Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 08:55 AM EDT

PDB ID	:	2EXK
Title	:	Structure of the family43 beta-Xylosidase E187G 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:

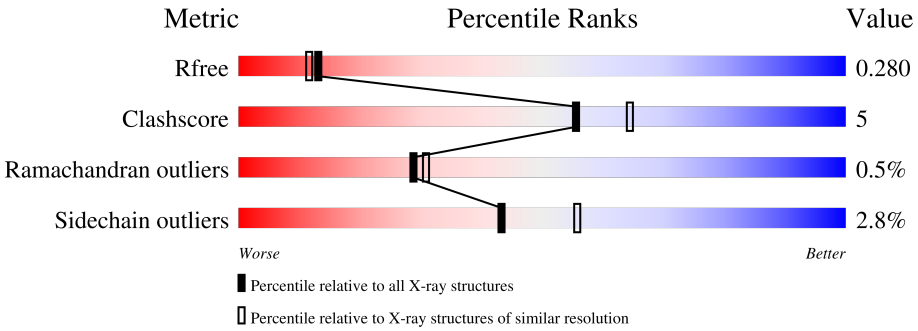
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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

Mol	Chain	Length	Quality of chain
1	A	535	85% 14% .
1	B	535	88% 10% .
1	C	535	84% 15% .
1	D	535	86% 13% .
2	E	2	50% 50%
2	F	2	100%
2	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
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	-	-	-
2	XYS	G	2	X	-	-	-
2	XYS	H	1	X	-	-	-
2	XYS	H	2	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18715 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
1	A	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	B	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	C	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	D	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			

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	187	GLY	GLU	engineered mutation	UNP Q68HB3
B	2	ALA	SER	engineered mutation	UNP Q68HB3
B	187	GLY	GLU	engineered mutation	UNP Q68HB3
C	2	ALA	SER	engineered mutation	UNP Q68HB3
C	187	GLY	GLU	engineered mutation	UNP Q68HB3
D	2	ALA	SER	engineered mutation	UNP Q68HB3
D	187	GLY	GLU	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
2	E	2	Total	C	O		0	0	0
			19	10	9				
2	F	2	Total	C	O		0	0	0
			19	10	9				

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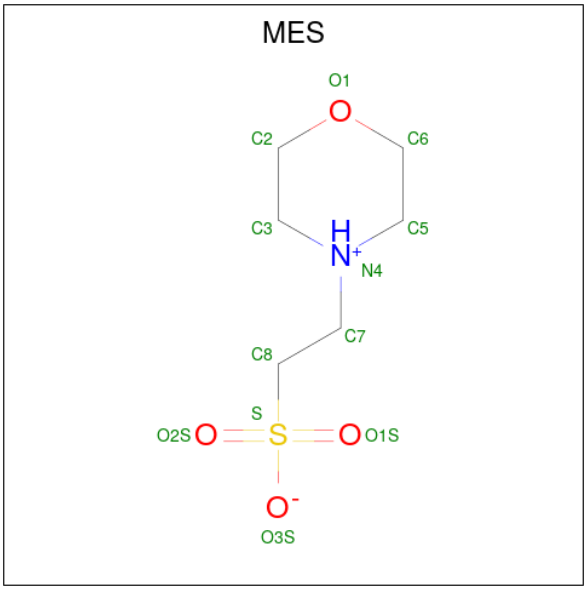
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	2	Total C O 19 10 9	0	0	0
2	H	2	Total C O 19 10 9	0	0	0

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

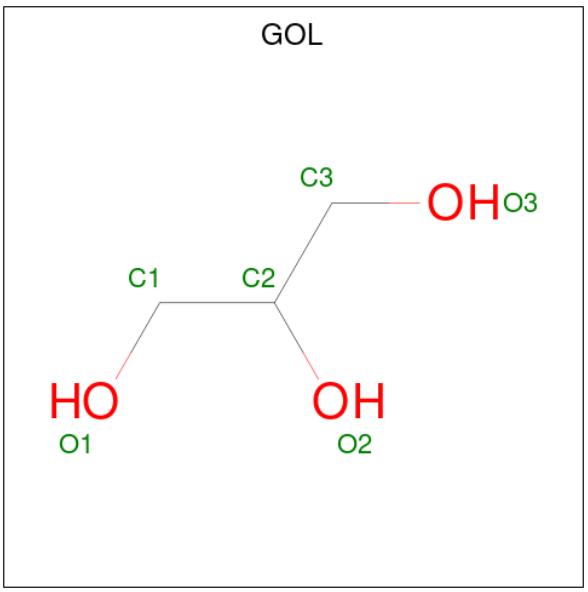
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	B	1	Total C N O S 12 6 1 4 1	0	0
4	D	1	Total C N O S 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
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

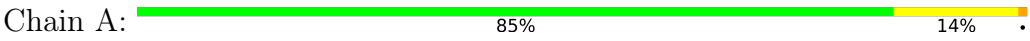
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	325	Total O 325 325	0	0
6	B	361	Total O 361 361	0	0
6	C	140	Total O 140 140	0	0
6	D	265	Total O 265 265	0	0

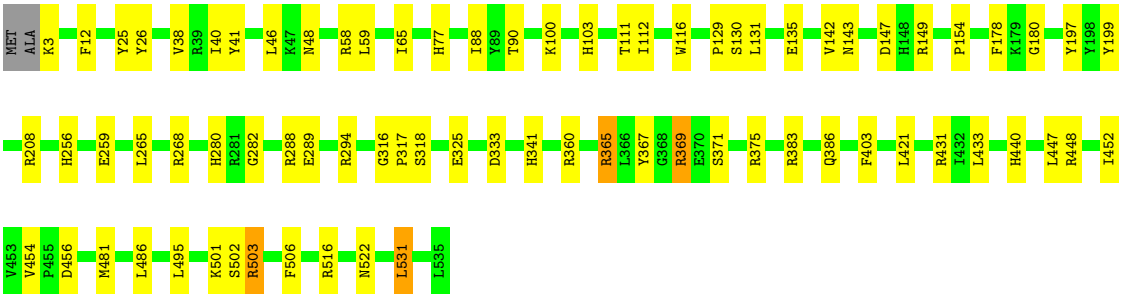
3 Residue-property plots (i)

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

• Molecule 1: beta-D-xylosidase

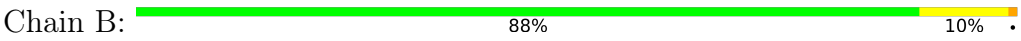
Chain A:

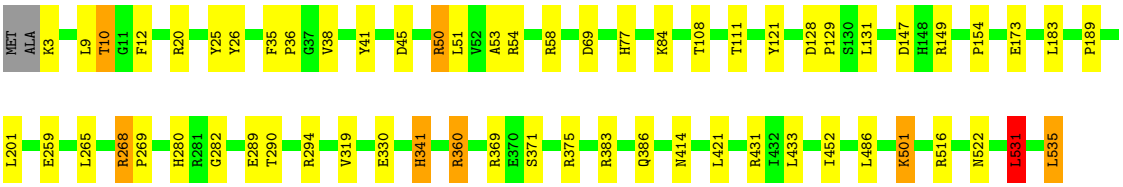




• Molecule 1: beta-D-xylosidase

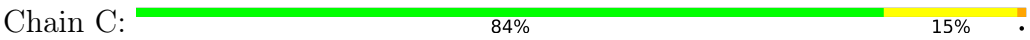
Chain B:

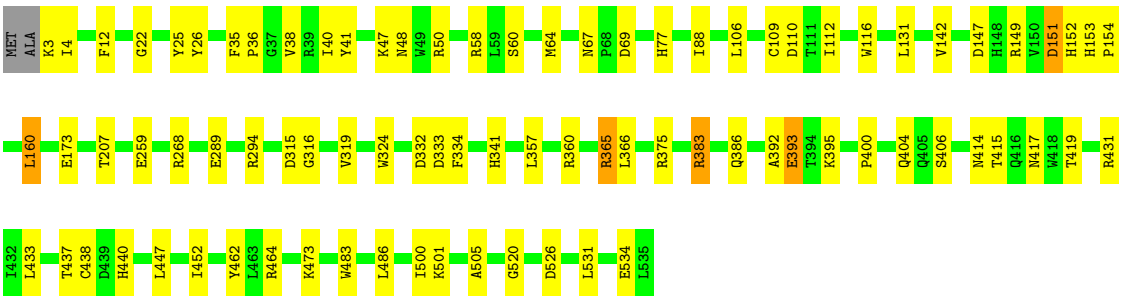




• Molecule 1: beta-D-xylosidase

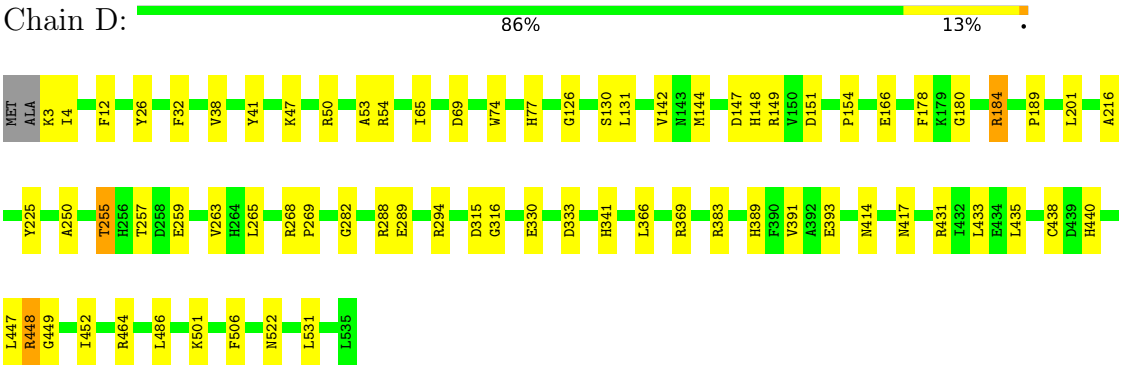
Chain C:





• Molecule 1: beta-D-xylosidase

Chain D:

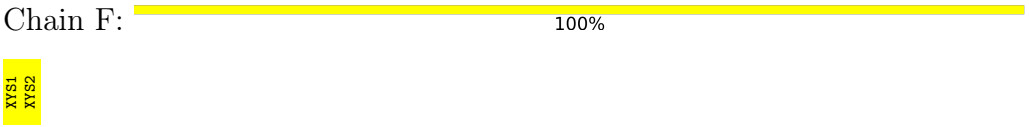


• Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-xylopyranose

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	139.87Å 139.87Å 232.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	2.23 – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (2.23-2.20) 99.5 (19.99-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.43 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.238 0.240 , 0.280	Depositor DCC
R_{free} test set	5803 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18715	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: CA, MES, XYS, 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	0.45	0/4515	0.62	2/6153 (0.0%)
1	B	0.45	0/4515	0.62	2/6153 (0.0%)
1	C	0.72	13/4515 (0.3%)	0.62	3/6153 (0.0%)
1	D	0.44	0/4515	0.60	0/6153
All	All	0.53	13/18060 (0.1%)	0.61	7/24612 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	GLU	CD-OE2	12.34	1.39	1.25
1	C	50	ARG	CZ-NH1	9.67	1.45	1.33
1	C	393	GLU	CD-OE1	9.63	1.36	1.25
1	C	259	GLU	CD-OE1	9.59	1.36	1.25
1	C	383	ARG	CZ-NH1	9.37	1.45	1.33
1	C	319	VAL	C-O	8.28	1.39	1.23
1	C	393	GLU	CG-CD	7.52	1.63	1.51
1	C	393	GLU	CD-OE2	7.19	1.33	1.25
1	C	315	ASP	CG-OD2	6.92	1.41	1.25
1	C	294	ARG	NE-CZ	6.51	1.41	1.33
1	C	386	GLN	CD-OE1	5.73	1.36	1.24
1	C	534	GLU	CD-OE1	5.71	1.31	1.25
1	C	25	TYR	CG-CD2	5.20	1.46	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	383	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	C	50	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	B	531	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	531	LEU	CA-CB-CG	6.69	130.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	383	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	369	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	268	ARG	NE-CZ-NH2	-5.41	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4371	0	4160	48	0
1	B	4371	0	4160	47	0
1	C	4371	0	4160	38	0
1	D	4371	0	4160	42	0
2	E	19	0	17	1	0
2	F	19	0	17	0	0
2	G	19	0	17	2	0
2	H	19	0	17	1	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	4	0
4	D	12	0	12	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	325	0	0	11	0
6	B	361	0	0	14	0
6	C	140	0	0	0	0
6	D	265	0	0	5	0
All	All	18715	0	16776	174	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 5.

