Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:42 PM EDT

PDB ID	:	6NCZ
Title	:	Crystal structure of hybrid beta-glucuronidase/beta-galacturonidase from Fusicatenibacter saccharivorans bound to phenyl-thio-beta-D-glucuronide
Authors	:	Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-12-12
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

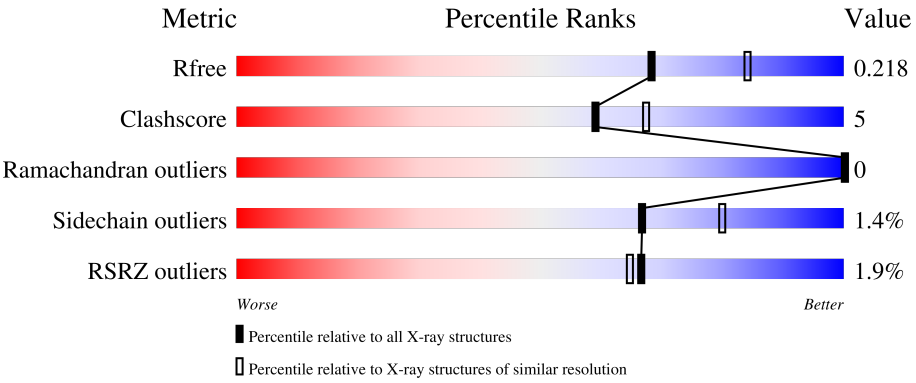
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	610	83% 13%
1	B	610	84% 12%
1	C	610	85% 11%
1	D	610	89% 7%
1	E	610	82% 14%

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Mol	Chain	Length	Quality of chain
1	F	610	2% 86% 10%

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
3	GOL	B	702	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30846 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-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4816	3064	823	901	28			
1	B	588	Total	C	N	O	S	0	0	0
			4816	3064	823	901	28			
1	C	589	Total	C	N	O	S	0	0	0
			4824	3070	824	902	28			
1	D	589	Total	C	N	O	S	0	0	0
			4824	3070	824	902	28			
1	E	589	Total	C	N	O	S	0	0	0
			4824	3070	824	902	28			
1	F	589	Total	C	N	O	S	0	0	0
			4824	3070	824	902	28			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	587	GLU	-	expression tag	UNP A0A174EHD1
A	588	ASN	-	expression tag	UNP A0A174EHD1
A	589	LEU	-	expression tag	UNP A0A174EHD1
A	590	TYR	-	expression tag	UNP A0A174EHD1
A	591	PHE	-	expression tag	UNP A0A174EHD1
A	592	GLN	-	expression tag	UNP A0A174EHD1
A	593	SER	-	expression tag	UNP A0A174EHD1
A	594	GLY	-	expression tag	UNP A0A174EHD1
A	595	SER	-	expression tag	UNP A0A174EHD1
A	596	HIS	-	expression tag	UNP A0A174EHD1
A	597	HIS	-	expression tag	UNP A0A174EHD1
A	598	HIS	-	expression tag	UNP A0A174EHD1
A	599	HIS	-	expression tag	UNP A0A174EHD1
A	600	HIS	-	expression tag	UNP A0A174EHD1
A	601	HIS	-	expression tag	UNP A0A174EHD1
B	587	GLU	-	expression tag	UNP A0A174EHD1
B	588	ASN	-	expression tag	UNP A0A174EHD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	589	LEU	-	expression tag	UNP A0A174EHD1
B	590	TYR	-	expression tag	UNP A0A174EHD1
B	591	PHE	-	expression tag	UNP A0A174EHD1
B	592	GLN	-	expression tag	UNP A0A174EHD1
B	593	SER	-	expression tag	UNP A0A174EHD1
B	594	GLY	-	expression tag	UNP A0A174EHD1
B	595	SER	-	expression tag	UNP A0A174EHD1
B	596	HIS	-	expression tag	UNP A0A174EHD1
B	597	HIS	-	expression tag	UNP A0A174EHD1
B	598	HIS	-	expression tag	UNP A0A174EHD1
B	599	HIS	-	expression tag	UNP A0A174EHD1
B	600	HIS	-	expression tag	UNP A0A174EHD1
B	601	HIS	-	expression tag	UNP A0A174EHD1
C	587	GLU	-	expression tag	UNP A0A174EHD1
C	588	ASN	-	expression tag	UNP A0A174EHD1
C	589	LEU	-	expression tag	UNP A0A174EHD1
C	590	TYR	-	expression tag	UNP A0A174EHD1
C	591	PHE	-	expression tag	UNP A0A174EHD1
C	592	GLN	-	expression tag	UNP A0A174EHD1
C	593	SER	-	expression tag	UNP A0A174EHD1
C	594	GLY	-	expression tag	UNP A0A174EHD1
C	595	SER	-	expression tag	UNP A0A174EHD1
C	596	HIS	-	expression tag	UNP A0A174EHD1
C	597	HIS	-	expression tag	UNP A0A174EHD1
C	598	HIS	-	expression tag	UNP A0A174EHD1
C	599	HIS	-	expression tag	UNP A0A174EHD1
C	600	HIS	-	expression tag	UNP A0A174EHD1
C	601	HIS	-	expression tag	UNP A0A174EHD1
D	587	GLU	-	expression tag	UNP A0A174EHD1
D	588	ASN	-	expression tag	UNP A0A174EHD1
D	589	LEU	-	expression tag	UNP A0A174EHD1
D	590	TYR	-	expression tag	UNP A0A174EHD1
D	591	PHE	-	expression tag	UNP A0A174EHD1
D	592	GLN	-	expression tag	UNP A0A174EHD1
D	593	SER	-	expression tag	UNP A0A174EHD1
D	594	GLY	-	expression tag	UNP A0A174EHD1
D	595	SER	-	expression tag	UNP A0A174EHD1
D	596	HIS	-	expression tag	UNP A0A174EHD1
D	597	HIS	-	expression tag	UNP A0A174EHD1
D	598	HIS	-	expression tag	UNP A0A174EHD1
D	599	HIS	-	expression tag	UNP A0A174EHD1
D	600	HIS	-	expression tag	UNP A0A174EHD1

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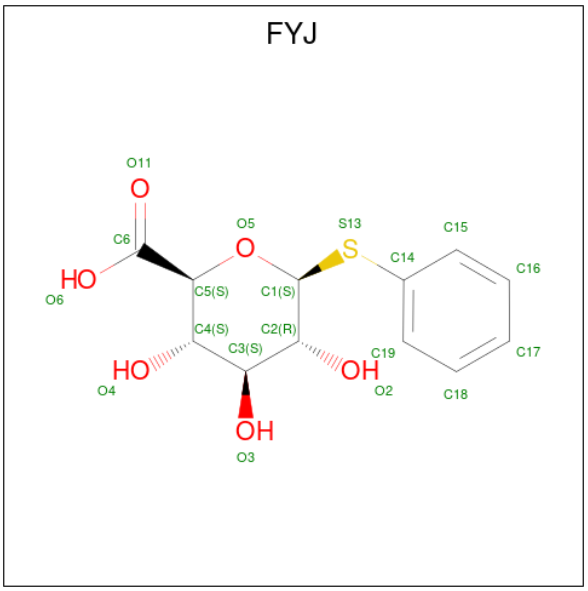
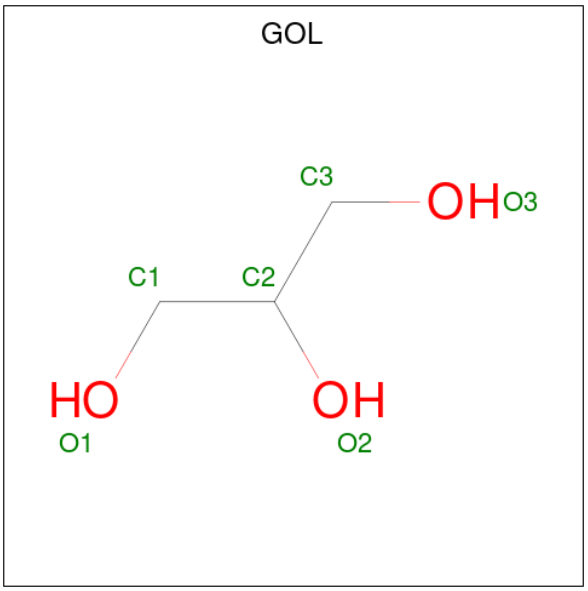
Chain	Residue	Modelled	Actual	Comment	Reference
D	601	HIS	-	expression tag	UNP A0A174EHD1
E	587	GLU	-	expression tag	UNP A0A174EHD1
E	588	ASN	-	expression tag	UNP A0A174EHD1
E	589	LEU	-	expression tag	UNP A0A174EHD1
E	590	TYR	-	expression tag	UNP A0A174EHD1
E	591	PHE	-	expression tag	UNP A0A174EHD1
E	592	GLN	-	expression tag	UNP A0A174EHD1
E	593	SER	-	expression tag	UNP A0A174EHD1
E	594	GLY	-	expression tag	UNP A0A174EHD1
E	595	SER	-	expression tag	UNP A0A174EHD1
E	596	HIS	-	expression tag	UNP A0A174EHD1
E	597	HIS	-	expression tag	UNP A0A174EHD1
E	598	HIS	-	expression tag	UNP A0A174EHD1
E	599	HIS	-	expression tag	UNP A0A174EHD1
E	600	HIS	-	expression tag	UNP A0A174EHD1
E	601	HIS	-	expression tag	UNP A0A174EHD1
F	587	GLU	-	expression tag	UNP A0A174EHD1
F	588	ASN	-	expression tag	UNP A0A174EHD1
F	589	LEU	-	expression tag	UNP A0A174EHD1
F	590	TYR	-	expression tag	UNP A0A174EHD1
F	591	PHE	-	expression tag	UNP A0A174EHD1
F	592	GLN	-	expression tag	UNP A0A174EHD1
F	593	SER	-	expression tag	UNP A0A174EHD1
F	594	GLY	-	expression tag	UNP A0A174EHD1
F	595	SER	-	expression tag	UNP A0A174EHD1
F	596	HIS	-	expression tag	UNP A0A174EHD1
F	597	HIS	-	expression tag	UNP A0A174EHD1
F	598	HIS	-	expression tag	UNP A0A174EHD1
F	599	HIS	-	expression tag	UNP A0A174EHD1
F	600	HIS	-	expression tag	UNP A0A174EHD1
F	601	HIS	-	expression tag	UNP A0A174EHD1

