Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 11:31 AM EDT

PDB ID	:	2WYS
Title	:	High resolution crystallographic structure of the Clostridium thermocellum N-terminal endo-1,4-beta-D-xylanase 10B (Xyn10B) CBM22-1- GH10 modules complexed with xylohexaose
Authors	:	Najmudin, S.; Pinheiro, B.A.; Romao, M.J.; Prates, J.A.M.; Fontes, C.M.G.A.
Deposited on	:	2009-11-20
Resolution	:	2.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

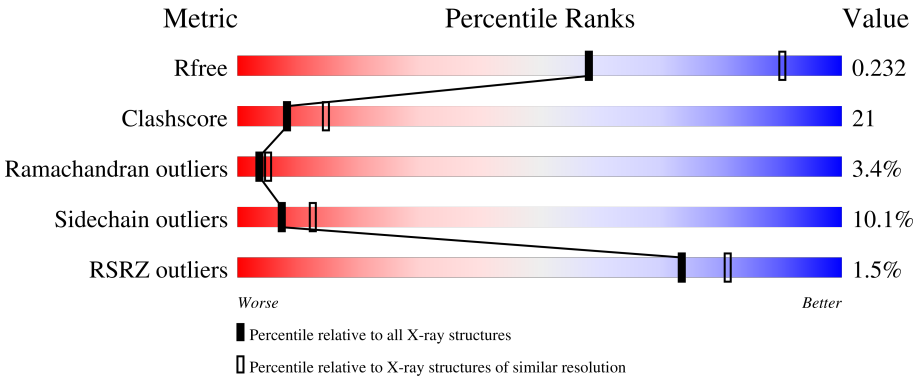
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	540	% 57% 31% 6% • 5%
1	B	540	% 59% 32% 5% •
2	C	2	50% 50%
3	D	3	33% 67%

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	XYP	C	1	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8545 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 ENDO-1,4-BETA-XYLANASE Y.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	Se	0	2	0
			4043	2538	688	799	8	10			
1	B	517	Total	C	N	O	S	Se	0	1	1
			4054	2543	692	802	8	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	expression tag	UNP P51584
A	13	GLY	-	expression tag	UNP P51584
A	14	SER	-	expression tag	UNP P51584
A	15	SER	-	expression tag	UNP P51584
A	16	HIS	-	expression tag	UNP P51584
A	17	HIS	-	expression tag	UNP P51584
A	18	HIS	-	expression tag	UNP P51584
A	19	HIS	-	expression tag	UNP P51584
A	20	HIS	-	expression tag	UNP P51584
A	21	HIS	-	expression tag	UNP P51584
A	22	SER	-	expression tag	UNP P51584
A	23	SER	-	expression tag	UNP P51584
A	24	GLY	-	expression tag	UNP P51584
A	25	LEU	-	expression tag	UNP P51584
A	26	VAL	-	expression tag	UNP P51584
A	27	PRO	-	expression tag	UNP P51584
A	28	ARG	-	expression tag	UNP P51584
A	29	GLY	-	expression tag	UNP P51584
A	30	SER	-	expression tag	UNP P51584
A	31	HIS	-	expression tag	UNP P51584
A	32	MSE	-	expression tag	UNP P51584
A	337	ALA	GLU	engineered mutation	UNP P51584
B	12	MSE	-	expression tag	UNP P51584
B	13	GLY	-	expression tag	UNP P51584
B	14	SER	-	expression tag	UNP P51584

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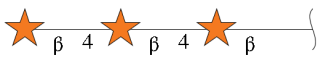
Chain	Residue	Modelled	Actual	Comment	Reference
B	15	SER	-	expression tag	UNP P51584
B	16	HIS	-	expression tag	UNP P51584
B	17	HIS	-	expression tag	UNP P51584
B	18	HIS	-	expression tag	UNP P51584
B	19	HIS	-	expression tag	UNP P51584
B	20	HIS	-	expression tag	UNP P51584
B	21	HIS	-	expression tag	UNP P51584
B	22	SER	-	expression tag	UNP P51584
B	23	SER	-	expression tag	UNP P51584
B	24	GLY	-	expression tag	UNP P51584
B	25	LEU	-	expression tag	UNP P51584
B	26	VAL	-	expression tag	UNP P51584
B	27	PRO	-	expression tag	UNP P51584
B	28	ARG	-	expression tag	UNP P51584
B	29	GLY	-	expression tag	UNP P51584
B	30	SER	-	expression tag	UNP P51584
B	31	HIS	-	expression tag	UNP P51584
B	32	MSE	-	expression tag	UNP P51584
B	337	ALA	GLU	engineered mutation	UNP P51584

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

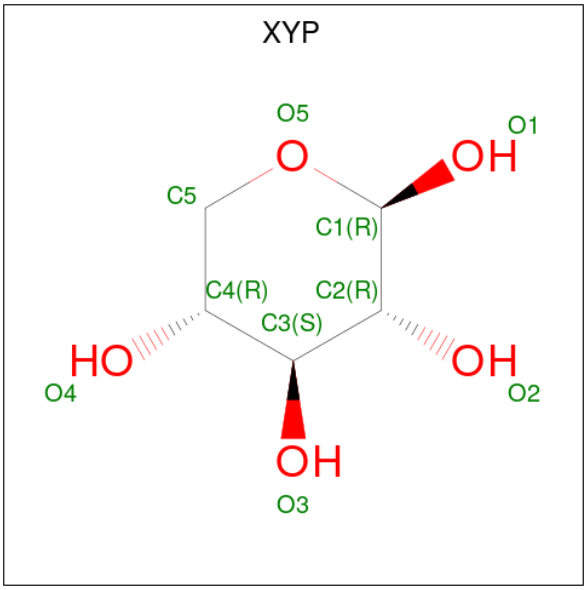
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			18	10	8			

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 4 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$).