All (174) 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:A:369:ARG:HH22	1:A:522:ASN:ND2	1.34	1.24
1:A:369:ARG:HH22	1:A:522:ASN:HD22	1.08	1.02
1:B:54:ARG:HE	4:B:2014:MES:H82	1.27	0.98
1:A:369:ARG:NH2	1:A:522:ASN:HD22	1.63	0.97
1:A:369:ARG:NH2	1:A:522:ASN:ND2	2.14	0.95
1:D:255:THR:HG22	1:D:259:GLU:H	1.37	0.88
1:A:503:ARG:HG3	6:A:2241:HOH:O	1.81	0.79
1:A:360:ARG:HB2	1:A:365:ARG:HH12	1.50	0.76
1:A:25:TYR:OH	1:A:256:HIS:HD2	1.70	0.75
1:A:369:ARG:HH22	1:A:522:ASN:HD21	1.32	0.75
1:D:268:ARG:HD3	1:D:289:GLU:OE1	1.86	0.74
1:C:268:ARG:HD3	1:C:289:GLU:OE1	1.87	0.73
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.70	0.73
1:C:77:HIS:CD2	1:C:131:LEU:H	2.07	0.72
1:B:3:LYS:HG3	6:B:2093:HOH:O	1.89	0.71
1:B:53:ALA:HA	4:B:2014:MES:H51	1.71	0.71
1:B:10:THR:CG2	1:B:386:GLN:O	2.40	0.69
1:D:53:ALA:HA	4:D:2015:MES:H81	1.76	0.68
1:B:147:ASP:OD1	1:B:149:ARG:HD3	1.93	0.68
1:A:111:THR:HG21	6:A:2193:HOH:O	1.93	0.68
1:B:10:THR:HG23	1:B:386:GLN:O	1.94	0.68
1:C:58:ARG:NH2	1:C:116:TRP:O	2.26	0.68
1:D:147:ASP:OD1	1:D:149:ARG:HD3	1.94	0.67
1:B:111:THR:HG22	6:B:2101:HOH:O	1.94	0.67
1:D:294:ARG:NH1	1:D:315:ASP:O	2.29	0.66
1:C:3:LYS:HD3	1:C:316:GLY:H	1.62	0.65
1:B:121:TYR:OH	1:C:520:GLY:HA3	1.98	0.64
1:C:40:ILE:HG21	1:C:112:ILE:HD11	1.81	0.63
1:C:433:LEU:HB2	1:C:452:ILE:HB	1.83	0.61
1:B:77:HIS:CD2	1:B:131:LEU:H	2.19	0.61
1:D:433:LEU:HB2	1:D:452:ILE:HB	1.82	0.60
1:A:365:ARG:HD3	1:A:367:TYR:CZ	2.37	0.59
1:D:288:ARG:HH12	2:H:2:XYS:H52	1.67	0.59
1:A:502:SER:O	1:A:503:ARG:HB2	2.03	0.58
1:C:147:ASP:OD1	1:C:149:ARG:HD3	2.03	0.58
1:B:54:ARG:NE	4:B:2014:MES:H82	2.08	0.57
1:B:58:ARG:NH1	6:B:2032:HOH:O	2.19	0.57
1:D:77:HIS:CD2	1:D:131:LEU:H	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:HD3	1:C:526:ASP:OD1	2.04	0.57
1:C:417:ASN:HA	1:C:438:CYS:O	2.04	0.57
1:B:10:THR:HG22	1:B:386:GLN:HB3	1.87	0.57
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.53	0.57
1:D:435:LEU:HD12	1:D:447:LEU:HD13	1.85	0.56
1:D:255:THR:HG23	1:D:257:THR:H	1.69	0.56
1:A:433:LEU:HB2	1:A:452:ILE:HB	1.88	0.56
1:A:280:HIS:CD2	1:A:282:GLY:H	2.24	0.56
1:D:255:THR:HG22	1:D:259:GLU:N	2.16	0.56
1:C:375:ARG:HG3	1:C:415:THR:HG21	1.88	0.55
1:D:54:ARG:H	4:D:2015:MES:H32	1.71	0.55
1:B:84:LYS:HD3	1:B:108:THR:HB	1.87	0.55
1:D:330:GLU:O	1:D:531:LEU:HA	2.07	0.55
1:A:147:ASP:O	1:A:154:PRO:HA	2.07	0.55
1:C:392:ALA:HA	1:C:531:LEU:O	2.08	0.54
1:D:178:PHE:CE2	1:D:180:GLY:HA2	2.43	0.54
1:A:147:ASP:OD1	1:A:149:ARG:HD3	2.08	0.54
1:A:383:ARG:HD2	6:A:2164:HOH:O	2.06	0.54
1:B:50:ARG:HH11	1:B:50:ARG:HB3	1.73	0.54
1:A:58:ARG:NH2	1:A:116:TRP:O	2.31	0.53
1:C:334:PHE:HB3	1:C:357:LEU:HD22	1.89	0.53
1:D:147:ASP:O	1:D:154:PRO:HA	2.08	0.53
1:C:393:GLU:HG3	1:C:464:ARG:HB2	1.90	0.53
1:A:208:ARG:CZ	6:A:2241:HOH:O	2.55	0.53
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.08	0.53
1:B:280:HIS:HE1	6:B:2194:HOH:O	1.91	0.53
1:D:3:LYS:HD3	1:D:316:GLY:H	1.73	0.53
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.44	0.52
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.92	0.52
1:B:58:ARG:NH2	6:B:2032:HOH:O	2.36	0.52
1:A:448:ARG:NH2	6:A:2269:HOH:O	2.42	0.52
1:B:433:LEU:HB3	1:B:452:ILE:HB	1.91	0.52
1:B:369:ARG:NH2	1:B:522:ASN:OD1	2.43	0.51
1:D:151:ASP:HB3	6:D:2159:HOH:O	2.09	0.51
1:B:375:ARG:NH2	6:B:2171:HOH:O	2.43	0.51
1:A:421:LEU:HD13	1:A:486:LEU:HD13	1.92	0.51
1:B:9:LEU:HB2	1:B:290:THR:HB	1.91	0.51
1:A:365:ARG:HB2	1:A:365:ARG:HH11	1.75	0.51
1:A:431:ARG:HD2	6:A:2092:HOH:O	2.10	0.51
1:C:4:ILE:HG12	1:C:47:LYS:HB2	1.93	0.50
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LYS:HD2	1:C:462:TYR:CE1	2.47	0.50
1:D:184:ARG:HD3	6:D:2161:HOH:O	2.10	0.49
1:C:142:VAL:HG13	1:C:160:LEU:HD12	1.93	0.49
1:C:334:PHE:HB3	1:C:357:LEU:CD2	2.43	0.49
1:B:421:LEU:HD13	1:B:486:LEU:HD13	1.93	0.49
1:C:147:ASP:O	1:C:154:PRO:HA	2.11	0.49
6:B:2063:HOH:O	1:C:404:GLN:HG2	2.13	0.48
1:A:375:ARG:NH2	6:A:2142:HOH:O	2.46	0.48
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.96	0.48
6:A:2136:HOH:O	2:E:2:XYS:O2	2.19	0.48
1:D:216:ALA:HB1	1:D:225:TYR:HB3	1.96	0.48
1:A:3:LYS:HB3	1:A:316:GLY:H	1.80	0.47
1:C:207:THR:N	2:G:1:XYS:O3	2.47	0.47
1:D:259:GLU:OE1	1:D:294:ARG:NH2	2.47	0.47
1:A:383:ARG:NH2	1:A:386:GLN:OE1	2.47	0.47
1:A:501:LYS:HE2	6:A:2076:HOH:O	2.14	0.47
1:D:189:PRO:HA	1:D:201:LEU:O	2.14	0.47
1:B:20:ARG:HG3	1:B:25:TYR:CE1	2.49	0.47
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.97	0.47
1:A:440:HIS:NE2	1:A:501:LYS:HG2	2.30	0.47
1:A:40:ILE:HG21	1:A:112:ILE:HD11	1.97	0.46
1:A:288:ARG:NH2	1:A:506:PHE:HB3	2.30	0.46
1:B:421:LEU:HD13	1:B:486:LEU:CD1	2.45	0.46
1:D:126:GLY:HA3	1:D:144:MET:O	2.16	0.46
1:A:130:SER:HB3	1:A:142:VAL:HG23	1.97	0.46
1:A:403:PHE:O	1:D:148:HIS:HE1	1.99	0.46
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.63	0.46
1:A:90:THR:HA	1:A:103:HIS:O	2.15	0.46
1:B:54:ARG:H	4:B:2014:MES:H51	1.80	0.46
1:C:26:TYR:HA	1:C:41:TYR:O	2.15	0.46
1:C:151:ASP:OD2	1:C:152:HIS:CE1	2.69	0.46
1:B:51:LEU:HD23	1:B:341:HIS:CG	2.51	0.46
1:B:189:PRO:HA	1:B:201:LEU:O	2.16	0.46
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.37	0.46
1:D:250:ALA:HA	1:D:263:VAL:O	2.15	0.46
1:B:371:SER:HA	1:B:516:ARG:HD3	1.98	0.45
1:B:501:LYS:HD2	6:B:2075:HOH:O	2.15	0.45
1:D:69:ASP:CG	1:D:414:ASN:HB2	2.36	0.45
1:A:197:TYR:HB2	1:A:199:TYR:CE1	2.52	0.45
1:A:265:LEU:HA	1:A:289:GLU:O	2.16	0.45
1:B:360:ARG:HD3	6:B:2257:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.32	0.45
1:A:129:PRO:HA	1:A:143:ASN:HB3	1.98	0.44
1:A:88:ILE:HG21	1:A:129:PRO:HB2	1.98	0.44
1:B:26:TYR:HA	1:B:41:TYR:O	2.18	0.44
1:A:280:HIS:HD2	1:A:282:GLY:H	1.63	0.44
1:A:447:LEU:HD11	1:A:486:LEU:HD22	2.00	0.44
1:D:391:VAL:CG2	1:D:464:ARG:HD2	2.48	0.44
1:B:259:GLU:OE1	1:B:294:ARG:NH2	2.47	0.44
1:B:535:LEU:HD11	6:B:2097:HOH:O	2.17	0.44
1:A:259:GLU:OE1	1:A:294:ARG:NH2	2.43	0.43
1:B:3:LYS:CE	6:B:2118:HOH:O	2.65	0.43
1:D:448:ARG:HA	1:D:449:GLY:HA2	1.83	0.43
1:B:501:LYS:NZ	6:B:2192:HOH:O	2.51	0.43
1:C:48:ASN:HB3	1:C:324:TRP:CD1	2.53	0.43
1:B:3:LYS:HE3	6:B:2118:HOH:O	2.18	0.43
1:B:265:LEU:HA	1:B:289:GLU:O	2.18	0.43
1:A:48:ASN:HB3	6:A:2236:HOH:O	2.18	0.43
1:D:393:GLU:OE1	1:D:464:ARG:HD3	2.18	0.43
1:C:88:ILE:HD13	1:C:106:LEU:HD13	2.01	0.43
1:C:440:HIS:NE2	1:C:501:LYS:HD3	2.34	0.43
1:A:77:HIS:CD2	1:A:131:LEU:H	2.37	0.42
1:B:69:ASP:CG	1:B:414:ASN:HB2	2.38	0.42
1:C:500:ILE:HB	1:C:505:ALA:HB2	2.00	0.42
1:D:389:HIS:HD2	6:D:2250:HOH:O	2.01	0.42
1:B:45:ASP:HA	1:B:319:VAL:HG21	2.01	0.42
1:C:3:LYS:HD3	1:C:316:GLY:N	2.31	0.42
1:C:35:PHE:CG	1:C:36:PRO:HA	2.54	0.42
1:C:77:HIS:HD2	1:C:131:LEU:H	1.64	0.42
1:D:440:HIS:NE2	1:D:501:LYS:HG2	2.35	0.42
1:D:417:ASN:HA	1:D:438:CYS:O	2.20	0.42
1:A:26:TYR:HA	1:A:41:TYR:O	2.20	0.42
1:A:365:ARG:HD3	1:A:367:TYR:CE2	2.55	0.42
1:B:330:GLU:O	1:B:531:LEU:HA	2.20	0.42
1:C:64:MET:O	1:C:67:ASN:HB2	2.20	0.42
1:C:419:THR:HG22	1:C:437:THR:HG22	2.02	0.42
1:C:109:CYS:HB2	1:C:116:TRP:CD2	2.55	0.41
1:B:147:ASP:O	1:B:154:PRO:HA	2.20	0.41
1:C:207:THR:HG22	2:G:1:XYS:H3	2.02	0.41
1:A:371:SER:HA	1:A:516:ARG:HD3	2.03	0.41
1:D:50:ARG:HA	6:D:2129:HOH:O	2.20	0.41
1:C:153:HIS:HA	1:C:154:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:C	1:D:265:LEU:HD12	2.40	0.41
1:B:128:ASP:N	1:B:129:PRO:CD	2.84	0.41
1:D:77:HIS:CD2	6:D:2055:HOH:O	2.74	0.41
1:B:35:PHE:CG	1:B:36:PRO:HA	2.55	0.41
1:D:130:SER:HB3	1:D:142:VAL:HG23	2.02	0.41
1:B:280:HIS:CD2	1:B:282:GLY:H	2.39	0.40
1:C:462:TYR:HB3	1:C:483:TRP:CH2	2.56	0.40
1:D:26:TYR:HA	1:D:41:TYR:O	2.21	0.40
1:D:32:PHE:CE2	1:D:74:TRP:CD1	3.10	0.40
1:A:111:THR:HG22	6:A:2183:HOH:O	2.22	0.40
1:D:369:ARG:NH2	1:D:522:ASN:OD1	2.41	0.40
1:B:50:ARG:HD2	6:B:2083:HOH:O	2.20	0.40
1:D:269:PRO:HB3	1:D:282:GLY:HA3	2.03	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%)	505 (95%)	23 (4%)	3 (1%)	25	26
1	B	531/535 (99%)	508 (96%)	21 (4%)	2 (0%)	34	37
1	C	531/535 (99%)	503 (95%)	25 (5%)	3 (1%)	25	26
1	D	531/535 (99%)	501 (94%)	28 (5%)	2 (0%)	34	37
All	All	2124/2140 (99%)	2017 (95%)	97 (5%)	10 (0%)	29	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	38	VAL

