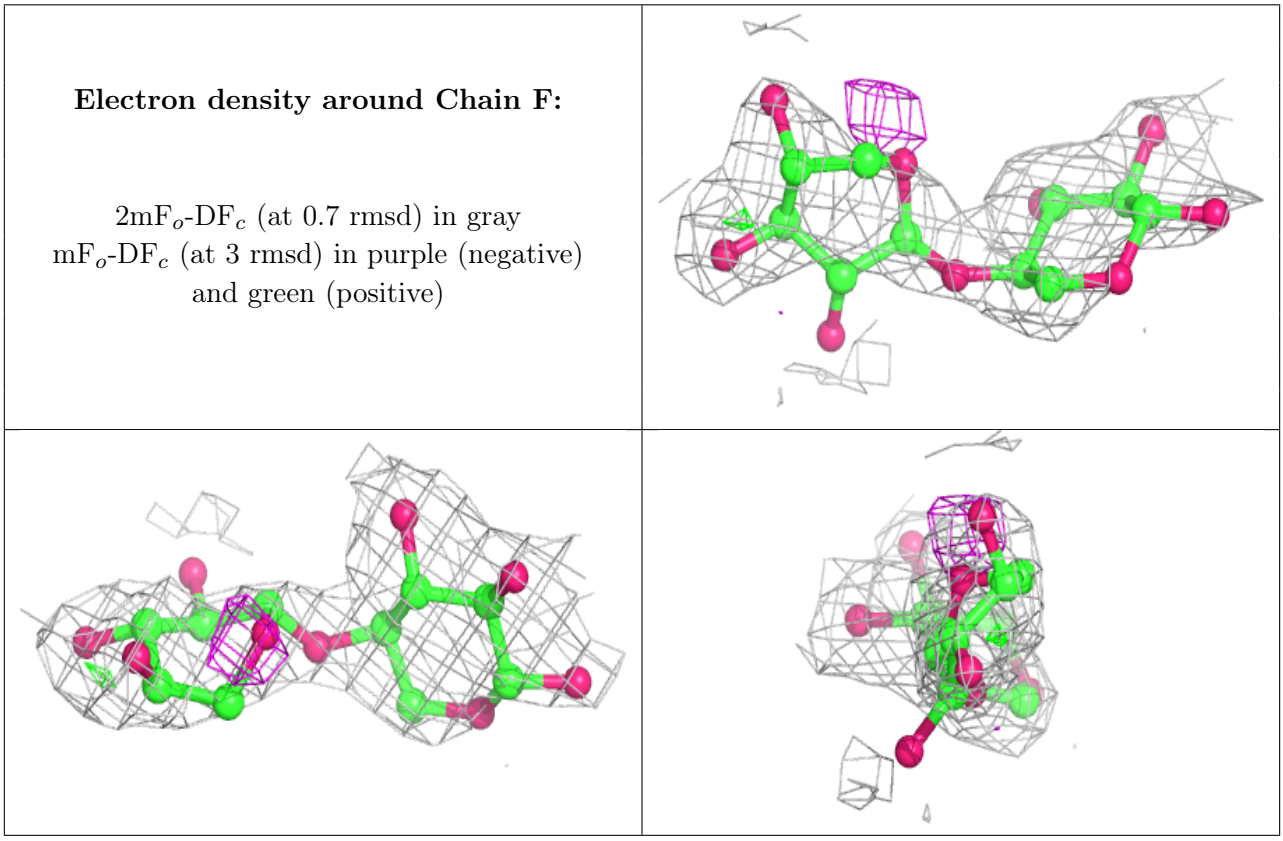
Electron density around Chain E:

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



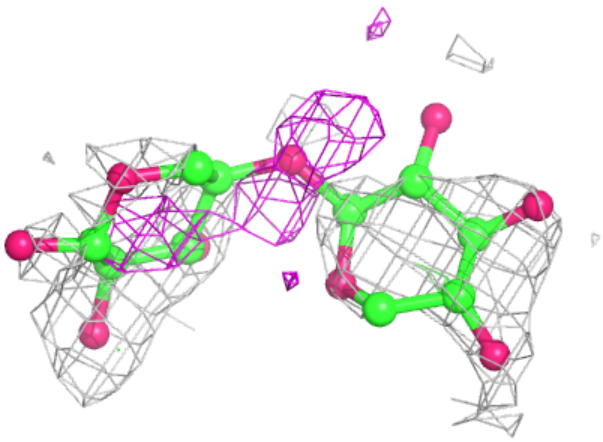
Electron density around Chain F:

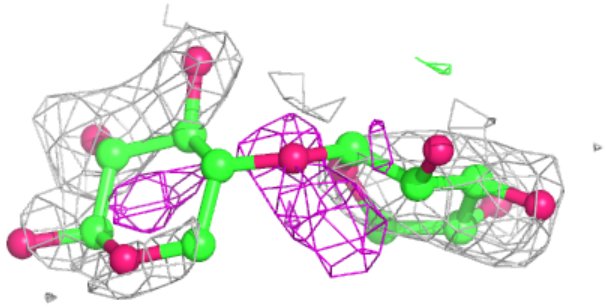
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

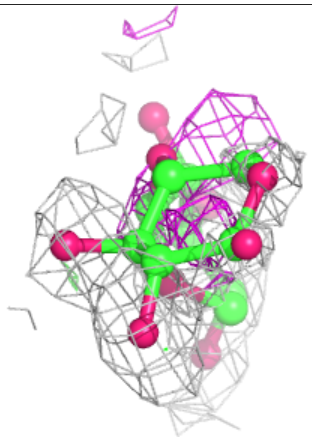


Electron density around Chain G:

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

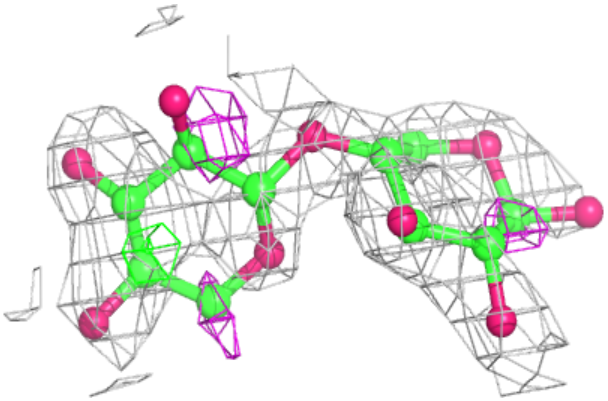


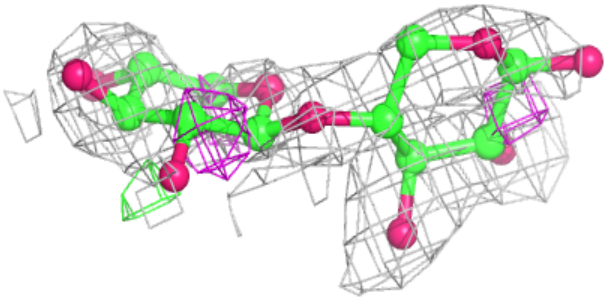


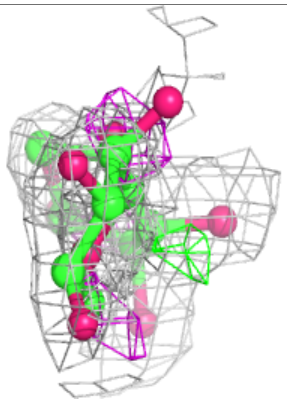


Electron density around Chain H:

$2mF_o$-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(Å^2)	Q<0.9
4	MES	D	2015	12/12	0.48	0.46	116,116,118,118	0
4	MES	B	2014	12/12	0.71	0.36	81,83,84,85	0
5	GOL	B	2017	6/6	0.86	0.12	40,41,43,46	0
3	CA	C	2003	1/1	0.88	0.10	50,50,50,50	0
5	GOL	A	2016	6/6	0.89	0.13	26,28,29,31	0
5	GOL	C	2018	6/6	0.91	0.12	33,37,40,41	0
5	GOL	D	2019	6/6	0.93	0.11	25,25,27,32	0
3	CA	D	2004	1/1	0.95	0.05	37,37,37,37	0
4	MES	A	2013	12/12	0.96	0.14	34,36,37,38	0
3	CA	B	2002	1/1	0.97	0.06	29,29,29,29	0
3	CA	A	2001	1/1	0.98	0.06	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.