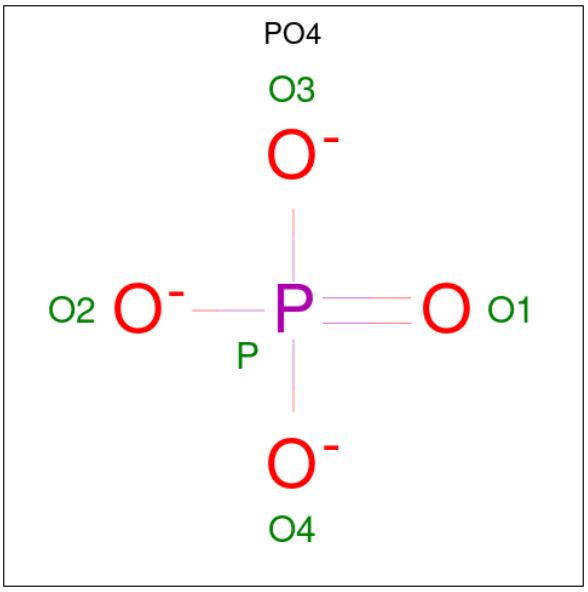


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

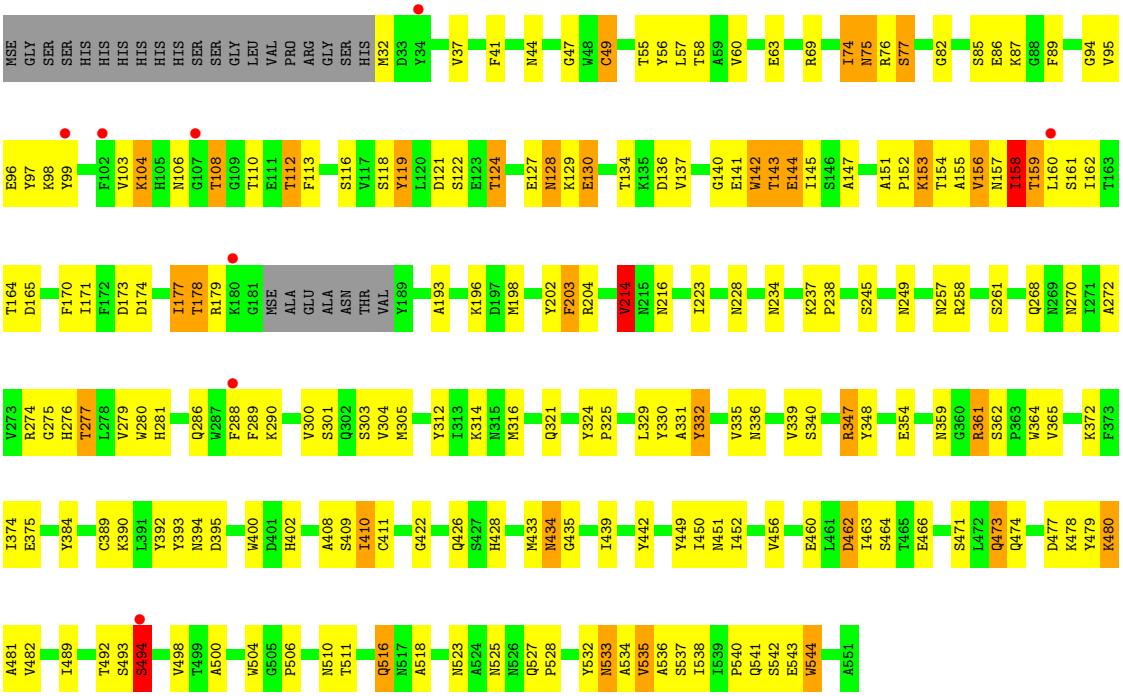
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	151	Total O 151 151	0	0
7	B	227	Total O 227 227	0	0

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.

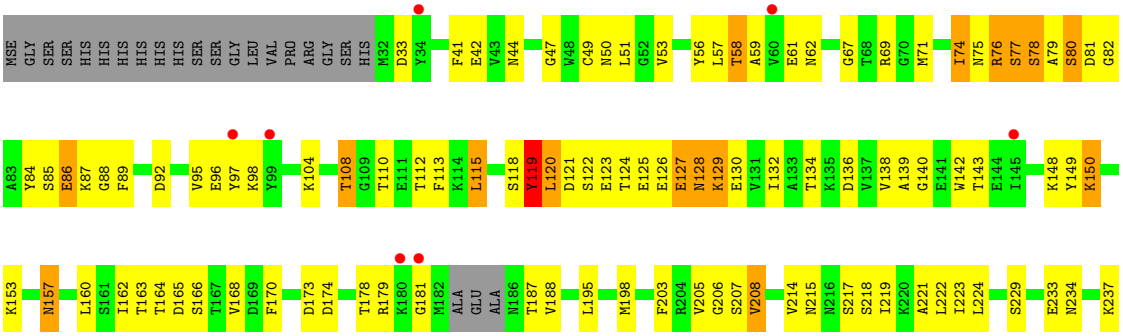
• Molecule 1: ENDO-1,4-BETA-XYLANASE Y

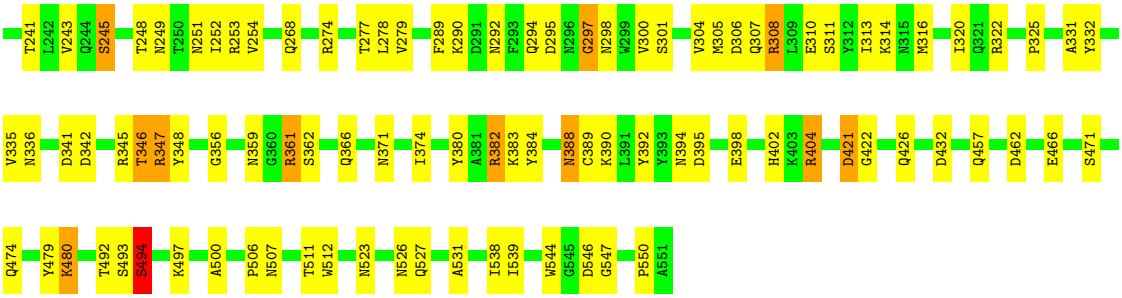
Chain A:



• Molecule 1: ENDO-1,4-BETA-XYLANASE Y

Chain B:





• Molecule 2: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose

Chain C:

• Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.70Å 173.70Å 135.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.85 – 2.75 86.85 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.85-2.75) 98.9 (86.85-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.236 0.187 , 0.232	Depositor DCC
R_{free} test set	3077 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8545	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PO4, XYP

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	0.99	2/4128 (0.0%)	0.94	5/5591 (0.1%)
1	B	1.06	5/4135 (0.1%)	0.98	5/5602 (0.1%)
All	All	1.03	7/8263 (0.1%)	0.96	10/11193 (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	A	0	1
1	B	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	SER	C-N	-10.25	1.10	1.34
1	B	389	CYS	CB-SG	-7.09	1.70	1.82
1	B	86	GLU	CG-CD	6.00	1.60	1.51
1	B	348	TYR	CE2-CZ	5.56	1.45	1.38
1	B	86	GLU	CB-CG	5.51	1.62	1.52
1	B	42	GLU	CB-CG	5.31	1.62	1.52
1	A	473	GLN	CG-CD	5.13	1.62	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	494	SER	O-C-N	6.78	133.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	432	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	494	SER	CA-C-N	-5.89	104.23	117.20
1	A	258	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	274	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	462	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	404	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	308	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	SER	Peptide
1	B	494	SER	Peptide
1	B	80	SER	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	4043	0	3849	173	0
1	B	4054	0	3848	158	0
2	C	18	0	0	3	0
3	D	28	0	0	2	0
4	A	10	0	0	3	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	151	0	0	26	0
7	B	227	0	0	30	0
All	All	8545	0	7697	335	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 21.