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Mol	Chain	Res	Type
1	B	12	PHE
1	B	38	VAL
1	C	12	PHE
1	C	38	VAL
1	D	38	VAL
1	C	22	GLY
1	D	12	PHE
1	A	318	SER

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%)	454 (97%)	14 (3%)	41	53
1	B	468/469 (100%)	457 (98%)	11 (2%)	49	62
1	C	468/469 (100%)	452 (97%)	16 (3%)	37	47
1	D	468/469 (100%)	457 (98%)	11 (2%)	49	62
All	All	1872/1876 (100%)	1820 (97%)	52 (3%)	43	56

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	65	ILE
1	A	100	LYS
1	A	135	GLU
1	A	268	ARG
1	A	325	GLU
1	A	333	ASP
1	A	341	HIS
1	A	365	ARG
1	A	456	ASP
1	A	481	MET
1	A	495	LEU
1	A	503	ARG

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Mol	Chain	Res	Type
1	A	531	LEU
1	B	10	THR
1	B	50	ARG
1	B	173	GLU
1	B	183	LEU
1	B	341	HIS
1	B	360	ARG
1	B	383	ARG
1	B	431	ARG
1	B	501	LYS
1	B	531	LEU
1	B	535	LEU
1	C	60	SER
1	C	110	ASP
1	C	151	ASP
1	C	160	LEU
1	C	173	GLU
1	C	332	ASP
1	C	333	ASP
1	C	341	HIS
1	C	360	ARG
1	C	365	ARG
1	C	366	LEU
1	C	383	ARG
1	C	406	SER
1	C	447	LEU
1	C	473	LYS
1	C	486	LEU
1	D	65	ILE
1	D	166	GLU
1	D	184	ARG
1	D	255	THR
1	D	333	ASP
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	431	ARG
1	D	448	ARG
1	D	486	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	210	ASN
1	A	254	HIS
1	A	256	HIS
1	A	280	HIS
1	A	422	GLN
1	A	522	ASN
1	B	77	HIS
1	B	254	HIS
1	B	280	HIS
1	C	77	HIS
1	C	152	HIS
1	C	195	ASN
1	C	254	HIS
1	C	280	HIS
1	C	411	ASN
1	C	422	GLN
1	D	77	HIS
1	D	280	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	2.50	4 (40%)	14,14,14	2.72	6 (42%)
2	XYS	E	2	2	9,9,10	1.04	0	10,12,14	1.43	1 (10%)
2	XYS	F	1	2	10,10,10	2.04	3 (30%)	14,14,14	1.92	3 (21%)
2	XYS	F	2	2	9,9,10	1.23	1 (11%)	10,12,14	2.14	3 (30%)
2	XYS	G	1	2	10,10,10	1.99	3 (30%)	14,14,14	1.67	2 (14%)
2	XYS	G	2	2	9,9,10	1.28	1 (11%)	10,12,14	1.02	1 (10%)
2	XYS	H	1	2	10,10,10	2.24	3 (30%)	14,14,14	1.41	2 (14%)
2	XYS	H	2	2	9,9,10	0.98	0	10,12,14	1.29	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	-	0/1/1/1
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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	XYS	O5-C1	5.77	1.51	1.43
2	H	1	XYS	O5-C1	4.82	1.49	1.43
2	F	1	XYS	O5-C1	4.20	1.48	1.43
2	G	1	XYS	O5-C1	3.75	1.48	1.43
2	E	1	XYS	O4-C4	3.28	1.50	1.43
2	H	1	XYS	O4-C4	2.90	1.49	1.43
2	F	1	XYS	O5-C5	2.88	1.48	1.43
2	G	1	XYS	O4-C4	2.73	1.49	1.43
2	F	1	XYS	O4-C4	2.54	1.48	1.43
2	G	1	XYS	O5-C5	2.36	1.47	1.43
2	G	2	XYS	O5-C1	2.35	1.47	1.42
2	H	1	XYS	C4-C3	2.34	1.56	1.52
2	E	1	XYS	O5-C5	2.29	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	XYS	O1-C1	2.19	1.46	1.39
2	F	2	XYS	C2-C3	2.16	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	XYS	O5-C1-C2	5.58	117.72	109.43
2	E	1	XYS	O4-C4-C3	4.95	120.05	110.14
2	F	2	XYS	C1-C2-C3	4.80	115.56	109.67
2	G	1	XYS	O4-C4-C5	4.77	118.91	109.15
2	F	1	XYS	O4-C4-C3	4.76	119.67	110.14
2	F	2	XYS	C4-C3-C2	4.05	115.73	110.92
2	E	2	XYS	C1-C2-C3	3.94	114.51	109.67
2	F	1	XYS	O5-C5-C4	3.75	116.57	110.77
2	E	1	XYS	C5-C4-C3	-3.65	105.18	109.67
2	E	1	XYS	O5-C5-C4	-3.59	105.23	110.77
2	H	1	XYS	O4-C4-C5	3.38	116.07	109.15
2	E	1	XYS	O4-C4-C5	3.06	115.40	109.15
2	H	2	XYS	C1-C2-C3	2.82	113.14	109.67
2	H	1	XYS	O4-C4-C3	2.45	115.04	110.14
2	G	2	XYS	C5-O5-C1	2.38	115.18	111.52
2	G	1	XYS	O5-C1-C2	2.31	112.86	109.43
2	F	2	XYS	C5-C4-C3	2.28	112.47	109.67
2	E	1	XYS	C5-O5-C1	2.23	116.46	112.71
2	F	1	XYS	O1-C1-O5	2.15	115.32	109.72