- Molecule 2 is phenyl 1-thio-beta-D-glucopyranosiduronic acid (three-letter code: FYJ) (formula: $C_{12}H_{14}O_6S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			19	12	6	1		
2	B	1	Total	C	O	S	0	0
			19	12	6	1		
2	C	1	Total	C	O	S	0	0
			19	12	6	1		
2	D	1	Total	C	O	S	0	0
			19	12	6	1		
2	E	1	Total	C	O	S	0	0
			19	12	6	1		
2	F	1	Total	C	O	S	0	0
			19	12	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

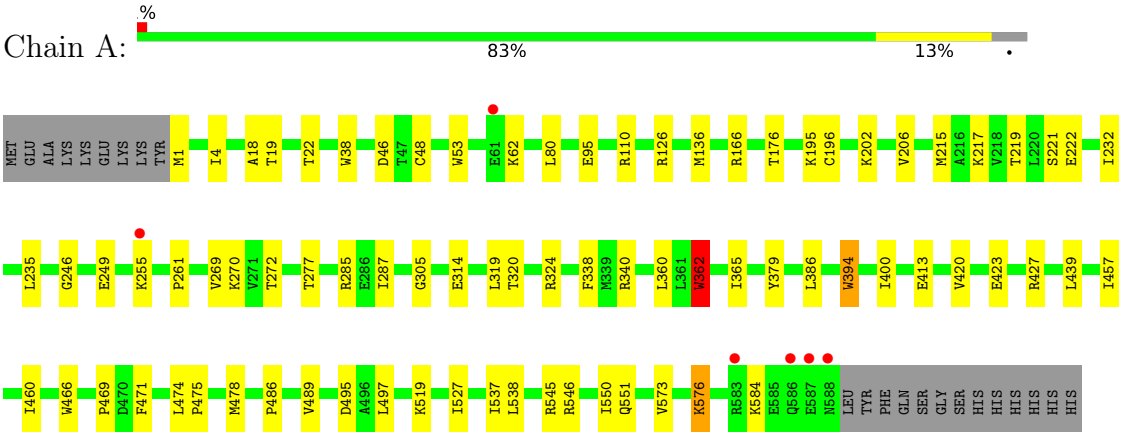
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	316	Total O 316 316	0	0
4	B	311	Total O 311 311	0	0
4	C	309	Total O 309 309	0	0
4	D	304	Total O 304 304	0	0
4	E	246	Total O 246 246	0	0
4	F	282	Total O 282 282	0	0

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.

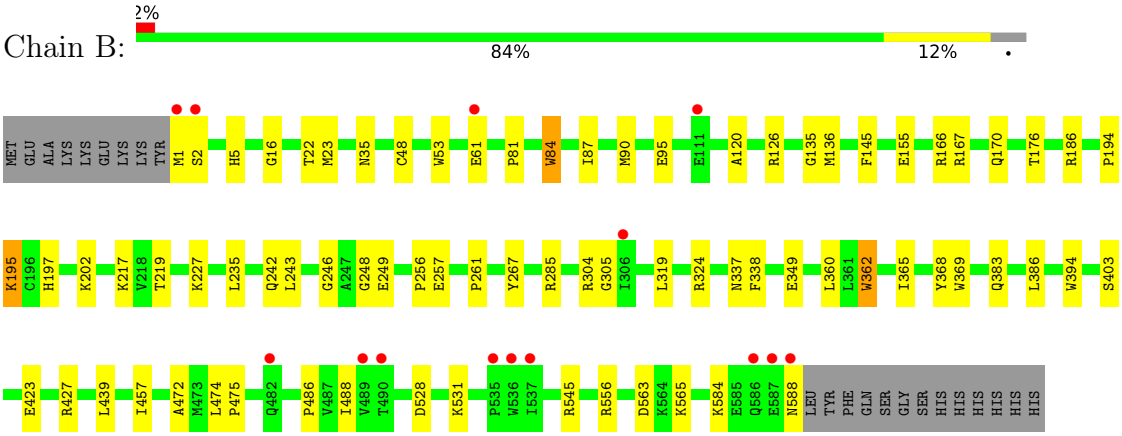
• Molecule 1: Beta-glucuronidase

Chain A:



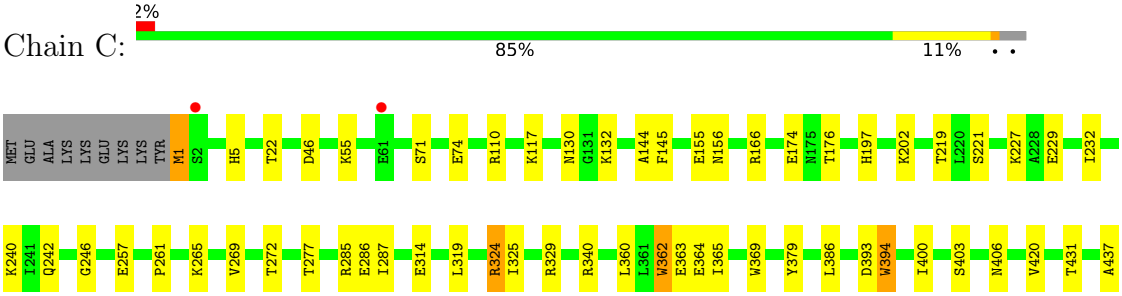
• Molecule 1: Beta-glucuronidase

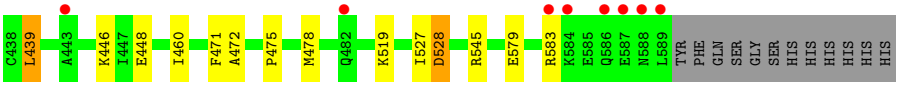
Chain B:



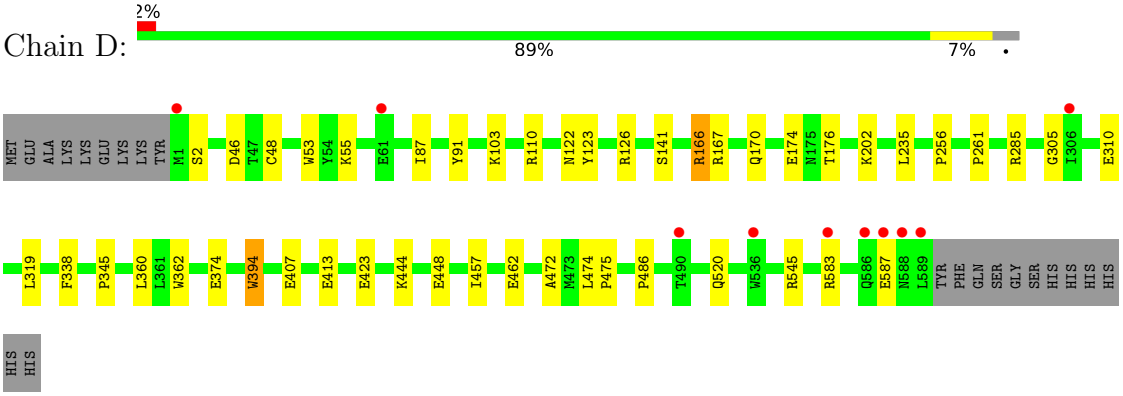
• Molecule 1: Beta-glucuronidase

Chain C:

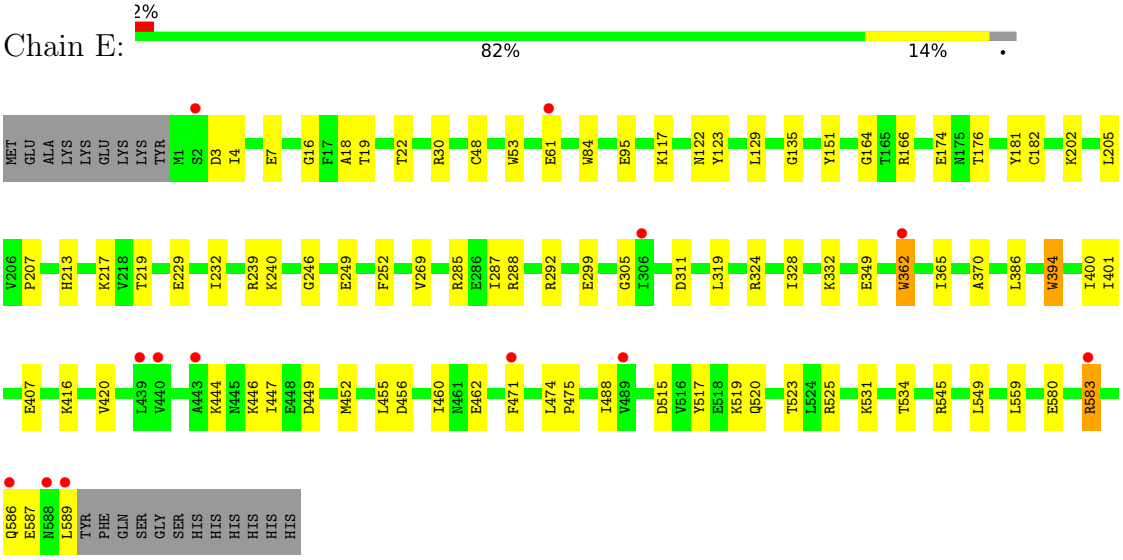




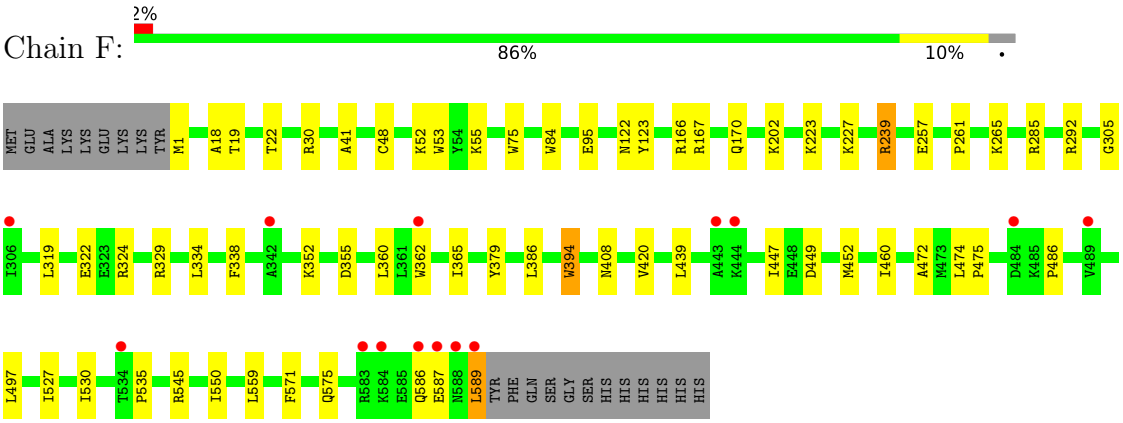
• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	109.13Å 116.92Å 117.60Å 60.32° 62.53° 87.09°	Depositor
Resolution (Å)	29.67 – 2.20 29.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.67-2.20) 97.4 (29.67-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.181 , 0.218 0.180 , 0.218	Depositor DCC
R_{free} test set	2010 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h-k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30846	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: FYJ, 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	0.44	0/4929	0.59	1/6669 (0.0%)
1	B	0.45	0/4929	0.59	0/6669
1	C	0.49	0/4937	0.63	4/6680 (0.1%)
1	D	0.46	1/4937 (0.0%)	0.61	1/6680 (0.0%)
1	E	0.44	0/4937	0.60	0/6680
1	F	0.45	0/4937	0.60	0/6680
All	All	0.46	1/29606 (0.0%)	0.60	6/40058 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	GLU	CB-CG	5.40	1.62	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	110	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	C	110	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	C	324	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	166	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	362	TRP	CA-CB-CG	5.45	124.05	113.70
1	C	110	ARG	NE-CZ-NH1	5.44	123.02	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	4816	0	4709	52	0
1	B	4816	0	4709	48	0
1	C	4824	0	4720	44	0
1	D	4824	0	4720	29	0
1	E	4824	0	4720	61	0
1	F	4824	0	4720	39	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	1	0
2	E	19	0	0	0	0
2	F	19	0	0	0	0
3	A	6	0	7	0	0
3	B	6	0	8	4	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
3	E	6	0	8	0	0
3	F	6	0	8	2	0
4	A	316	0	0	7	0
4	B	311	0	0	4	0
4	C	309	0	0	8	0
4	D	304	0	0	5	0
4	E	246	0	0	5	0
4	F	282	0	0	5	0
All	All	30846	0	28345	269	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 (269) 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:F:319:LEU:O	1:F:324:ARG:NH2	1.76	1.17
1:E:471:PHE:CZ	1:E:474:LEU:HD23	2.05	0.91
1:C:431:THR:O	4:C:801:HOH:O	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LYS:NZ	4:E:801:HOH:O	2.06	0.82
1:A:217:LYS:NZ	4:A:803:HOH:O	2.13	0.80
1:B:84:TRP:O	1:B:87:ILE:HG22	1.82	0.80
1:A:439:LEU:H	1:A:439:LEU:HD23	1.51	0.75
1:F:322:GLU:OE2	4:F:801:HOH:O	2.05	0.74
1:C:319:LEU:O	1:C:324:ARG:NH2	2.21	0.74
1:B:319:LEU:O	1:B:324:ARG:NH2	2.21	0.73
1:B:545:ARG:HH22	3:B:702:GOL:H2	1.54	0.72
1:D:583:ARG:NH2	1:D:587:GLU:OE1	2.23	0.72
1:D:374:GLU:CB	1:D:413:GLU:OE1	2.38	0.71
1:A:439:LEU:O	4:A:802:HOH:O	2.11	0.69
1:B:588:ASN:O	4:B:801:HOH:O	2.08	0.69
1:E:471:PHE:HZ	1:E:474:LEU:HD23	1.54	0.69
1:E:589:LEU:O	4:E:802:HOH:O	2.10	0.69
1:F:19:THR:O	1:F:22:THR:HG22	1.93	0.69
1:A:413:GLU:OE1	4:A:801:HOH:O	2.10	0.68
1:A:1:MET:CE	1:A:4:ILE:HD11	2.24	0.67
1:A:319:LEU:O	1:A:324:ARG:NH2	2.27	0.67
1:F:18:ALA:HA	1:F:22:THR:HG21	1.76	0.67
1:E:471:PHE:CZ	1:E:474:LEU:CD2	2.79	0.66
1:E:287:ILE:O	1:E:288:ARG:HD2	1.96	0.65
1:E:18:ALA:HA	1:E:22:THR:HG21	1.78	0.65
1:C:528:ASP:OD2	4:C:802:HOH:O	2.15	0.65
1:A:18:ALA:HA	1:A:22:THR:HG21	1.80	0.64
1:E:207:PRO:HB2	1:E:288:ARG:HD3	1.80	0.64
1:B:61:GLU:CD	1:B:61:GLU:H	2.02	0.63
1:F:497:LEU:HD22	1:F:550:ILE:HA	1.80	0.63
1:A:110:ARG:NH1	4:A:804:HOH:O	2.27	0.62
1:C:365:ILE:HD13	1:C:386:LEU:HB2	1.82	0.62
1:E:19:THR:O	1:E:22:THR:HG22	1.99	0.62
1:E:319:LEU:O	1:E:324:ARG:NH2	2.32	0.62
1:C:55:LYS:NZ	4:C:810:HOH:O	2.32	0.62
1:E:95:GLU:OE1	1:E:166:ARG:HD3	2.01	0.61
1:F:1:MET:N	4:F:806:HOH:O	2.33	0.60
1:B:439:LEU:HD23	1:B:439:LEU:H	1.67	0.60
1:E:239:ARG:HE	1:E:252:PHE:CB	2.14	0.60
1:B:362:TRP:HZ3	1:B:488:ILE:HD12	1.66	0.59
1:D:202:LYS:HB3	1:D:394:TRP:CE3	2.37	0.59
1:D:374:GLU:HB2	1:D:413:GLU:OE1	2.02	0.58
1:C:446:LYS:HE3	1:C:448:GLU:OE2	2.03	0.58
1:C:439:LEU:O	4:C:803:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ARG:NH2	1:E:580:GLU:OE2	2.34	0.57
1:D:310:GLU:HG2	1:D:319:LEU:HD13	1.86	0.57
1:A:255:LYS:NZ	4:A:808:HOH:O	2.37	0.57
1:E:229:GLU:HB2	1:E:240:LYS:HE2	1.87	0.57
1:F:95:GLU:OE1	1:F:166:ARG:HD3	2.05	0.56
1:E:370:ALA:HB3	4:E:1024:HOH:O	2.05	0.56
1:B:235:LEU:HD11	1:B:256:PRO:HB3	1.87	0.56
1:A:217:LYS:HG2	1:A:249:GLU:HG2	1.88	0.56
1:C:1:MET:HG2	1:C:5:HIS:CD2	2.40	0.56
1:F:408:ASN:O	1:F:439:LEU:HD13	2.04	0.56
1:B:167:ARG:HB2	1:B:170:GLN:HG3	1.87	0.55
1:F:19:THR:H	1:F:22:THR:HG22	1.71	0.55
1:A:19:THR:O	1:A:22:THR:HG22	2.06	0.55
1:F:52:LYS:HD3	1:F:55:LYS:HE3	1.89	0.55
1:C:329:ARG:NH1	4:C:814:HOH:O	2.39	0.54
1:E:232:ILE:HG12	1:E:269:VAL:HG12	1.88	0.54
1:B:120:ALA:HB3	1:B:186:ARG:HG3	1.88	0.54
1:C:202:LYS:HB3	1:C:394:TRP:CE3	2.43	0.54
1:A:1:MET:HE1	1:A:4:ILE:HD11	1.88	0.54
1:D:545:ARG:HH22	3:D:702:GOL:H2	1.73	0.54
1:C:166:ARG:HB3	1:C:174:GLU:HA	1.89	0.54