All (335) 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:155:ALA:HA	7:A:2033:HOH:O	1.17	1.34
4:A:1001:XYP:O4	2:C:1:XYP:C5	1.81	1.28
1:B:157:ASN:HB3	7:B:2018:HOH:O	1.39	1.19
1:B:492:THR:HG22	1:B:493:SER:H	1.05	1.19
1:A:270:ASN:HB3	7:A:2068:HOH:O	1.44	1.18
1:B:241:THR:HB	1:B:316:MSE:HE1	1.16	1.15
1:A:119:TYR:HE1	1:A:128:ASN:HB3	1.10	1.12
1:B:241:THR:HB	1:B:316:MSE:CE	1.80	1.12
1:A:85:SER:OG	1:A:87:LYS:HE2	1.51	1.10
1:B:493:SER:HA	1:B:494:SER:CB	1.80	1.10
1:B:49:CYS:HA	7:B:2005:HOH:O	1.49	1.09
1:A:119:TYR:CE1	1:A:128:ASN:HB3	1.88	1.08
1:A:158:ILE:CG2	1:A:159:THR:H	1.67	1.08
1:B:118:SER:HB3	1:B:129:LYS:HE2	1.34	1.05
1:B:85:SER:OG	1:B:87:LYS:HE2	1.58	1.02
1:A:289:PHE:HA	1:A:305:MSE:CE	1.89	1.02
1:A:119:TYR:HE2	1:A:152:PRO:HD2	1.25	1.00
1:A:121:ASP:HB3	1:A:124:THR:OG1	1.62	1.00
1:A:158:ILE:HG22	1:A:159:THR:N	1.78	0.96
1:A:434:ASN:HD22	1:A:435:GLY:H	1.04	0.95
1:A:288:PHE:O	1:A:305:MSE:HE1	1.66	0.95
1:B:361:ARG:HD3	7:B:2136:HOH:O	1.64	0.94
1:A:312:TYR:CE1	1:A:316:MSE:HE3	2.04	0.93
1:B:492:THR:HG22	1:B:493:SER:N	1.82	0.93
1:B:58:THR:HG22	7:B:2010:HOH:O	1.68	0.91
1:B:493:SER:HA	1:B:494:SER:HB3	1.49	0.91
1:A:289:PHE:HA	1:A:305:MSE:HE1	1.53	0.91
1:A:158:ILE:CG2	1:A:159:THR:N	2.29	0.91
1:A:158:ILE:HG22	1:A:159:THR:H	1.30	0.90
1:B:120:LEU:HD12	1:B:121:ASP:N	1.87	0.90
3:D:2:XYP:O4	3:D:3:XYP:C2	2.22	0.88
1:B:471:SER:H	1:B:474:GLN:HE21	1.21	0.88
1:A:492:THR:HG22	1:A:493:SER:H	1.36	0.88
1:A:141:GLU:HG2	7:A:2030:HOH:O	1.71	0.87
1:A:493:SER:HA	1:A:494:SER:CB	2.03	0.87
1:A:119:TYR:CE2	1:A:152:PRO:HD2	2.09	0.87
1:A:119:TYR:HE1	1:A:128:ASN:CB	1.88	0.86
1:A:270:ASN:HB2	7:A:2069:HOH:O	1.72	0.86
4:A:1001:XYP:C4	2:C:1:XYP:C5	2.53	0.86
1:B:289:PHE:O	1:B:300:VAL:HG13	1.75	0.86
1:A:516:GLN:H	1:A:516:GLN:HE21	1.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:HA	1:A:305:MSE:HE3	1.58	0.83
1:A:44:ASN:OD1	1:A:325:PRO:HD2	1.79	0.83
3:D:2:XYP:C4	3:D:3:XYP:C1	2.58	0.82
1:A:129:LYS:HG2	1:A:130:GLU:H	1.44	0.81
1:A:89:PHE:CE2	1:A:214:VAL:HG22	2.17	0.80
1:B:119:TYR:HD1	1:B:120:LEU:N	1.80	0.80
1:B:128:ASN:O	1:B:129:LYS:HD2	1.82	0.79
1:B:122:SER:HA	7:B:2032:HOH:O	1.83	0.78
1:A:136:ASP:HB2	7:A:2029:HOH:O	1.83	0.78
1:A:158:ILE:HG23	1:A:159:THR:H	1.46	0.78
1:A:96:GLU:O	7:A:2021:HOH:O	2.02	0.78
1:A:329:LEU:O	1:A:389:CYS:HB2	1.82	0.78
1:B:241:THR:CB	1:B:316:MSE:CE	2.61	0.77
1:B:380:TYR:HE1	7:B:2146:HOH:O	1.66	0.77
1:A:193:ALA:HA	1:A:198:MSE:CE	2.16	0.76
1:A:347:ARG:HH11	1:A:348:TYR:HE1	1.34	0.76
1:A:155:ALA:C	1:A:156:VAL:HG22	2.05	0.76
1:A:434:ASN:ND2	1:A:435:GLY:H	1.83	0.75
1:A:434:ASN:HD22	1:A:435:GLY:N	1.82	0.75
1:B:41:PHE:O	1:B:69:ARG:HD3	1.85	0.75
1:B:241:THR:CB	1:B:316:MSE:HE1	2.08	0.75
1:B:251:ASN:HB3	7:B:2085:HOH:O	1.87	0.75
1:B:493:SER:HA	1:B:494:SER:OG	1.87	0.74
1:B:119:TYR:HD1	1:B:120:LEU:H	1.35	0.74
1:B:290:LYS:HA	1:B:298:ASN:O	1.88	0.74
1:A:478:LYS:O	1:A:482:VAL:HG23	1.88	0.73
1:B:492:THR:CG2	1:B:493:SER:H	1.88	0.73
1:B:254:VAL:HB	1:B:316:MSE:HE2	1.71	0.73
1:B:245:SER:HB3	7:B:2083:HOH:O	1.89	0.73
1:B:119:TYR:CD1	1:B:120:LEU:N	2.57	0.72
1:B:44:ASN:OD1	1:B:325:PRO:HD2	1.91	0.71
1:B:134:THR:O	7:B:2033:HOH:O	2.08	0.71
1:A:121:ASP:HA	7:A:2033:HOH:O	1.89	0.71
1:A:312:TYR:CZ	1:A:316:MSE:HE3	2.26	0.71
1:A:41:PHE:O	1:A:69:ARG:HD3	1.91	0.70
1:A:85:SER:OG	1:A:87:LYS:CE	2.35	0.70
1:A:234:ASN:HA	1:A:237:LYS:HD2	1.72	0.70
1:A:527[A]:GLN:OE1	7:A:2140:HOH:O	2.09	0.70
1:B:395:ASP:O	1:B:426:GLN:HG3	1.92	0.70
1:A:112:THR:HG23	1:A:136:ASP:OD1	1.92	0.70
1:B:278:LEU:HD13	1:B:313:ILE:HG12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HD3	7:B:2132:HOH:O	1.91	0.70
1:B:493:SER:CA	1:B:494:SER:CB	2.67	0.70
1:B:471:SER:H	1:B:474:GLN:NE2	1.89	0.70
1:A:137:VAL:HG22	1:A:143:THR:HG21	1.74	0.70
1:A:301:SER:HB3	1:A:304:VAL:HG23	1.74	0.69
1:B:108:THR:HA	7:B:2028:HOH:O	1.94	0.68
1:A:533:ASN:HA	1:A:536:ALA:HB3	1.76	0.68
1:A:144:GLU:HG3	1:A:145:ILE:N	2.09	0.68
1:A:312:TYR:CE1	1:A:316:MSE:CE	2.76	0.67
1:B:215:ASN:HB3	7:B:2066:HOH:O	1.94	0.67
1:B:493:SER:HB2	7:B:2208:HOH:O	1.94	0.66
1:A:493:SER:HA	1:A:494:SER:HB3	1.76	0.66
1:A:155:ALA:CA	7:A:2033:HOH:O	1.99	0.66
1:B:59:ALA:HB2	1:B:71:MSE:HE1	1.78	0.65
1:B:457:GLN:HG2	1:B:500:ALA:HB3	1.78	0.65
1:B:74:ILE:HG13	1:B:75:ASN:N	2.10	0.64
1:A:121:ASP:CB	1:A:124:THR:OG1	2.40	0.63
1:A:493:SER:HA	1:A:494:SER:OG	1.98	0.63
1:B:76:ARG:HH12	1:B:164:THR:HG23	1.64	0.63
1:A:155:ALA:O	1:A:156:VAL:HG22	1.98	0.63
1:A:89:PHE:CE2	1:A:214:VAL:CG2	2.82	0.62
1:B:241:THR:OG1	1:B:316:MSE:HE3	2.00	0.62
1:A:155:ALA:C	1:A:156:VAL:CG2	2.67	0.62
1:A:314:LYS:HG3	1:A:384:TYR:CE1	2.34	0.62
4:A:1001:XYP:O4	2:C:1:XYP:C4	2.47	0.62
1:A:193:ALA:HA	1:A:198:MSE:HE3	1.80	0.61
1:B:224:LEU:HB2	7:B:2071:HOH:O	1.99	0.61
1:A:433:MSE:CE	1:A:477:ASP:HB3	2.29	0.61
1:A:55:THR:HG21	1:A:82:GLY:O	2.01	0.60
1:B:347:ARG:HH11	1:B:347:ARG:HG3	1.66	0.60
1:B:292:ASN:HB3	7:B:2103:HOH:O	1.99	0.60