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
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.

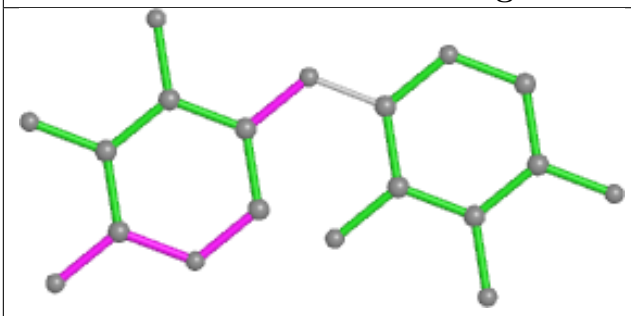
There are no ring outliers.

3 monomers are involved in 4 short contacts:

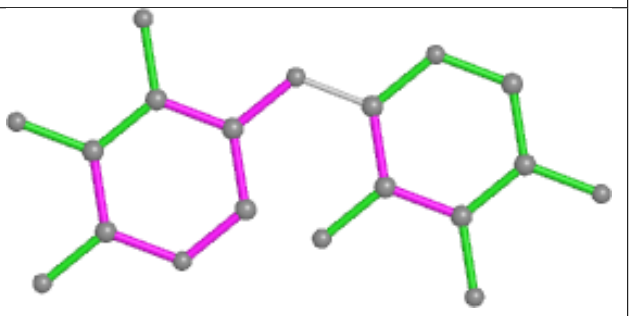
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	XYS	1	0
2	G	1	XYS	2	0
2	E	2	XYS	1	0