1:C:229:GLU:OE2	1:C:240:LYS:HE3	2.08	0.53
1:B:563:ASP:OD2	1:B:565:LYS:HD2	2.09	0.53
1:E:217:LYS:HG2	1:E:249:GLU:HG2	1.91	0.53
1:E:456:ASP:OD2	4:E:803:HOH:O	2.18	0.53
1:C:325:ILE:HG22	1:C:329:ARG:HD3	1.90	0.53
1:C:478:MET:HG3	1:C:527:ILE:HG13	1.91	0.53
1:B:423:GLU:O	1:B:427:ARG:HG3	2.09	0.53
1:E:19:THR:H	1:E:22:THR:HG22	1.73	0.53
1:A:195:LYS:HE3	1:A:222:GLU:OE1	2.08	0.52
1:A:340:ARG:HG3	1:A:362:TRP:CD1	2.44	0.52
1:C:379:TYR:OH	1:C:420:VAL:HG12	2.09	0.52
1:D:444:LYS:HE3	1:D:448:GLU:OE2	2.09	0.52
1:C:74:GLU:HB3	1:E:549:LEU:HD22	1.92	0.52
1:F:449:ASP:O	1:F:452:MET:HG3	2.09	0.52
1:F:586:GLN:O	1:F:589:LEU:HB2	2.09	0.52
1:C:1:MET:CE	1:E:407:GLU:OE1	2.57	0.52
1:B:305:GLY:HA2	1:B:338:PHE:O	2.10	0.52
1:D:110:ARG:NH1	4:D:817:HOH:O	2.43	0.52
1:D:141:SER:HB2	1:D:345:PRO:HD2	1.90	0.52
1:D:261:PRO:HG3	1:D:360:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LYS:HE2	1:B:242:GLN:OE1	2.10	0.52
1:B:324:ARG:NH1	1:B:349:GLU:OE1	2.41	0.52
1:F:19:THR:H	1:F:22:THR:CG2	2.23	0.52
1:E:61:GLU:CD	1:E:61:GLU:H	2.13	0.51
1:A:573:VAL:O	1:A:576:LYS:HE3	2.10	0.51
1:B:22:THR:HG21	1:B:145:PHE:O	2.10	0.51
1:F:48:CYS:HB2	1:F:53:TRP:CE3	2.45	0.51
1:D:110:ARG:HG3	1:D:110:ARG:HH11	1.75	0.51
1:E:7:GLU:OE2	4:E:804:HOH:O	2.19	0.51
1:E:239:ARG:HE	1:E:252:PHE:HB3	1.75	0.50
1:E:362:TRP:HZ3	1:E:488:ILE:HD12	1.75	0.50
1:E:583:ARG:O	1:E:587:GLU:HG3	2.12	0.50
1:F:305:GLY:HA2	1:F:338:PHE:O	2.11	0.50
1:A:126:ARG:HG3	1:A:136:MET:HB3	1.93	0.50
1:E:474:LEU:HG	1:E:523:THR:HG21	1.93	0.49
1:C:1:MET:HE1	1:E:407:GLU:OE1	2.12	0.49
1:A:202:LYS:HB3	1:A:394:TRP:CE3	2.48	0.49
1:E:19:THR:H	1:E:22:THR:CG2	2.25	0.49
1:D:457:ILE:HG12	1:D:486:PRO:HG2	1.94	0.49
1:A:48:CYS:HB2	1:A:53:TRP:CE3	2.47	0.49
1:E:305:GLY:HA3	1:E:534:THR:HG22	1.93	0.49
1:B:1:MET:HE3	1:B:5:HIS:CE1	2.47	0.49
1:B:528:ASP:O	1:B:531:LYS:HE2	2.13	0.49
1:E:474:LEU:HB3	1:E:475:PRO:HD3	1.95	0.49
1:A:95:GLU:OE1	1:A:166:ARG:HD3	2.13	0.49
1:D:407:GLU:HG3	2:D:701:FYJ:S13	2.52	0.49
1:F:527:ILE:HB	1:F:530:ILE:HD12	1.95	0.49
1:F:202:LYS:HB3	1:F:394:TRP:CE3	2.47	0.48
1:B:155:GLU:HG2	4:D:961:HOH:O	2.12	0.48
1:E:299:GLU:OE2	1:E:299:GLU:HA	2.12	0.48
1:B:195:LYS:O	4:B:802:HOH:O	2.20	0.48
1:C:22:THR:CG2	1:C:145:PHE:O	2.62	0.48
1:D:103:LYS:NZ	4:D:801:HOH:O	2.14	0.48
1:E:239:ARG:HE	1:E:252:PHE:HB2	1.78	0.48
1:F:447:ILE:HG23	1:F:460:ILE:HD11	1.95	0.48
1:D:462:GLU:OE2	1:D:520:GLN:NE2	2.38	0.48
1:F:379:TYR:OH	1:F:420:VAL:HG12	2.13	0.48
1:A:320:THR:HB	4:A:837:HOH:O	2.14	0.48
1:B:243:LEU:HD23	1:B:248:GLY:HA3	1.96	0.47
1:F:223:LYS:HG2	4:F:1008:HOH:O	2.13	0.47
1:C:257:GLU:HB2	1:C:265:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:LYS:HB3	1:E:394:TRP:CE3	2.49	0.47
1:E:219:THR:HA	1:E:246:GLY:O	2.15	0.47
1:F:167:ARG:HB2	1:F:170:GLN:HG3	1.96	0.47
1:A:439:LEU:H	1:A:439:LEU:CD2	2.24	0.47
1:B:545:ARG:HH12	3:B:702:GOL:H2	1.79	0.47
1:F:474:LEU:HB3	1:F:475:PRO:HD3	1.97	0.47
1:C:272:THR:HG22	1:C:277:THR:HG23	1.96	0.46
1:C:579:GLU:O	1:C:583:ARG:HG3	2.14	0.46
1:F:559:LEU:HD13	1:F:571:PHE:HA	1.97	0.46
1:A:261:PRO:HG3	1:A:360:LEU:HG	1.96	0.46
1:E:400:ILE:HG13	1:E:401:ILE:HG13	1.97	0.46
1:A:1:MET:HE2	1:A:4:ILE:HD11	1.95	0.46
1:E:449:ASP:O	1:E:452:MET:HE2	2.15	0.46
1:F:305:GLY:O	1:F:535:PRO:HD2	2.15	0.46
1:F:329:ARG:NE	4:F:816:HOH:O	2.47	0.46
1:A:232:ILE:HG12	1:A:269:VAL:HG22	1.98	0.46
1:E:122:ASN:HA	1:E:123:TYR:HA	1.70	0.46
1:E:515:ASP:OD2	1:E:519:LYS:HE2	2.15	0.46
1:F:122:ASN:HA	1:F:123:TYR:HA	1.67	0.46
1:D:87:ILE:HG22	1:D:91:TYR:HD2	1.80	0.45
1:E:416:LYS:O	1:E:420:VAL:HG23	2.15	0.45
1:B:219:THR:HA	1:B:246:GLY:O	2.15	0.45
1:B:365:ILE:HD13	1:B:386:LEU:HB2	1.97	0.45
1:F:365:ILE:HD13	1:F:386:LEU:HB2	1.98	0.45
1:A:19:THR:H	1:A:22:THR:HG22	1.81	0.45
1:B:95:GLU:OE1	1:B:166:ARG:HD3	2.16	0.45
1:B:249:GLU:HG3	4:B:1001:HOH:O	2.16	0.45
1:D:48:CYS:HB2	1:D:53:TRP:CE3	2.51	0.45
1:C:155:GLU:OE2	4:C:804:HOH:O	2.21	0.45
1:D:374:GLU:HA	1:D:413:GLU:OE1	2.17	0.45
1:E:181:TYR:HE2	1:E:311:ASP:OD1	2.00	0.45
1:E:16:GLY:O	1:E:135:GLY:HA3	2.17	0.45
1:B:545:ARG:NH2	3:B:702:GOL:H2	2.25	0.45
1:F:334:LEU:HD12	1:F:575:GLN:HB2	1.98	0.45
1:A:469:PRO:HD2	4:A:1050:HOH:O	2.17	0.45
1:E:452:MET:HA	1:E:455:LEU:HD12	1.98	0.45
1:A:1:MET:HE2	1:A:4:ILE:CD1	2.47	0.44
1:C:176:THR:O	1:C:545:ARG:HD2	2.17	0.44
1:C:314:GLU:CD	1:C:314:GLU:H	2.20	0.44
1:B:474:LEU:HB3	1:B:475:PRO:HD3	1.99	0.44
1:C:286:GLU:HA	4:C:976:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:ARG:HH12	3:F:702:GOL:HO2	1.63	0.44
1:A:497:LEU:HD22	1:A:550:ILE:HA	1.99	0.44
1:B:176:THR:O	1:B:545:ARG:HD2	2.17	0.44
1:C:340:ARG:HG3	1:C:362:TRP:CD1	2.52	0.44
1:A:460:ILE:HG22	1:A:489:VAL:HA	2.00	0.44
1:A:537:ILE:HG12	1:A:538:LEU:H	1.83	0.44
1:C:71:SER:HB3	4:C:944:HOH:O	2.18	0.44
1:A:474:LEU:HB3	1:A:475:PRO:HD3	2.00	0.44
1:C:471:PHE:CE2	1:C:519:LYS:HD2	2.53	0.44