1:B:221:ALA:O	7:B:2071:HOH:O	2.16	0.60
1:A:533:ASN:O	1:A:534:ALA:C	2.36	0.60
1:A:127:GLU:HG3	1:B:126:GLU:OE1	2.02	0.60
1:B:58:THR:HG23	1:B:322:ARG:NH1	2.17	0.60
1:A:49:CYS:HB3	1:A:257:ASN:OD1	2.03	0.59
1:A:516:GLN:HE21	1:A:516:GLN:N	1.97	0.59
1:B:347:ARG:HH11	1:B:347:ARG:CG	2.15	0.59
1:A:237:LYS:HE2	1:A:280:TRP:CZ3	2.37	0.59
1:B:234:ASN:HA	1:B:237:LYS:HD2	1.85	0.58
1:B:41:PHE:CD1	1:B:71:MSE:HE3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:VAL:O	1:B:308:ARG:HG3	2.04	0.58
1:B:120:LEU:HD12	1:B:121:ASP:H	1.65	0.58
1:B:546:ASP:N	7:B:2226:HOH:O	2.22	0.58
1:A:162:ILE:HG22	1:A:170:PHE:CZ	2.39	0.58
1:A:359:ASN:HB2	1:A:361:ARG:HH21	1.69	0.58
1:A:44:ASN:OD1	1:A:325:PRO:CD	2.52	0.57
1:B:346:THR:CG2	7:B:2046:HOH:O	2.52	0.57
1:B:361:ARG:CD	7:B:2136:HOH:O	2.35	0.57
1:A:492:THR:HG22	1:A:493:SER:N	2.15	0.57
1:B:98:LYS:HB2	1:B:148:LYS:HE3	1.85	0.57
1:B:96:GLU:HA	1:B:149:TYR:O	2.06	0.56
1:B:480:LYS:HG2	1:B:538:ILE:HD11	1.88	0.56
1:A:129:LYS:HG2	1:A:130:GLU:N	2.19	0.56
1:B:249:ASN:O	1:B:307:GLN:HB3	2.06	0.56
1:B:314:LYS:HD2	1:B:384:TYR:CZ	2.40	0.56
1:B:241:THR:CB	1:B:316:MSE:HE3	2.33	0.55
1:A:442:TYR:CE2	1:A:482:VAL:HG13	2.41	0.55
1:A:76:ARG:HH22	1:A:164:THR:H	1.53	0.55
1:B:49:CYS:O	1:B:84:TYR:N	2.33	0.55
1:A:433:MSE:HE1	1:A:477:ASP:C	2.28	0.54
1:B:217:SER:HA	7:B:2020:HOH:O	2.06	0.54
1:B:84:TYR:HA	1:B:160:LEU:O	2.08	0.54
1:A:463:ILE:HG22	1:A:463:ILE:O	2.07	0.54
1:A:94:GLY:N	1:A:151:ALA:O	2.38	0.54
1:B:112:THR:O	1:B:164:THR:HA	2.07	0.54
1:B:233:GLU:O	1:B:237:LYS:HE3	2.08	0.53
1:A:63:GLU:O	1:A:142:TRP:HZ2	1.90	0.53
1:B:356:GLY:H	1:B:366:GLN:HB2	1.74	0.52
1:B:61:GLU:HA	7:B:2012:HOH:O	2.09	0.52
1:A:37:VAL:HB	1:A:177:ILE:HG13	1.91	0.52
1:B:95:VAL:HB	1:B:97:TYR:CE2	2.44	0.52
1:B:388:ASN:HB3	7:B:2153:HOH:O	2.09	0.52
1:A:300:VAL:CG2	1:A:305:MSE:HG2	2.40	0.52
1:B:336:ASN:OD1	1:B:394:ASN:HB3	2.09	0.52
1:B:56:TYR:O	1:B:57:LEU:HD12	2.10	0.52
1:A:76:ARG:NH2	1:A:164:THR:H	2.08	0.51
1:B:49:CYS:N	1:B:84:TYR:O	2.39	0.51
1:A:272:ALA:HB1	1:A:330:TYR:CD2	2.45	0.51
1:B:88:GLY:HA3	1:B:215:ASN:OD1	2.10	0.51
1:B:392:TYR:CE2	1:B:422:GLY:HA3	2.46	0.51
1:A:134:THR:HG22	7:A:2028:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:OD1	1:A:174:ASP:N	2.44	0.51
1:B:547:GLY:O	1:B:550:PRO:HD3	2.12	0.50
1:A:157:ASN:O	1:A:158:ILE:O	2.30	0.50
1:A:339:VAL:HG23	1:A:393:TYR:OH	2.11	0.50
1:B:96:GLU:HG3	7:B:2022:HOH:O	2.10	0.50
1:B:493:SER:CA	1:B:494:SER:HB3	2.29	0.50
1:B:290:LYS:NZ	1:B:295:ASP:O	2.41	0.50
1:B:471:SER:N	1:B:474:GLN:HE21	2.01	0.50
1:A:347:ARG:NH1	1:A:348:TYR:HE1	2.08	0.50
1:B:166:SER:OG	1:B:168:VAL:HG12	2.12	0.49
1:A:354:GLU:HB2	1:A:361:ARG:HG3	1.94	0.49
1:A:450:ILE:C	1:A:452:ILE:H	2.16	0.49
1:B:342:ASP:HA	7:B:2128:HOH:O	2.13	0.49
1:A:439:ILE:HD13	1:A:481:ALA:HB1	1.94	0.49
1:A:56:TYR:HE2	1:A:58:THR:HB	1.77	0.49
1:A:408:ALA:HB2	1:A:449:TYR:CE1	2.47	0.49
1:B:195:LEU:HB3	1:B:205:VAL:HG11	1.94	0.49
1:B:206:GLY:HA3	1:B:229:SER:HB3	1.95	0.49
1:B:279:VAL:HB	1:B:335:VAL:HG22	1.93	0.49
1:B:110:THR:CG2	1:B:138:VAL:HG12	2.43	0.49
1:B:207:SER:OG	1:B:208:VAL:N	2.46	0.49
1:A:112:THR:HG22	7:A:2028:HOH:O	2.12	0.48
1:B:187:THR:HA	7:B:2053:HOH:O	2.12	0.48
1:A:348:TYR:CD1	1:A:348:TYR:N	2.82	0.48
1:B:398:GLU:O	1:B:404:ARG:HB2	2.14	0.48
1:A:156:VAL:O	1:A:157:ASN:HB3	2.14	0.48
1:B:538:ILE:HG22	1:B:539:ILE:HD13	1.94	0.48
1:A:119:TYR:CD2	1:A:155:ALA:HB1	2.49	0.48
1:B:58:THR:HG23	1:B:322:ARG:HH12	1.77	0.48
1:B:119:TYR:O	1:B:127:GLU:OE1	2.31	0.48
1:A:336:ASN:OD1	1:A:394:ASN:HB3	2.13	0.48
1:B:181:GLY:HA3	7:B:2051:HOH:O	2.14	0.48
1:B:50:ASN:CG	1:B:50:ASN:O	2.52	0.47
1:B:305:MSE:O	1:B:306:ASP:C	2.50	0.47
1:B:289:PHE:CE1	1:B:305:MSE:HE2	2.49	0.47
1:B:62:ASN:HA	1:B:67:GLY:O	2.14	0.47
1:A:157:ASN:N	7:A:2034:HOH:O	2.48	0.47
1:A:428:HIS:HD1	1:A:462:ASP:CG	2.16	0.47
1:B:395:ASP:C	1:B:426:GLN:HG3	2.34	0.47
1:B:342:ASP:O	1:B:345:ARG:HB2	2.15	0.47
1:A:456:VAL:O	1:A:498:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASP:O	1:B:163:THR:HG22	2.15	0.47
1:B:162:ILE:HG22	1:B:170:PHE:CE1	2.49	0.47
1:A:108:THR:HA	7:A:2026:HOH:O	2.15	0.47
1:A:238:PRO:HD3	1:A:277:THR:O	2.14	0.47
1:A:480:LYS:HB2	1:A:534:ALA:HB1	1.96	0.47
1:B:92:ASP:HB2	1:B:95:VAL:CG2	2.45	0.47
1:B:292:ASN:ND2	1:B:294:GLN:HG3	2.30	0.47
1:B:300:VAL:HG23	1:B:301:SER:O	2.15	0.47
1:B:129:LYS:O	1:B:130:GLU:CG	2.63	0.46
1:A:152:PRO:O	1:A:154:THR:N	2.48	0.46
1:A:178:THR:HG23	7:A:2024:HOH:O	2.15	0.46
1:A:544:TRP:CD1	1:A:544:TRP:N	2.83	0.46
1:A:119:TYR:CE1	1:A:128:ASN:CB	2.74	0.46
1:A:410:ILE:HG22	1:A:411:CYS:N	2.31	0.46
1:A:202:TYR:HA	7:A:2043:HOH:O	2.16	0.46
1:A:528:PRO:HB3	1:A:532:TYR:CD2	2.51	0.46
1:A:279:VAL:HG13	1:A:364:TRP:CE2	2.51	0.46
1:B:219:ILE:O	1:B:223:ILE:HG12	2.16	0.46
1:A:158:ILE:O	1:A:159:THR:CB	2.64	0.45
1:A:348:TYR:N	1:A:348:TYR:HD1	2.14	0.45
1:A:162:ILE:CG2	1:A:170:PHE:CE1	2.98	0.45
1:A:103:VAL:HB	1:A:113:PHE:CE2	2.52	0.45