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

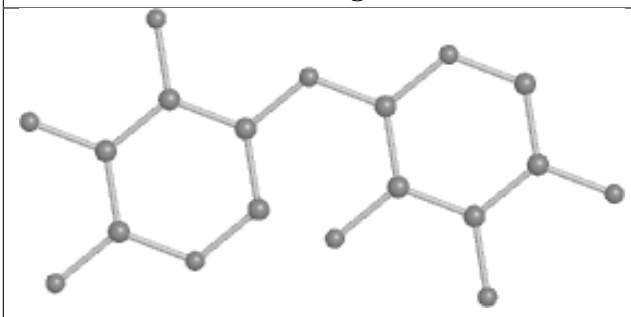
Oligosaccharide Chain E



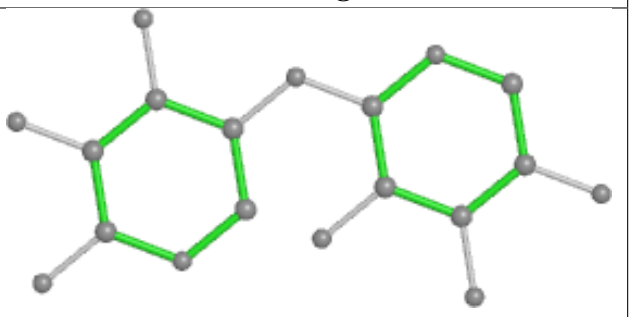
Bond lengths



Bond angles

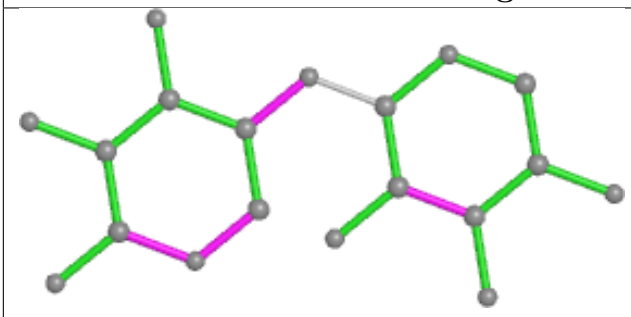


Torsions

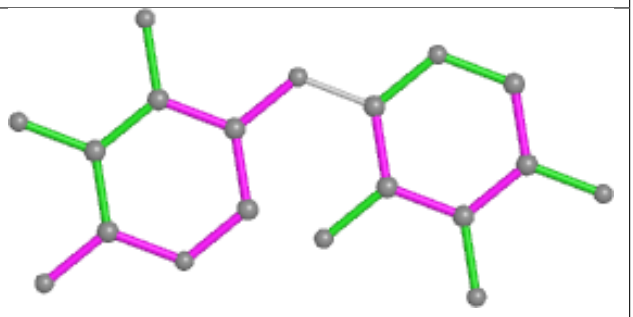


Rings

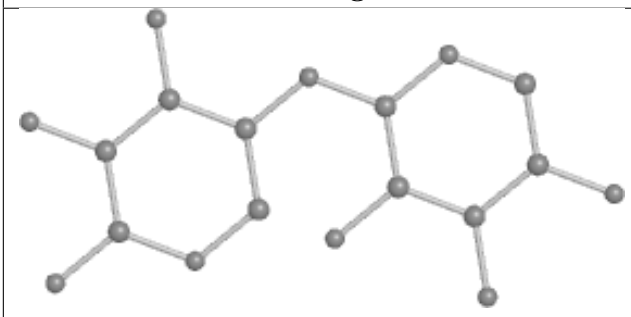
Oligosaccharide Chain F



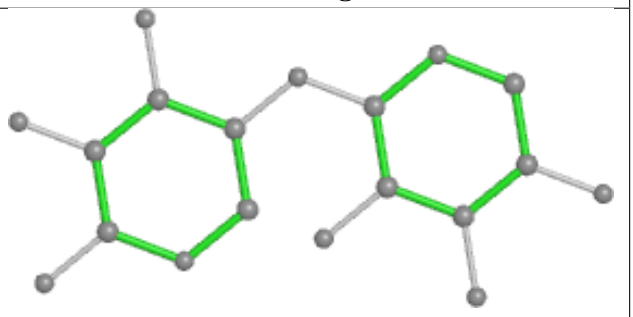
Bond lengths



Bond angles

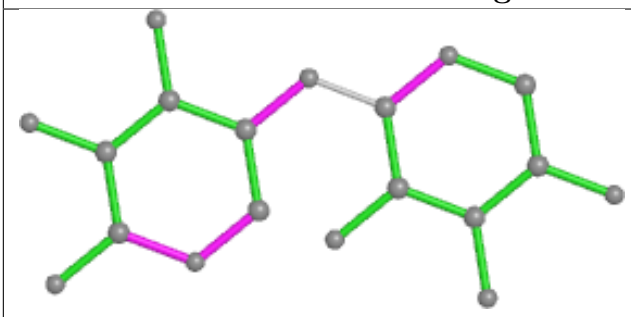


Torsions

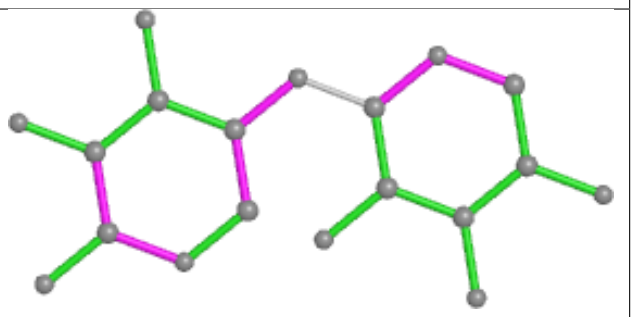


Rings

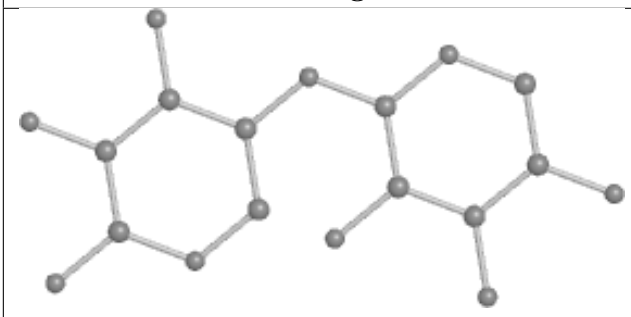
Oligosaccharide Chain G



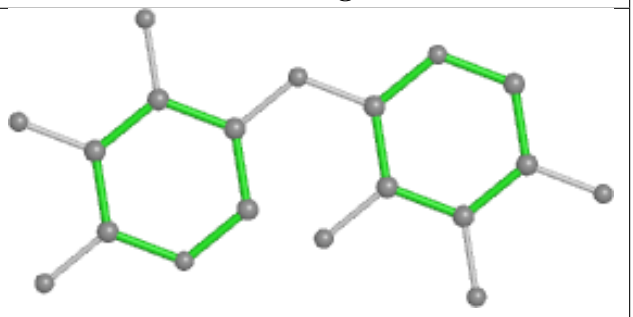
Bond lengths



Bond angles

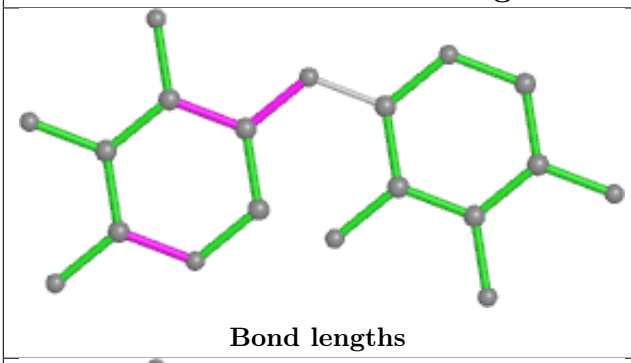


Torsions

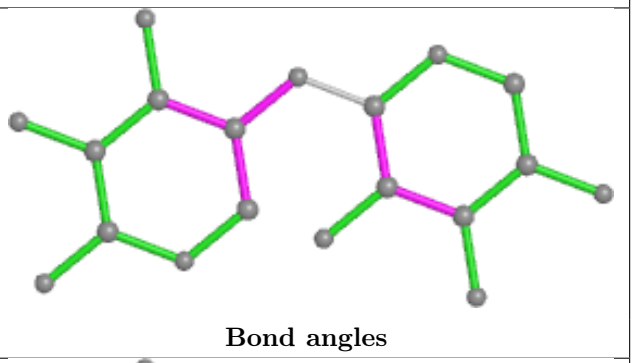


Rings

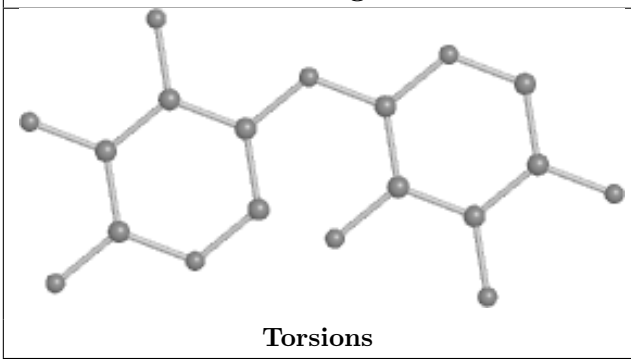
Oligosaccharide Chain H



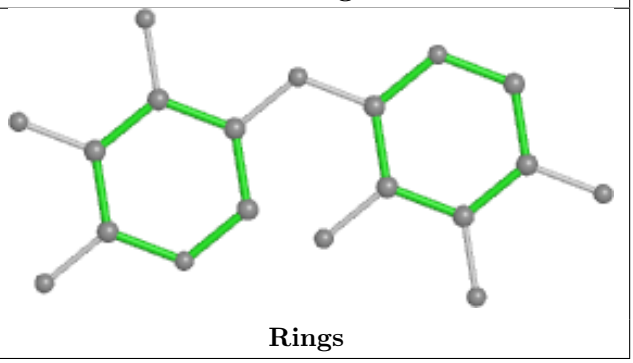
Bond lengths



Bond angles



Torsions



Rings

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	B	2017	-	5,5,5	0.39	0	5,5,5	0.31	0
4	MES	A	2013	-	12,12,12	1.78	3 (25%)	14,16,16	7.07	10 (71%)
5	GOL	C	2018	-	5,5,5	0.31	0	5,5,5	0.30	0
5	GOL	D	2019	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	A	2016	-	5,5,5	0.46	0	5,5,5	0.53	0
4	MES	B	2014	-	12,12,12	1.94	2 (16%)	14,16,16	7.65	10 (71%)
4	MES	D	2015	-	12,12,12	3.99	4 (33%)	14,16,16	7.42	9 (64%)

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	B	2017	-	-	4/4/4/4	-
4	MES	A	2013	-	-	2/6/14/14	0/1/1/1
5	GOL	C	2018	-	-	0/4/4/4	-
5	GOL	D	2019	-	-	0/4/4/4	-
5	GOL	A	2016	-	-	4/4/4/4	-
4	MES	B	2014	-	-	4/6/14/14	0/1/1/1
4	MES	D	2015	-	-	3/6/14/14	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2015	MES	O1S-S	8.87	1.71	1.45
4	D	2015	MES	C8-S	7.01	1.87	1.77
4	D	2015	MES	O2S-S	6.79	1.65	1.45
4	B	2014	MES	C8-S	5.35	1.85	1.77
4	A	2013	MES	C8-S	4.92	1.84	1.77
4	D	2015	MES	O3S-S	3.23	1.59	1.47
4	B	2014	MES	O2S-S	2.27	1.51	1.45
4	A	2013	MES	O1S-S	2.18	1.51	1.45
4	A	2013	MES	O2S-S	2.03	1.51	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2015	MES	O2S-S-C8	-19.83	83.04	106.92
4	B	2014	MES	O1S-S-C8	-19.49	83.45	106.92
4	A	2013	MES	O1S-S-C8	-17.07	86.36	106.92
4	D	2015	MES	O3S-S-O2S	-11.46	83.28	111.27
4	B	2014	MES	O3S-S-O1S	-10.86	84.74	111.27
4	B	2014	MES	O2S-S-C8	10.62	119.70	106.92
4	A	2013	MES	O3S-S-O1S	-10.17	86.44	111.27
4	A	2013	MES	O2S-S-O1S	-9.38	81.50	113.95
4	D	2015	MES	O2S-S-O1S	-9.18	82.16	113.95
4	A	2013	MES	O2S-S-C8	9.14	117.92	106.92
4	B	2014	MES	O2S-S-O1S	-8.69	83.87	113.95
4	B	2014	MES	O3S-S-C8	8.16	118.97	105.77
4	D	2015	MES	O1S-S-C8	6.71	115.00	106.92
4	A	2013	MES	C5-N4-C3	6.66	123.82	108.83
4	A	2013	MES	O3S-S-C8	6.41	116.13	105.77
4	D	2015	MES	O3S-S-C8	5.86	115.25	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2015	MES	O3S-S-O1S	5.66	125.10	111.27
4	D	2015	MES	C5-N4-C3	5.29	120.73	108.83
4	B	2014	MES	C5-N4-C3	5.05	120.20	108.83
4	A	2013	MES	O3S-S-O2S	4.97	123.42	111.27
4	B	2014	MES	C7-N4-C5	3.85	121.09	111.23
4	D	2015	MES	C7-N4-C3	3.44	120.03	111.23
4	D	2015	MES	C7-N4-C5	3.13	119.23	111.23
4	B	2014	MES	C7-N4-C3	2.91	118.67	111.23
4	B	2014	MES	O3S-S-O2S	2.80	118.12	111.27
4	A	2013	MES	C7-N4-C5	2.80	118.39	111.23
4	A	2013	MES	O1-C6-C5	-2.68	105.89	111.80
4	A	2013	MES	C7-N4-C3	2.56	117.79	111.23
4	B	2014	MES	O1-C6-C5	2.11	116.44	111.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2014	MES	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2015	MES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