1:C:472:ALA:O	1:C:475:PRO:HD2	2.18	0.44
1:D:305:GLY:HA2	1:D:338:PHE:O	2.18	0.44
1:E:48:CYS:HB2	1:E:53:TRP:CE3	2.53	0.44
1:A:232:ILE:HG21	1:A:235:LEU:HD12	1.99	0.44
1:B:457:ILE:HG12	1:B:486:PRO:HG2	2.00	0.44
1:A:546:ARG:HB3	1:A:551:GLN:CD	2.39	0.44
1:C:227:LYS:HE3	1:C:242:GLN:OE1	2.18	0.44
1:E:166:ARG:HB3	1:E:174:GLU:HA	2.00	0.43
1:E:447:ILE:HG23	1:E:460:ILE:HD11	2.00	0.43
1:C:460:ILE:HD13	1:C:460:ILE:HA	1.88	0.43
1:B:23:MET:HA	1:B:145:PHE:CD1	2.53	0.43
1:C:232:ILE:HG12	1:C:269:VAL:HG23	2.01	0.43
1:E:328:ILE:O	1:E:332:LYS:HG3	2.18	0.43
1:A:95:GLU:OE2	1:A:166:ARG:NH1	2.51	0.43
1:E:176:THR:O	1:E:545:ARG:HD2	2.18	0.43
1:A:573:VAL:O	1:A:576:LYS:HG3	2.18	0.43
1:F:41:ALA:HB2	1:F:75:TRP:CE2	2.54	0.43
1:B:383:GLN:OE1	4:B:803:HOH:O	2.21	0.43
1:C:287:ILE:HG12	1:C:400:ILE:HB	1.99	0.43
1:A:38:TRP:CG	1:A:80:LEU:HD12	2.53	0.43
1:B:217:LYS:HG2	1:B:249:GLU:HG2	2.01	0.43
1:D:472:ALA:O	1:D:475:PRO:HD2	2.19	0.43
1:E:324:ARG:NH1	1:E:349:GLU:OE1	2.48	0.43
1:D:374:GLU:CA	1:D:413:GLU:OE1	2.66	0.43
1:F:329:ARG:HD2	4:F:1059:HOH:O	2.19	0.43
1:C:340:ARG:HA	1:C:362:TRP:HB3	2.01	0.43
1:F:123:TYR:CZ	1:F:170:GLN:HB3	2.54	0.43
1:F:257:GLU:HB2	1:F:265:LYS:HG2	2.01	0.43
1:A:270:LYS:HE2	1:A:270:LYS:HB3	1.85	0.43
1:B:194:PRO:O	1:B:197:HIS:ND1	2.42	0.43
1:B:202:LYS:HB3	1:B:394:TRP:CE3	2.53	0.43
1:A:272:THR:HG22	1:A:277:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ARG:O	1:E:531:LYS:HE3	2.19	0.42
1:C:261:PRO:HG3	1:C:360:LEU:HG	2.01	0.42
1:D:474:LEU:HB3	1:D:475:PRO:HD3	2.01	0.42
1:E:205:LEU:HD12	1:E:213:HIS:O	2.19	0.42
1:B:472:ALA:O	1:B:475:PRO:HD2	2.20	0.42
1:A:219:THR:HA	1:A:246:GLY:O	2.19	0.42
1:B:126:ARG:HG3	1:B:136:MET:HB3	2.02	0.42
1:B:362:TRP:NE1	1:B:403:SER:HB2	2.34	0.42
3:C:702:GOL:H12	1:E:3:ASP:OD1	2.19	0.42
1:D:167:ARG:HB2	1:D:170:GLN:HG3	2.02	0.42
1:F:239:ARG:HA	1:F:239:ARG:CZ	2.49	0.42
1:E:517:TYR:CZ	1:E:559:LEU:HD21	2.55	0.42
1:A:466:TRP:CZ2	1:A:495:ASP:HB2	2.55	0.42
1:B:545:ARG:HH22	3:B:702:GOL:C2	2.29	0.42
1:D:166:ARG:HB3	1:D:174:GLU:HA	2.01	0.42
1:C:197:HIS:CE1	1:C:221:SER:HB3	2.55	0.42
1:F:545:ARG:NH1	3:F:702:GOL:O2	2.45	0.42
1:C:219:THR:HA	1:C:246:GLY:O	2.20	0.42
1:A:206:VAL:HA	1:A:215:MET:HE3	2.01	0.41
1:A:305:GLY:HA2	1:A:338:PHE:O	2.20	0.41
1:D:55:LYS:HE2	4:D:839:HOH:O	2.20	0.41
1:E:129:LEU:HD23	1:E:151:TYR:HB2	2.01	0.41
1:B:35:ASN:CG	1:B:81:PRO:HD3	2.40	0.41
1:E:365:ILE:HD13	1:E:386:LEU:HB2	2.01	0.41
1:E:462:GLU:OE2	1:E:520:GLN:NE2	2.45	0.41
1:A:471:PHE:CD1	1:A:519:LYS:HD2	2.55	0.41
1:C:364:GLU:HB2	1:C:403:SER:HB3	2.01	0.41
1:D:122:ASN:HA	1:D:123:TYR:HA	1.67	0.41
1:D:176:THR:O	1:D:545:ARG:HD2	2.19	0.41
1:D:235:LEU:HD11	1:D:256:PRO:HB3	2.02	0.41
1:A:62:LYS:HE3	1:A:62:LYS:HB3	1.88	0.41
1:B:257:GLU:HG3	1:B:267:TYR:OH	2.20	0.41
1:F:261:PRO:HG3	1:F:360:LEU:HG	2.02	0.41
1:C:369:TRP:CD1	1:E:4:ILE:HD12	2.56	0.41
1:E:586:GLN:HA	1:E:586:GLN:NE2	2.35	0.41
1:C:130:ASN:OD1	1:C:156:ASN:HA	2.20	0.41
1:C:406:ASN:HA	1:C:437:ALA:HB3	2.03	0.41
1:D:126:ARG:HD3	4:D:909:HOH:O	2.20	0.41
1:E:444:LYS:HZ2	1:E:446:LYS:HZ3	1.68	0.41
1:A:176:THR:O	1:A:545:ARG:HD2	2.21	0.41
1:A:478:MET:HG3	1:A:527:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLY:O	1:B:135:GLY:HA3	2.21	0.41
1:B:362:TRP:CZ3	1:B:488:ILE:HD12	2.53	0.41
1:B:368:TYR:CE1	1:B:369:TRP:CD2	3.09	0.41
1:B:556:ARG:HA	1:B:556:ARG:HD3	1.85	0.41
1:F:292:ARG:O	1:F:486:PRO:HB3	2.20	0.41
1:A:457:ILE:HG12	1:A:486:PRO:HG2	2.02	0.41
1:A:365:ILE:HD13	1:A:386:LEU:HB2	2.04	0.40
1:C:117:LYS:HA	1:C:144:ALA:O	2.21	0.40
1:C:363:GLU:OE1	1:C:393:ASP:OD2	2.39	0.40
1:E:586:GLN:O	1:E:589:LEU:HB2	2.22	0.40
1:A:287:ILE:HG12	1:A:400:ILE:HB	2.04	0.40
1:A:379:TYR:OH	1:A:420:VAL:HG12	2.21	0.40
1:E:164:GLY:HA3	1:E:182:CYS:SG	2.61	0.40
1:F:352:LYS:O	1:F:355:ASP:HB2	2.21	0.40
1:B:304:ARG:N	1:B:337:ASN:OD1	2.55	0.40
1:A:196:CYS:HA	1:A:221:SER:OG	2.21	0.40
1:A:423:GLU:O	1:A:427:ARG:HG3	2.21	0.40
1:B:48:CYS:HB2	1:B:53:TRP:CE3	2.57	0.40
1:F:472:ALA:O	1:F:475:PRO:HD2	2.22	0.40
1:B:261:PRO:HG3	1:B:360:LEU:HG	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	586/610 (96%)	566 (97%)	20 (3%)	0	100	100
1	B	586/610 (96%)	568 (97%)	18 (3%)	0	100	100
1	C	587/610 (96%)	565 (96%)	22 (4%)	0	100	100
1	D	587/610 (96%)	566 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	587/610 (96%)	561 (96%)	26 (4%)	0	100	100
1	F	587/610 (96%)	570 (97%)	17 (3%)	0	100	100
All	All	3520/3660 (96%)	3396 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	516/536 (96%)	509 (99%)	7 (1%)	67	80
1	B	516/536 (96%)	509 (99%)	7 (1%)	67	80
1	C	517/536 (96%)	509 (98%)	8 (2%)	65	78
1	D	517/536 (96%)	512 (99%)	5 (1%)	76	86
1	E	517/536 (96%)	511 (99%)	6 (1%)	71	83
1	F	517/536 (96%)	508 (98%)	9 (2%)	60	74
All	All	3100/3216 (96%)	3058 (99%)	42 (1%)	67	80