1:A:473:GLN:HB3	7:A:2125:HOH:O	2.15	0.45
1:B:222:LEU:HD13	1:B:526:ASN:HB3	1.98	0.45
1:A:203:PHE:HB2	1:A:500:ALA:HA	1.98	0.45
1:A:433:MSE:HE1	1:A:477:ASP:HB3	1.99	0.45
1:A:523:ASN:OD1	1:A:525:ASN:N	2.40	0.45
1:A:400:TRP:CE2	1:A:402:HIS:HE1	2.35	0.45
1:B:252:ILE:N	1:B:311:SER:OG	2.40	0.45
1:A:160:LEU:HD12	1:A:161:SER:H	1.81	0.45
1:B:492:THR:CG2	1:B:493:SER:N	2.53	0.45
1:A:392:TYR:CE2	1:A:422:GLY:HA3	2.51	0.45
1:A:541:GLN:HA	1:A:544:TRP:CE2	2.52	0.45
1:B:76:ARG:HH22	1:B:164:THR:H	1.65	0.45
1:A:286:GLN:NE2	1:A:290:LYS:NZ	2.65	0.45
1:A:493:SER:HB2	7:A:2132:HOH:O	2.17	0.45
1:B:120:LEU:HD12	1:B:120:LEU:C	2.37	0.45
1:B:523:ASN:ND2	1:B:527[B]:GLN:HB2	2.32	0.45
1:A:119:TYR:OH	1:A:152:PRO:HG2	2.17	0.44
1:B:82:GLY:HA3	1:B:163:THR:HG22	1.99	0.44
1:A:179:ARG:HB2	7:A:2021:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:HB3	1:A:365:VAL:HB	2.00	0.44
1:B:316:MSE:O	1:B:320:ILE:HG13	2.16	0.44
1:A:335:VAL:HG21	1:A:374:ILE:HG23	1.99	0.44
1:A:460:GLU:HG2	1:A:504:TRP:CZ3	2.52	0.44
1:B:78:SER:C	1:B:80:SER:H	2.21	0.44
1:B:78:SER:O	1:B:80:SER:N	2.50	0.44
1:A:74:ILE:HG13	1:A:75:ASN:N	2.32	0.44
1:A:156:VAL:N	7:A:2033:HOH:O	2.49	0.44
1:A:162:ILE:HG22	1:A:170:PHE:CE1	2.52	0.44
1:A:204:ARG:HG2	1:A:228:ASN:OD1	2.17	0.44
1:A:493:SER:CA	1:A:494:SER:CB	2.88	0.44
1:B:243:VAL:N	1:B:253:ARG:O	2.49	0.44
1:A:449:TYR:HA	1:A:452:ILE:HD12	2.00	0.44
1:A:471:SER:OG	1:A:474:GLN:HG3	2.18	0.44
1:A:493:SER:CB	7:A:2132:HOH:O	2.65	0.44
1:B:341:ASP:O	1:B:402:HIS:HE1	2.01	0.44
1:B:162:ILE:HG22	1:B:170:PHE:CZ	2.53	0.43
1:B:494:SER:HB2	1:B:497:LYS:HE2	2.00	0.43
1:A:98:LYS:O	1:A:177:ILE:HA	2.18	0.43
1:B:85:SER:OG	1:B:87:LYS:CE	2.49	0.43
1:B:382:ARG:NH2	1:B:421:ASP:OD1	2.45	0.43
1:A:159:THR:O	1:A:159:THR:HG22	2.14	0.43
1:A:193:ALA:CA	1:A:198:MSE:HE3	2.48	0.43
1:A:198:MSE:HE2	1:A:544:TRP:CH2	2.53	0.43
1:B:383:LYS:HD3	1:B:384:TYR:CZ	2.54	0.43
1:B:479:TYR:CD1	1:B:531:ALA:HB1	2.53	0.43
1:B:47:GLY:O	1:B:85:SER:CB	2.66	0.43
1:B:41:PHE:HD1	1:B:71:MSE:HE3	1.83	0.43
1:B:507:ASN:HB2	1:B:523:ASN:O	2.18	0.43
1:A:395:ASP:O	1:A:426:GLN:HG3	2.18	0.43
1:A:347:ARG:HB3	1:A:348:TYR:CD1	2.54	0.43
1:A:463:ILE:HD12	1:A:479:TYR:CD2	2.54	0.43
1:A:489:ILE:O	7:A:2129:HOH:O	2.21	0.43
1:B:331:ALA:HA	1:B:390:LYS:O	2.19	0.43
1:A:56:TYR:O	1:A:57:LEU:HD12	2.18	0.43
1:A:216:ASN:N	7:A:2049:HOH:O	2.52	0.43
1:B:120:LEU:CD1	1:B:121:ASP:N	2.72	0.42
1:B:44:ASN:HA	7:B:2002:HOH:O	2.19	0.42
1:A:118:SER:HB3	1:A:129:LYS:HG3	2.00	0.42
1:A:152:PRO:C	1:A:154:THR:H	2.22	0.42
1:A:193:ALA:CA	1:A:198:MSE:CE	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527[A]:GLN:NE2	7:A:2141:HOH:O	2.52	0.42
1:B:104:LYS:HD2	1:B:142:TRP:NE1	2.34	0.42
1:A:97:TYR:HB2	1:A:99:TYR:CE2	2.55	0.42
1:A:464:SER:C	1:A:466:GLU:H	2.23	0.42
1:B:404:ARG:HD3	7:B:2160:HOH:O	2.20	0.42
1:B:294:GLN:HE21	1:B:294:GLN:HA	1.85	0.42
1:B:341:ASP:O	1:B:402:HIS:CE1	2.72	0.42
1:B:119:TYR:O	1:B:127:GLU:CD	2.58	0.42
1:A:237:LYS:HE2	1:A:280:TRP:HZ3	1.80	0.41
1:B:110:THR:HG22	1:B:138:VAL:HG12	2.02	0.41
1:A:56:TYR:CE2	1:A:58:THR:HB	2.54	0.41
1:A:170:PHE:O	1:A:171:ILE:HG12	2.20	0.41
1:B:198:MSE:HG2	1:B:544:TRP:CE2	2.56	0.41
1:A:196:LYS:HB2	1:A:228:ASN:ND2	2.35	0.41
1:A:300:VAL:HG21	1:A:305:MSE:HE2	2.02	0.41
1:A:535:VAL:HA	1:A:538:ILE:HD12	2.02	0.41
1:B:50:ASN:N	7:B:2005:HOH:O	2.21	0.41
1:B:136:ASP:O	7:B:2035:HOH:O	2.22	0.41
1:B:471:SER:OG	1:B:474:GLN:HG3	2.20	0.41
1:A:223:ILE:H	1:A:223:ILE:HG12	1.70	0.41
1:A:245:SER:HB2	7:A:2057:HOH:O	2.20	0.41
1:A:541:GLN:C	1:A:543:GLU:H	2.23	0.41
1:A:275:GLY:HA3	1:A:332:TYR:CD1	2.55	0.41
1:A:510:ASN:HB3	7:A:2135:HOH:O	2.20	0.41
1:A:540:PRO:O	1:A:543:GLU:HB2	2.20	0.41
1:B:113:PHE:HE2	1:B:170:PHE:CD1	2.39	0.41
1:B:292:ASN:OD1	1:B:297:GLY:HA3	2.21	0.41
1:B:49:CYS:HB3	1:B:84:TYR:CE2	2.54	0.41
1:B:104:LYS:HD2	1:B:142:TRP:CD1	2.55	0.41
1:B:127:GLU:HB3	1:B:128:ASN:H	1.73	0.41
1:B:149:TYR:CG	1:B:150:LYS:N	2.88	0.41
1:A:47:GLY:HA2	1:A:324:TYR:OH	2.21	0.41
1:A:281:HIS:HB2	1:A:362:SER:HA	2.03	0.41
1:B:76:ARG:HH12	1:B:164:THR:CG2	2.32	0.41
1:B:115:LEU:O	1:B:132:ILE:HG13	2.21	0.41
1:B:162:ILE:CG2	1:B:170:PHE:CE1	3.03	0.41
1:B:53:VAL:O	1:B:53:VAL:HG22	2.21	0.41
1:A:75:ASN:ND2	1:A:75:ASN:O	2.54	0.40
1:A:112:THR:O	1:A:164:THR:HA	2.22	0.40
1:A:276:HIS:ND1	1:A:277:THR:HB	2.36	0.40
1:A:286:GLN:HE21	1:A:290:LYS:NZ	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:O	1:B:311:SER:C	2.59	0.40
1:A:204:ARG:HG2	1:A:204:ARG:HH11	1.87	0.40
1:A:537:SER:HB3	7:A:2143:HOH:O	2.21	0.40
1:B:371:ASN:HB3	1:B:374:ILE:HD12	2.03	0.40
1:A:331:ALA:HA	1:A:390:LYS:O	2.21	0.40
1:B:173:ASP:OD1	1:B:174:ASP:N	2.55	0.40
1:B:129:LYS:O	1:B:130:GLU:HG2	2.21	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	510/540 (94%)	427 (84%)	64 (12%)	19 (4%)	3 4
1	B	514/540 (95%)	451 (88%)	47 (9%)	16 (3%)	4 6
All	All	1024/1080 (95%)	878 (86%)	111 (11%)	35 (3%)	3 5