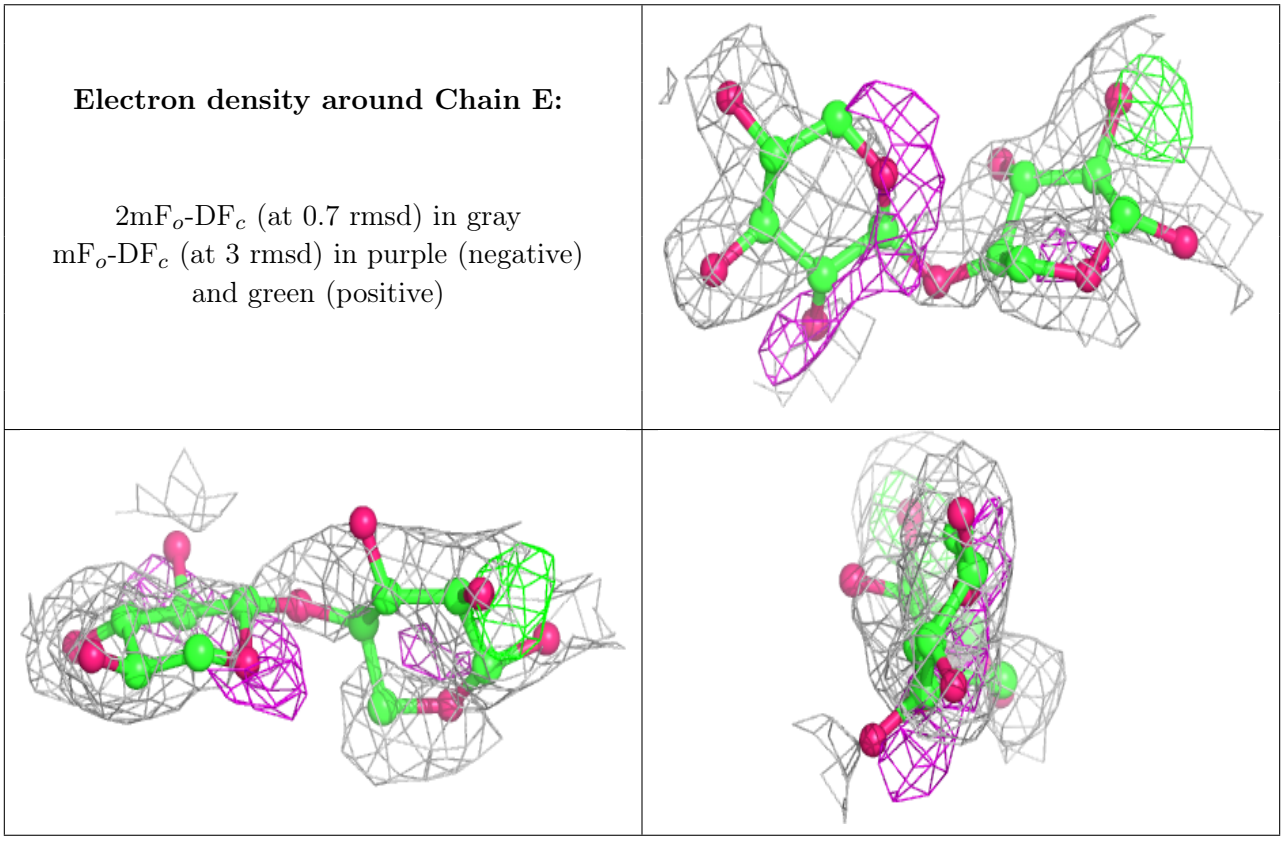
6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

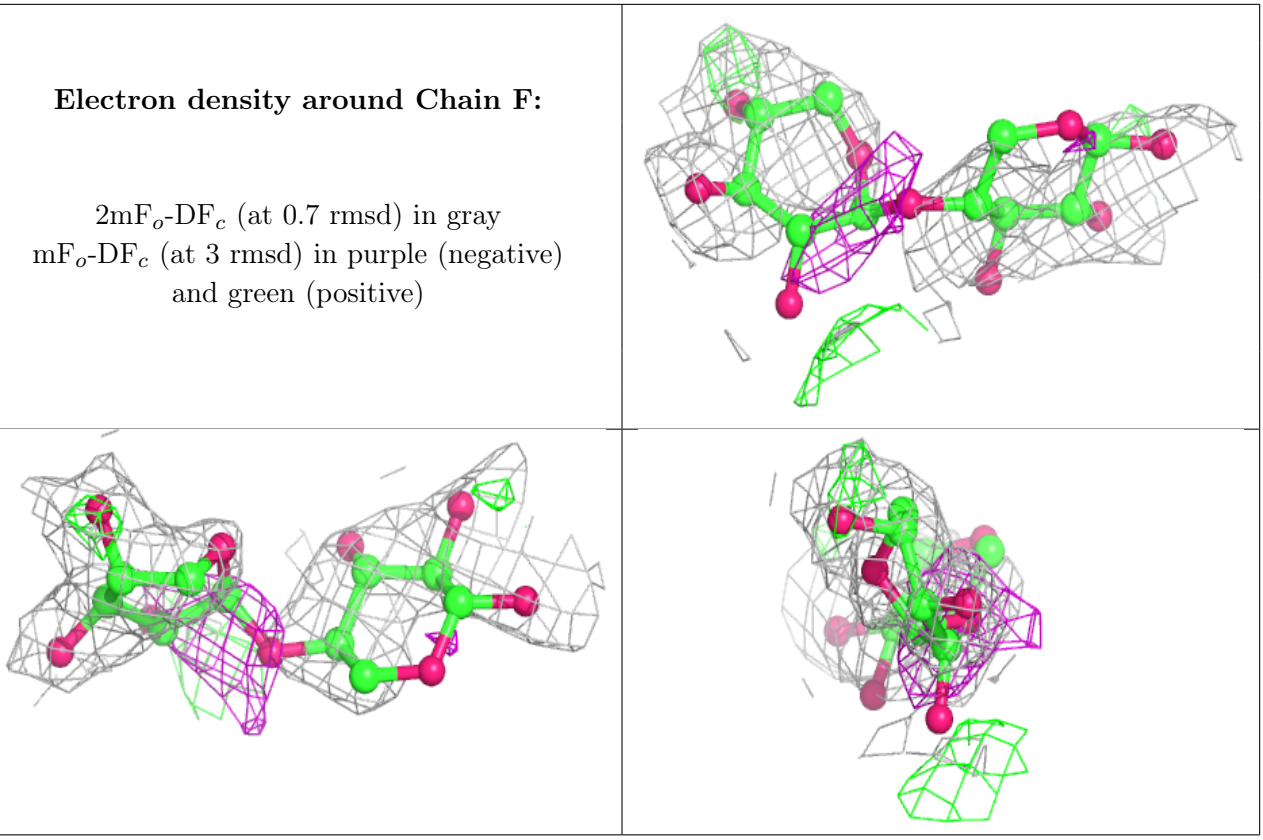
Unable to reproduce the depositors R factor - this section is therefore empty.