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	285	ARG
1	A	314	GLU
1	A	362	TRP
1	A	394	TRP
1	A	576	LYS
1	A	584	LYS
1	B	2	SER
1	B	84	TRP
1	B	90	MET
1	B	195	LYS
1	B	285	ARG

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Mol	Chain	Res	Type
1	B	362	TRP
1	B	584	LYS
1	C	1	MET
1	C	46	ASP
1	C	132	LYS
1	C	285	ARG
1	C	362	TRP
1	C	394	TRP
1	C	439	LEU
1	C	528	ASP
1	D	2	SER
1	D	46	ASP
1	D	285	ARG
1	D	362	TRP
1	D	394	TRP
1	E	30	ARG
1	E	84	TRP
1	E	285	ARG
1	E	362	TRP
1	E	394	TRP
1	E	583	ARG
1	F	30	ARG
1	F	84	TRP
1	F	227	LYS
1	F	239	ARG
1	F	285	ARG
1	F	362	TRP
1	F	394	TRP
1	F	587	GLU
1	F	589	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	588	ASN
1	E	586	GLN
1	F	482	GLN

5.3.3 RNA

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FYJ	C	701	-	20,20,20	0.81	1 (5%)	27,28,28	1.45	2 (7%)
2	FYJ	A	701	-	20,20,20	0.79	0	27,28,28	1.29	4 (14%)
2	FYJ	D	701	-	20,20,20	0.67	0	27,28,28	1.35	3 (11%)
3	GOL	A	702	-	5,5,5	1.05	0	5,5,5	1.02	0
3	GOL	D	702	-	5,5,5	0.84	0	5,5,5	0.98	0
2	FYJ	F	701	-	20,20,20	0.87	1 (5%)	27,28,28	1.46	4 (14%)
3	GOL	F	702	-	5,5,5	0.78	0	5,5,5	1.20	1 (20%)
2	FYJ	B	701	-	20,20,20	0.84	1 (5%)	27,28,28	1.54	3 (11%)
2	FYJ	E	701	-	20,20,20	0.82	1 (5%)	27,28,28	1.52	3 (11%)
3	GOL	E	702	-	5,5,5	1.12	0	5,5,5	0.86	0
3	GOL	C	702	-	5,5,5	1.08	0	5,5,5	0.71	0
3	GOL	B	702	-	5,5,5	0.77	0	5,5,5	1.11	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
2	FYJ	C	701	-	-	0/8/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FYJ	A	701	-	-	2/8/28/28	0/2/2/2
2	FYJ	D	701	-	-	0/8/28/28	0/2/2/2
3	GOL	A	702	-	-	2/4/4/4	-
3	GOL	D	702	-	-	0/4/4/4	-
2	FYJ	F	701	-	-	0/8/28/28	0/2/2/2
3	GOL	F	702	-	-	2/4/4/4	-
2	FYJ	B	701	-	-	1/8/28/28	0/2/2/2
2	FYJ	E	701	-	-	0/8/28/28	0/2/2/2
3	GOL	E	702	-	-	1/4/4/4	-
3	GOL	C	702	-	-	2/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	FYJ	C14-S13	2.34	1.81	1.77
2	F	701	FYJ	C14-S13	2.30	1.81	1.77
2	B	701	FYJ	C14-S13	2.28	1.81	1.77
2	E	701	FYJ	C14-S13	2.03	1.81	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	701	FYJ	C14-S13-C1	4.93	111.41	101.54
2	C	701	FYJ	C14-S13-C1	4.68	110.89	101.54
2	B	701	FYJ	O5-C1-C2	4.30	115.72	110.31
2	C	701	FYJ	O5-C1-C2	4.00	115.35	110.31
2	F	701	FYJ	O5-C1-C2	3.87	115.18	110.31
2	B	701	FYJ	C14-S13-C1	3.80	109.14	101.54
2	E	701	FYJ	O5-C1-C2	3.66	114.92	110.31
2	F	701	FYJ	C14-S13-C1	3.39	108.32	101.54
2	A	701	FYJ	O5-C1-C2	3.32	114.49	110.31
2	D	701	FYJ	O5-C1-C2	3.19	114.32	110.31
2	A	701	FYJ	C14-S13-C1	3.19	107.91	101.54
2	F	701	FYJ	C1-O5-C5	-3.14	107.62	113.38
2	D	701	FYJ	C14-S13-C1	3.13	107.79	101.54
2	B	701	FYJ	C1-O5-C5	-2.94	107.98	113.38
2	D	701	FYJ	O6-C6-C5	2.47	122.70	113.65
2	E	701	FYJ	C1-C2-C3	2.19	114.92	110.59
2	F	701	FYJ	O6-C6-O11	-2.13	119.25	124.09
2	A	701	FYJ	O4-C4-C5	2.04	114.32	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FYJ	C1-O5-C5	-2.01	109.69	113.38
3	F	702	GOL	C3-C2-C1	-2.00	103.92	111.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	GOL	C1-C2-C3-O3
3	C	702	GOL	O1-C1-C2-C3
3	F	702	GOL	O1-C1-C2-C3
3	A	702	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-C3
3	B	702	GOL	O2-C2-C3-O3
3	C	702	GOL	O1-C1-C2-O2
3	F	702	GOL	O1-C1-C2-O2
3	A	702	GOL	O2-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	E	702	GOL	O1-C1-C2-C3
2	A	701	FYJ	O5-C5-C6-O11
2	A	701	FYJ	O5-C5-C6-O6
2	B	701	FYJ	O5-C5-C6-O6

There are no ring outliers.

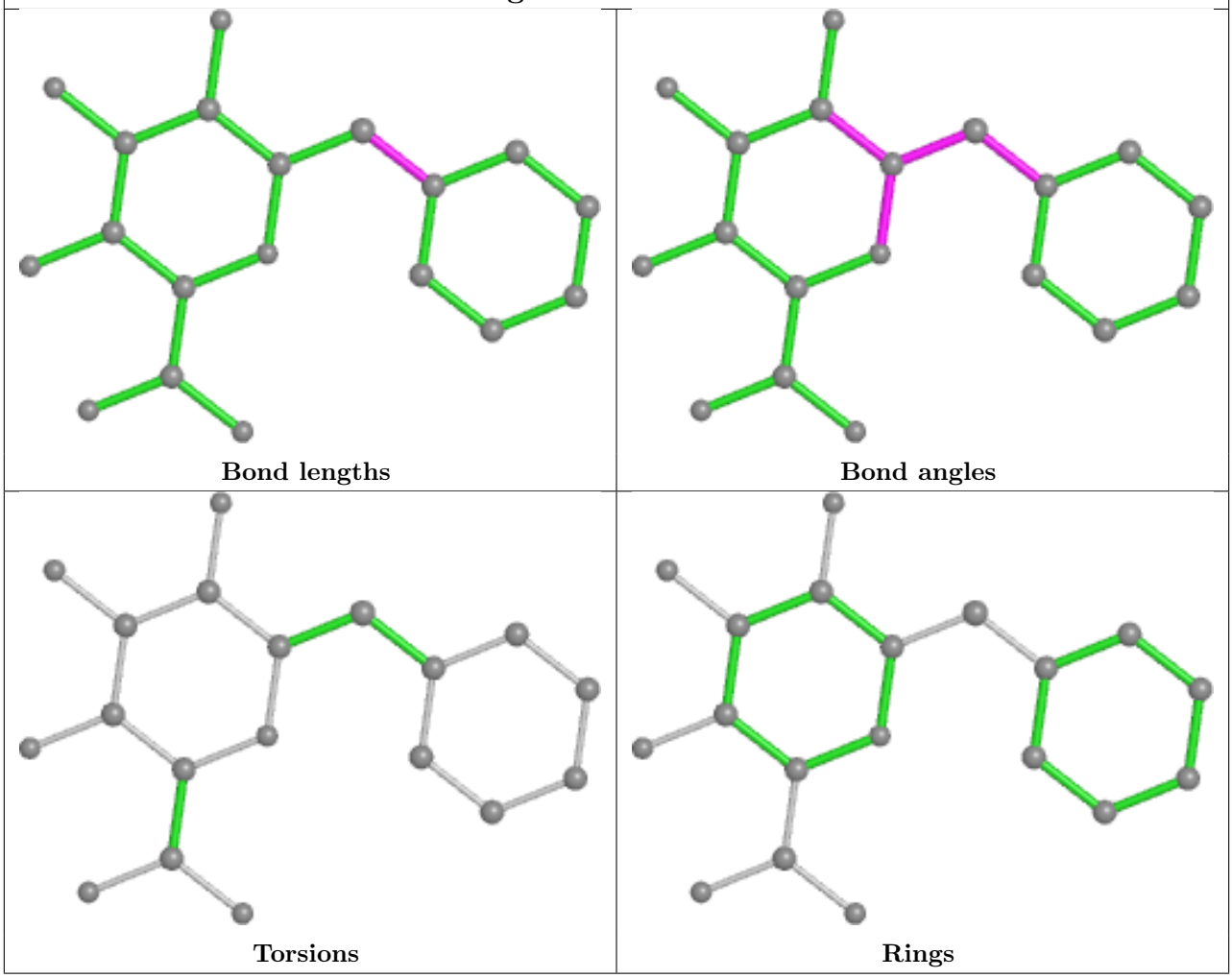
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	FYJ	1	0
3	D	702	GOL	1	0
3	F	702	GOL	2	0
3	C	702	GOL	1	0
3	B	702	GOL	4	0

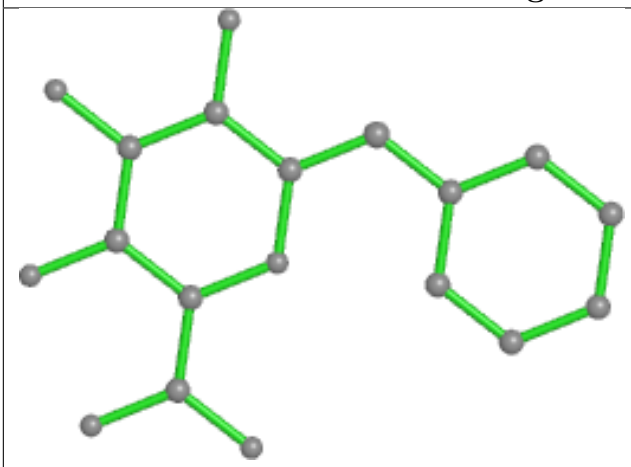
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