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	158	ILE
1	A	159	THR
1	A	494	SER
1	B	127	GLU
1	B	494	SER
1	A	153	LYS
1	A	542	SER
1	B	76	ARG
1	B	79	ALA
1	B	123	GLU

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Mol	Chain	Res	Type
1	B	125	GLU
1	B	139	ALA
1	B	140	GLY
1	B	153	LYS
1	B	188	VAL
1	B	214	VAL
1	A	142	TRP
1	A	147	ALA
1	A	214	VAL
1	A	249	ASN
1	B	119	TYR
1	A	451	ASN
1	A	506	PRO
1	A	544	TRP
1	B	77	SER
1	B	506	PRO
1	A	104	LYS
1	A	77	SER
1	A	410	ILE
1	B	165	ASP
1	A	140	GLY
1	A	74	ILE
1	A	518	ALA
1	B	297	GLY

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	434/443 (98%)	387 (89%)	47 (11%)	6 10
1	B	433/443 (98%)	392 (90%)	41 (10%)	8 15
All	All	867/886 (98%)	779 (90%)	88 (10%)	7 12

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32[A]	MSE
1	A	32[B]	MSE
1	A	49	CYS
1	A	60	VAL
1	A	77	SER
1	A	86	GLU
1	A	95	VAL
1	A	104	LYS
1	A	106	ASN
1	A	108	THR
1	A	110	THR
1	A	112	THR
1	A	116	SER
1	A	119	TYR
1	A	122	SER
1	A	124	THR
1	A	128	ASN
1	A	130	GLU
1	A	143	THR
1	A	144	GLU
1	A	153	LYS
1	A	156	VAL
1	A	158	ILE
1	A	165	ASP
1	A	177	ILE
1	A	178	THR
1	A	203	PHE
1	A	214	VAL
1	A	261	SER
1	A	268	GLN
1	A	277	THR
1	A	303	SER
1	A	321	GLN
1	A	332	TYR
1	A	340	SER
1	A	347	ARG
1	A	361	ARG
1	A	372	LYS
1	A	375	GLU
1	A	409	SER
1	A	434	ASN
1	A	480	LYS
1	A	494	SER

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Mol	Chain	Res	Type
1	A	511	THR
1	A	516	GLN
1	A	533	ASN
1	A	535	VAL
1	B	33	ASP
1	B	51	LEU
1	B	58	THR
1	B	74	ILE
1	B	77	SER
1	B	78	SER
1	B	86	GLU
1	B	89	PHE
1	B	108	THR
1	B	115	LEU
1	B	119	TYR
1	B	120	LEU
1	B	124	THR
1	B	128	ASN
1	B	129	LYS
1	B	143	THR
1	B	150	LYS
1	B	157	ASN
1	B	178	THR
1	B	179	ARG
1	B	203	PHE
1	B	208	VAL
1	B	218	SER
1	B	245	SER
1	B	248	THR
1	B	268	GLN
1	B	277	THR
1	B	332	TYR
1	B	346	THR
1	B	347	ARG
1	B	359	ASN
1	B	362	SER
1	B	382	ARG
1	B	388	ASN
1	B	421	ASP
1	B	462	ASP
1	B	466	GLU
1	B	480	LYS