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



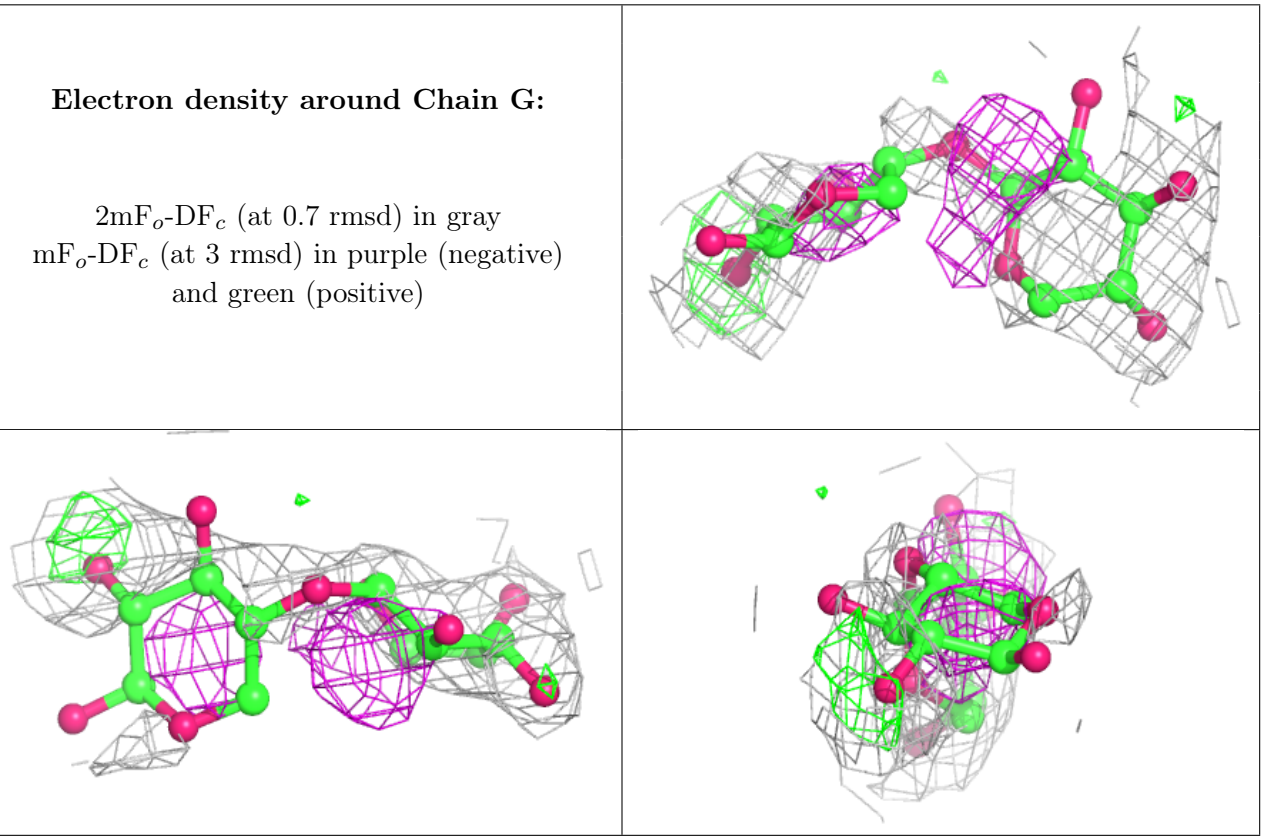
Electron density around Chain F:

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



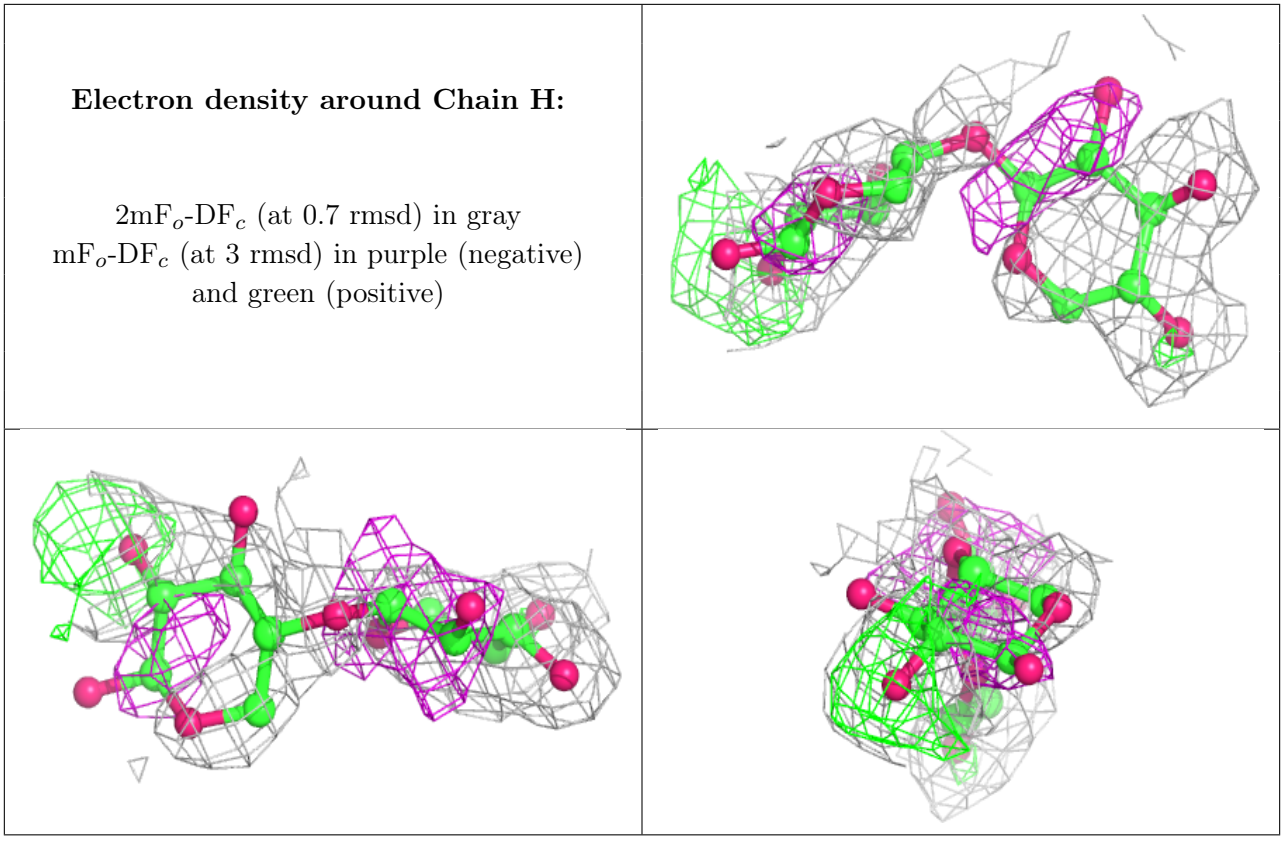
Electron density around Chain G:

$2mF_o$-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

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

6.5 Other polymers

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