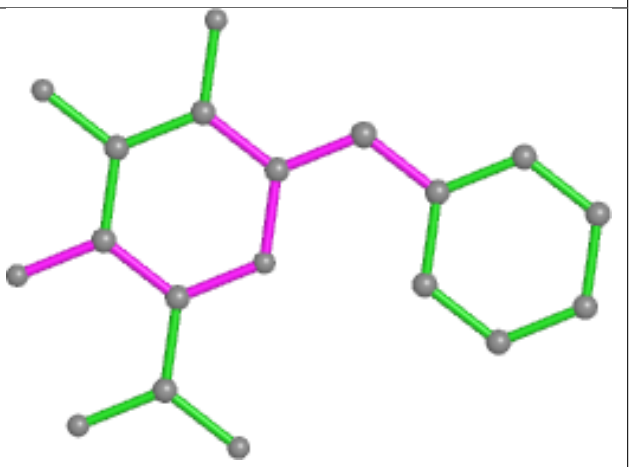
Ligand FYJ C 701



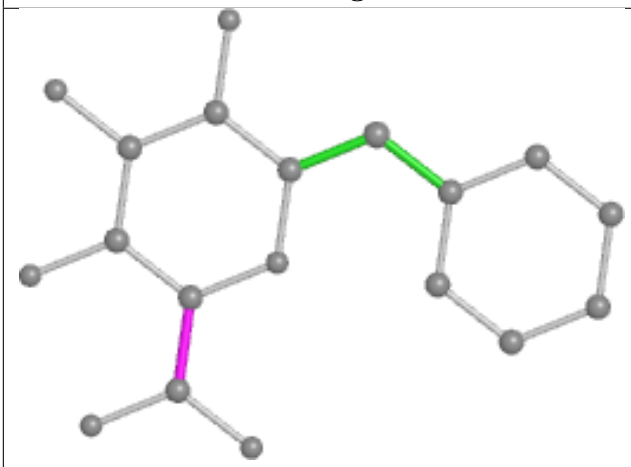
Ligand FYJ A 701



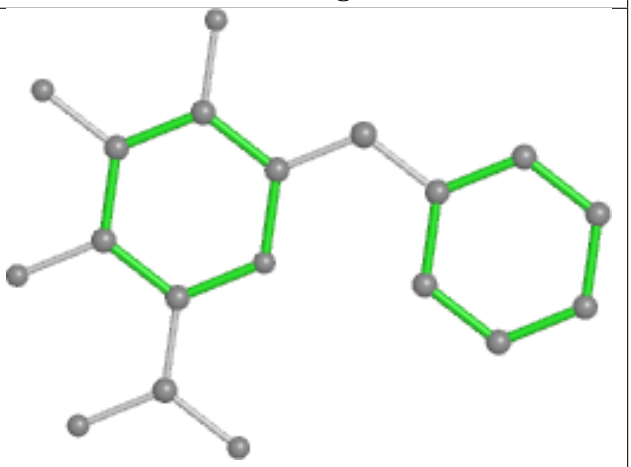
Bond lengths



Bond angles

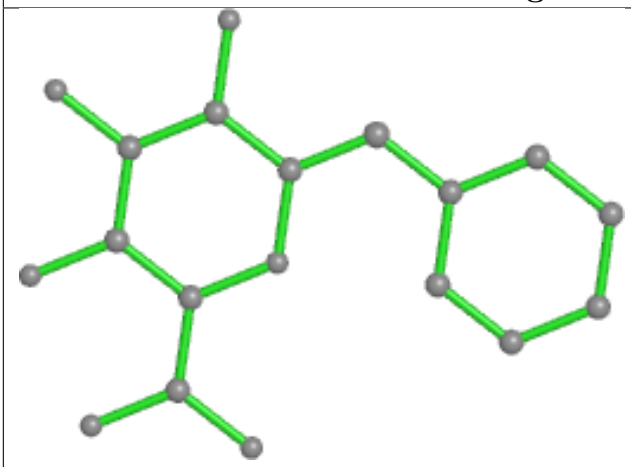


Torsions



Rings

Ligand FYJ D 701



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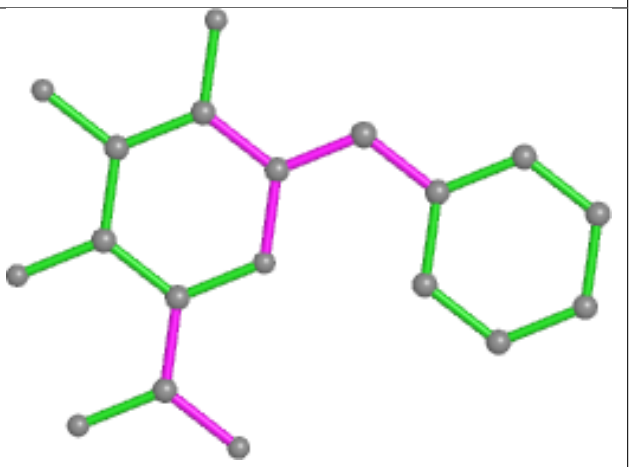

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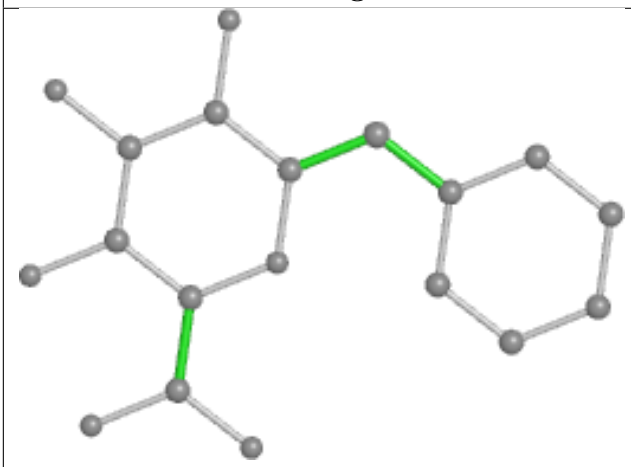

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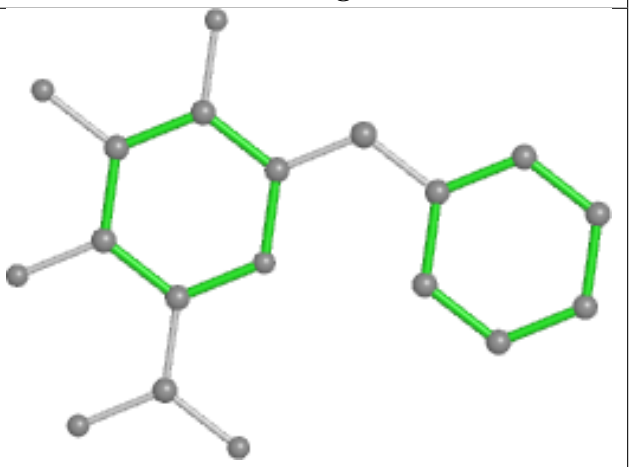
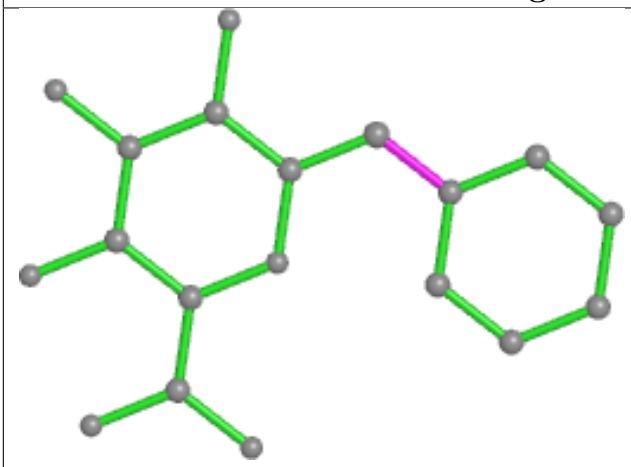
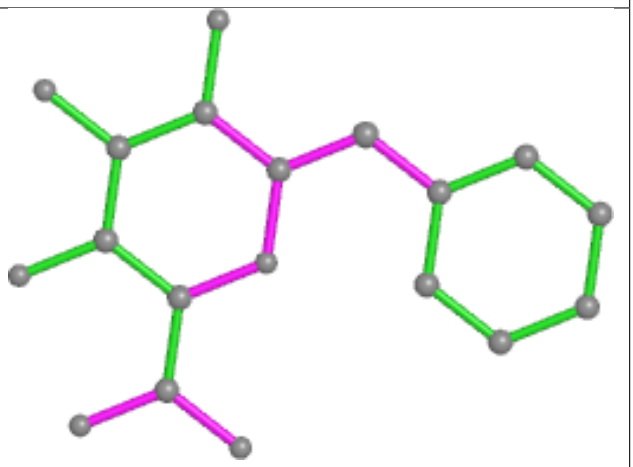