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Mol	Chain	Res	Type
1	B	494	SER
1	B	511	THR
1	B	512	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	294	GLN
1	A	388	ASN
1	A	402	HIS
1	A	416	ASN
1	A	434	ASN
1	A	447	GLN
1	A	516	GLN
1	A	541	GLN
1	B	128	ASN
1	B	294	GLN
1	B	298	ASN
1	B	474	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

5 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	XYP	C	1	2	9,9,10	0.50	0	10,12,14	1.87	2 (20%)
2	XYP	C	2	2	9,9,10	1.09	1 (11%)	10,12,14	1.62	1 (10%)
3	XYP	D	1	3	10,10,10	0.96	0	14,14,14	1.03	1 (7%)
3	XYP	D	2	3	9,9,10	1.09	1 (11%)	10,12,14	2.22	4 (40%)
3	XYP	D	3	3	9,9,10	1.23	1 (11%)	10,12,14	2.04	4 (40%)

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	XYP	C	1	2	3/3/3/4	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
3	XYP	D	1	3	-	-	0/1/1/1
3	XYP	D	2	3	-	-	0/1/1/1
3	XYP	D	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	XYP	C4-C3	2.14	1.55	1.52
3	D	2	XYP	C2-C3	2.11	1.55	1.52
3	D	3	XYP	C5-C4	2.02	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	XYP	C5-O5-C1	4.48	118.65	111.42
2	C	1	XYP	C4-C3-C2	-4.31	105.80	110.92
2	C	2	XYP	O4-C4-C3	3.68	117.77	110.15
3	D	2	XYP	O3-C3-C2	3.30	116.78	110.05
3	D	3	XYP	C4-C3-C2	2.95	114.42	110.92
3	D	3	XYP	C5-O5-C1	2.88	116.07	111.42
3	D	3	XYP	C1-C2-C3	2.59	113.42	109.64
3	D	2	XYP	C1-C2-C3	-2.57	105.90	109.64
3	D	3	XYP	C5-C4-C3	2.45	113.21	109.64
2	C	1	XYP	C1-C2-C3	2.33	113.03	109.64
3	D	2	XYP	O3-C3-C4	2.24	114.63	110.05
3	D	1	XYP	O3-C3-C4	-2.13	105.70	110.05

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	XYP	C3
2	C	1	XYP	C4
2	C	1	XYP	C2

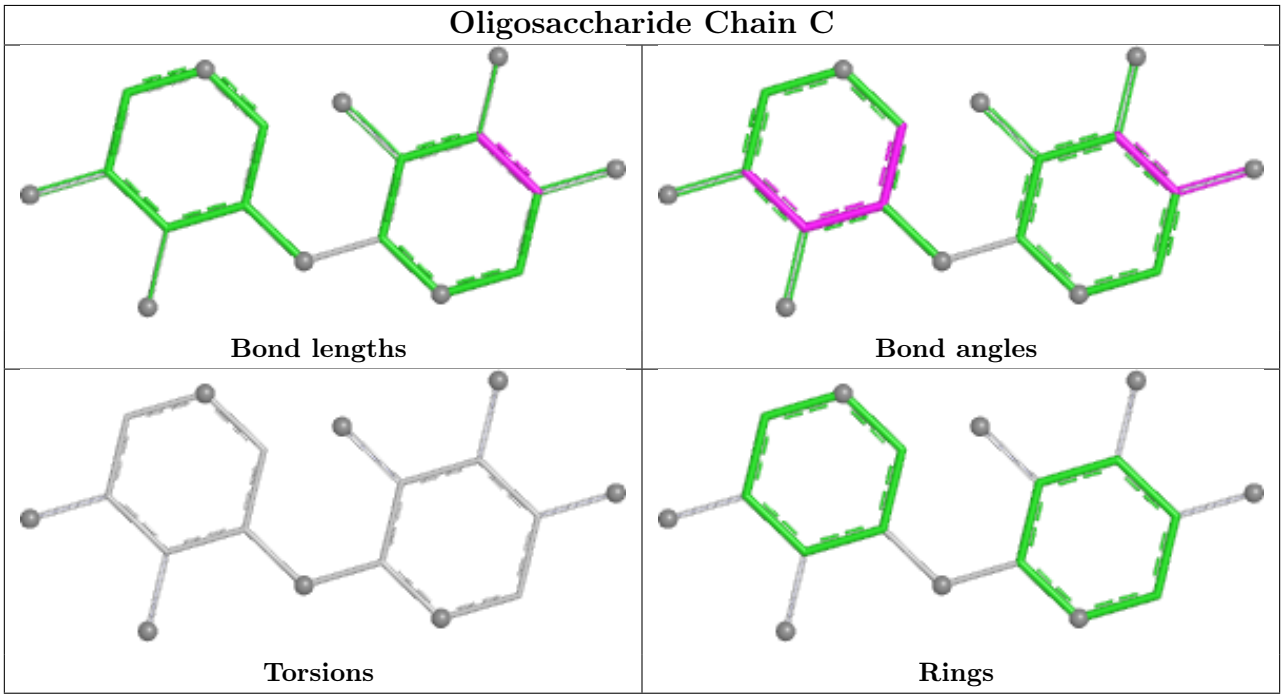
There are no torsion outliers.

There are no ring outliers.

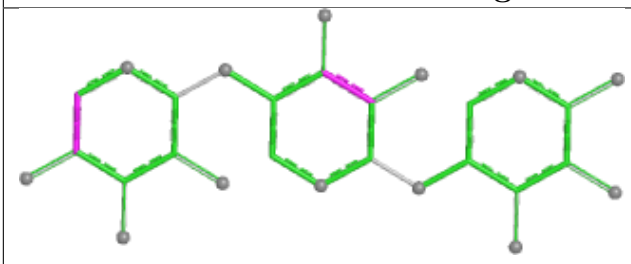
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	XYP	3	0
3	D	2	XYP	2	0
3	D	3	XYP	2	0

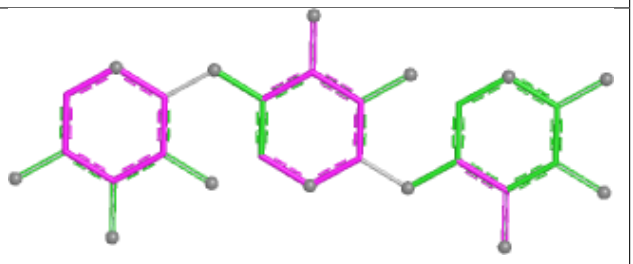
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



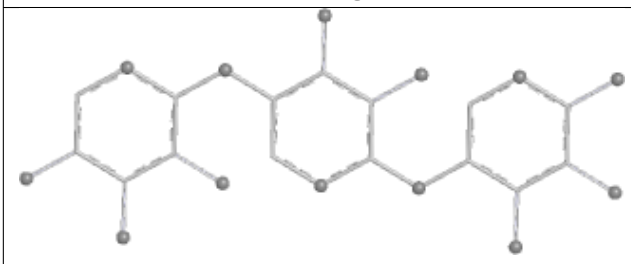
Oligosaccharide Chain D



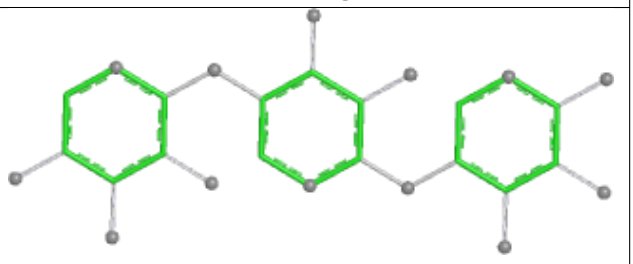
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
6	PO4	A	1555	-	4,4,4	0.94	0	6,6,6	0.69	0
6	PO4	B	1553	-	4,4,4	0.86	0	6,6,6	1.03	0
4	XYP	A	1001	-	10,10,10	0.67	0	14,14,14	1.46	1 (7%)

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
4	XYP	A	1001	-	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	XYP	O3-C3-C4	-3.19	103.54	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	XYP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	494:SER	C	495:LYS	N	1.10

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, 95^{th} 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	504/540 (93%)	0.23	8 (1%) 72 79	42, 69, 106, 123	0
1	B	507/540 (93%)	0.11	7 (1%) 75 82	35, 55, 99, 122	0
All	All	1011/1080 (93%)	0.17	15 (1%) 73 81	35, 63, 103, 123	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	3.6
1	B	145	ILE	3.2
1	A	160	LEU	2.8
1	A	288	PHE	2.8
1	A	99	TYR	2.7
1	A	180	LYS	2.6
1	A	34	TYR	2.4
1	B	34	TYR	2.4
1	B	97	TYR	2.3
1	A	107	GLY	2.2
1	A	102	PHE	2.2
1	B	180	LYS	2.1
1	A	494	SER	2.1
1	B	181	GLY	2.1
1	B	60	VAL	2.0

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

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

6.3 Carbohydrates (i)

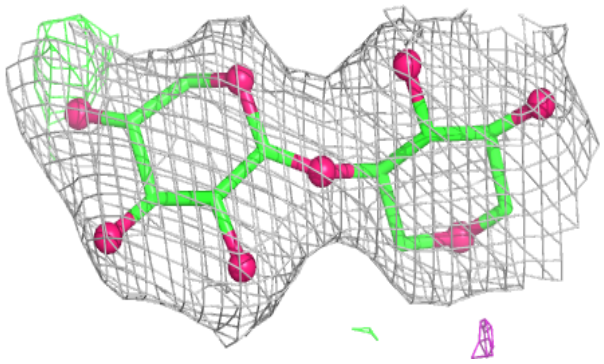
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

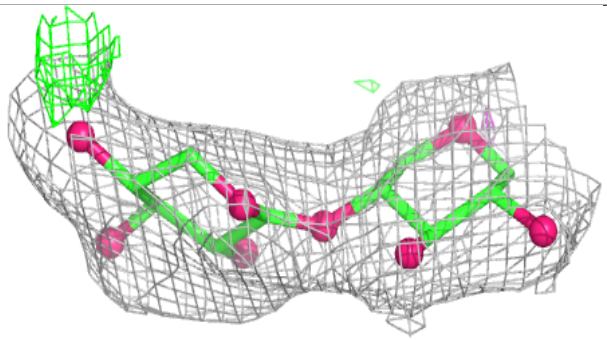
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XYP	D	3	9/10	0.95	0.18	76,80,84,84	0
2	XYP	C	2	9/10	0.96	0.12	55,70,73,73	0
3	XYP	D	2	9/10	0.98	0.19	40,46,48,48	0
2	XYP	C	1	9/10	0.99	0.17	42,44,46,50	0
3	XYP	D	1	10/10	0.99	0.17	40,42,44,44	0

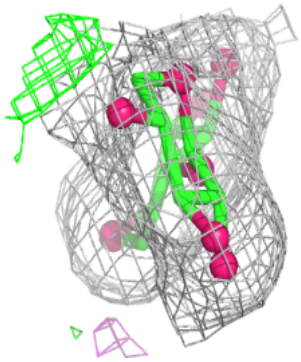
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

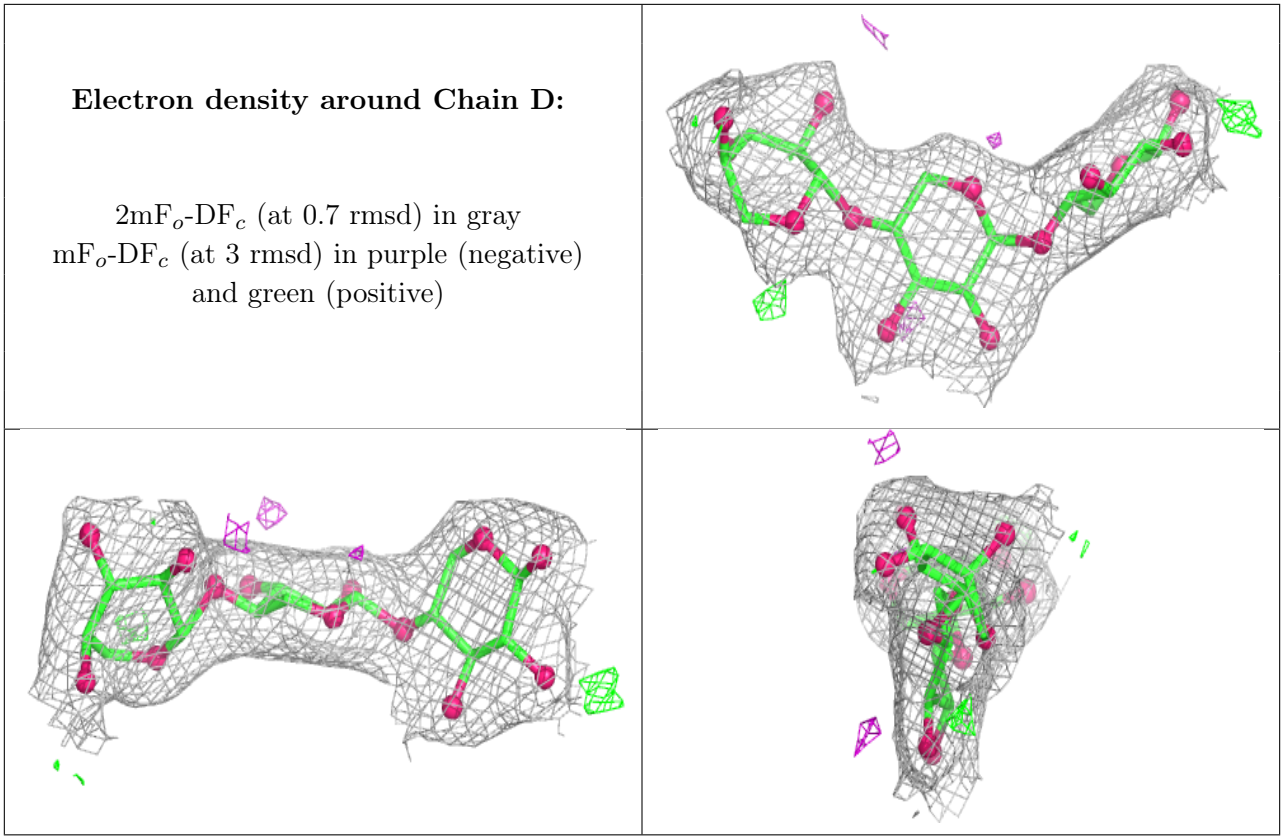
Electron density around Chain C:

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









6.4 Ligands

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, 95^{th} 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
5	CA	A	1553	1/1	0.88	0.14	95,95,95,95	0
5	CA	A	1552	1/1	0.91	0.13	81,81,81,81	0
6	PO4	B	1553	5/5	0.93	0.17	114,115,115,116	0
6	PO4	A	1555	5/5	0.94	0.24	101,101,103,104	0
4	XYP	A	1001	10/10	0.97	0.19	49,53,55,60	0
5	CA	A	1554	1/1	0.99	0.10	62,62,62,62	0
5	CA	B	1552	1/1	0.99	0.12	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.