Rings

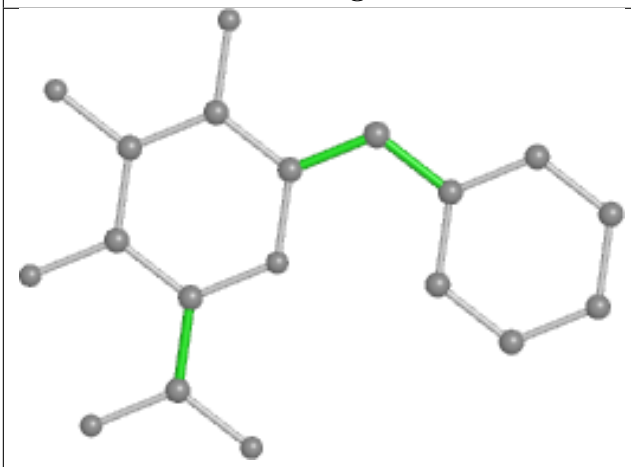
Ligand FYJ F 701



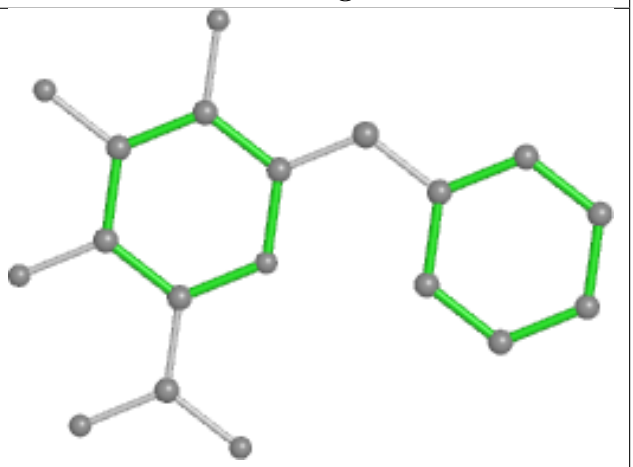
Bond lengths



Bond angles

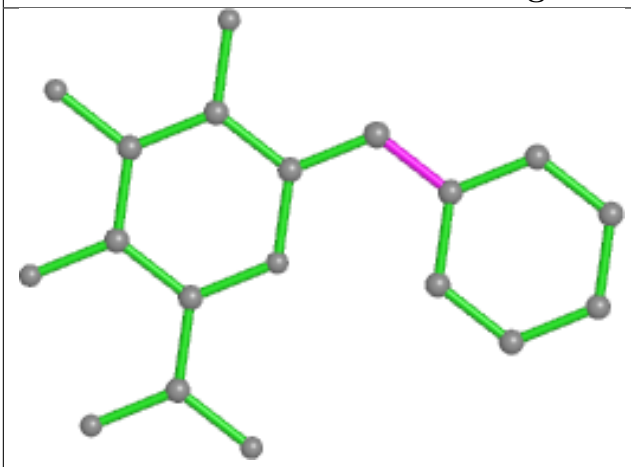


Torsions

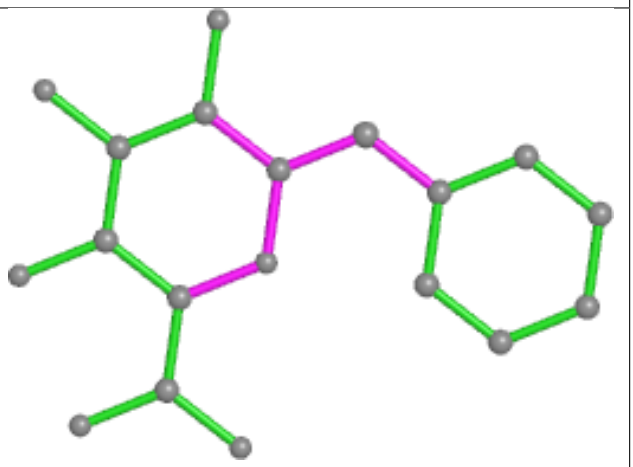


Rings

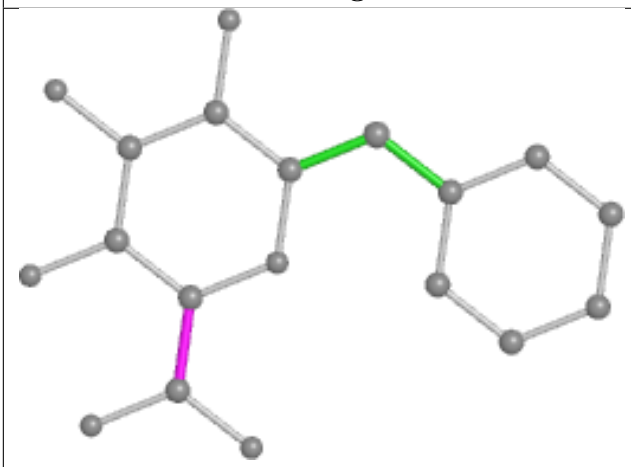
Ligand FYJ B 701



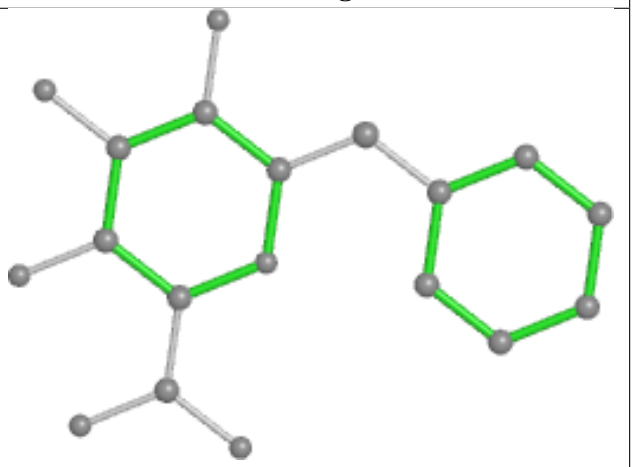
Bond lengths



Bond angles

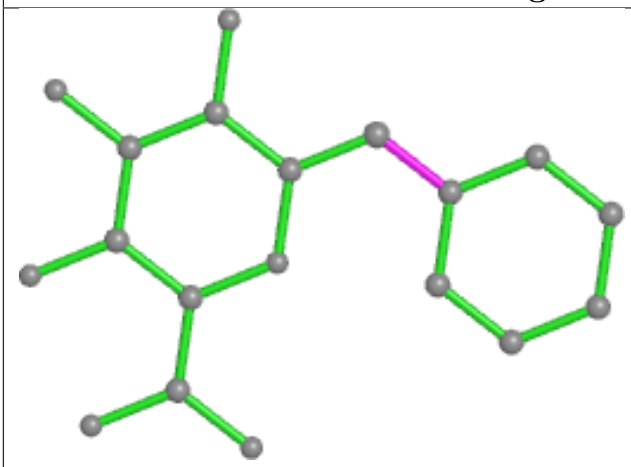


Torsions

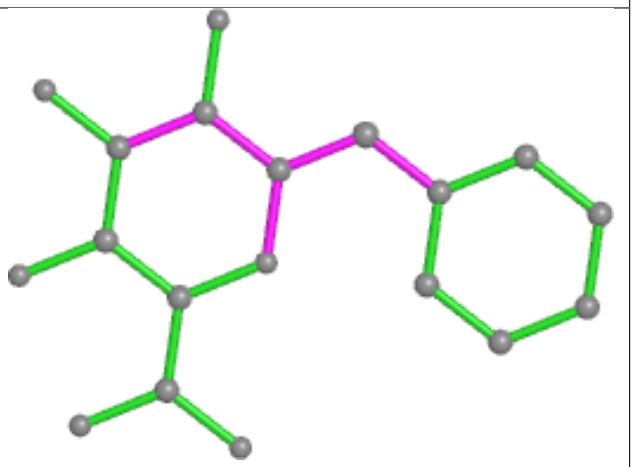


Rings

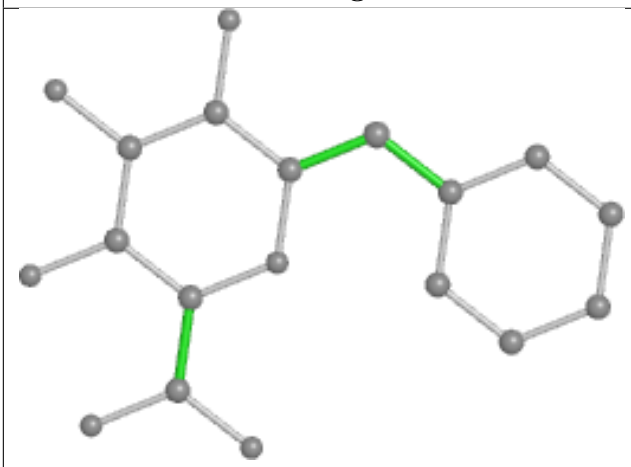
Ligand FYJ E 701



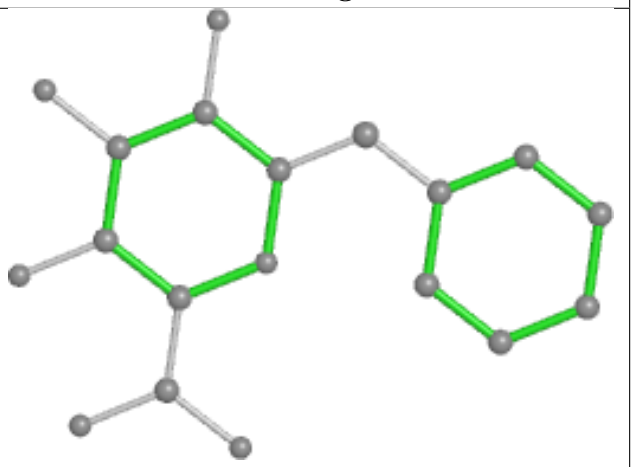
Bond lengths



Bond angles



Torsions



Rings

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

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	588/610 (96%)	-0.40	6 (1%)	82	81	18, 28, 47, 68	0
1	B	588/610 (96%)	-0.36	14 (2%)	59	56	19, 29, 46, 66	0
1	C	589/610 (96%)	-0.47	10 (1%)	70	68	20, 27, 44, 70	0
1	D	589/610 (96%)	-0.43	10 (1%)	70	68	21, 28, 45, 70	0
1	E	589/610 (96%)	-0.42	13 (2%)	62	59	19, 31, 48, 68	0
1	F	589/610 (96%)	-0.40	14 (2%)	59	56	20, 30, 48, 74	0
All	All	3532/3660 (96%)	-0.41	67 (1%)	66	65	18, 29, 47, 74	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	586	GLN	4.7
1	F	588	ASN	3.9
1	E	362	TRP	3.8
1	F	443	ALA	3.7
1	A	588	ASN	3.6
1	B	306	ILE	3.3
1	C	443	ALA	3.3
1	D	1	MET	3.2
1	A	586	GLN	3.2
1	E	440	VAL	3.1
1	C	588	ASN	3.1
1	C	586	GLN	3.1
1	A	61	GLU	3.1
1	A	587	GLU	3.1
1	E	61	GLU	3.0
1	D	588	ASN	2.9
1	C	587	GLU	2.8
1	E	586	GLN	2.8
1	E	588	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	589	LEU	2.8
1	B	61	GLU	2.8
1	C	583	ARG	2.7
1	B	587	GLU	2.7
1	E	443	ALA	2.7
1	C	589	LEU	2.7
1	D	589	LEU	2.7
1	D	61	GLU	2.6
1	E	439	LEU	2.5
1	F	444	LYS	2.5
1	F	583	ARG	2.5
1	E	471	PHE	2.5
1	C	61	GLU	2.4
1	A	583	ARG	2.4
1	F	584	LYS	2.4
1	F	587	GLU	2.4
1	B	586	GLN	2.4
1	B	489	VAL	2.4
1	B	536	TRP	2.4
1	D	587	GLU	2.4
1	D	583	ARG	2.4
1	D	306	ILE	2.3
1	D	490	THR	2.3
1	F	362	TRP	2.3
1	E	583	ARG	2.3
1	E	306	ILE	2.3
1	B	588	ASN	2.3
1	F	589	LEU	2.3
1	D	536	TRP	2.2
1	B	111	GLU	2.2
1	A	255	LYS	2.2
1	F	484	ASP	2.2
1	B	482	GLN	2.2
1	C	584	LYS	2.2
1	B	537	ILE	2.2
1	B	1	MET	2.2
1	B	535	PRO	2.2
1	F	306	ILE	2.1
1	C	482	GLN	2.1
1	B	490	THR	2.1
1	C	2	SER	2.1
1	F	342	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	534	THR	2.1
1	B	2	SER	2.1
1	E	489	VAL	2.0
1	F	489	VAL	2.0
1	D	586	GLN	2.0
1	E	2	SER	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

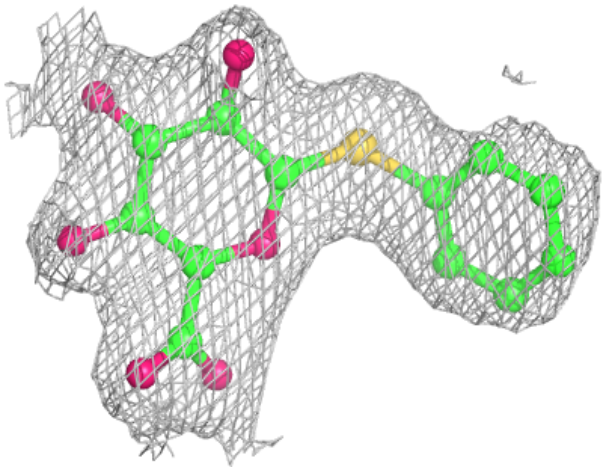
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

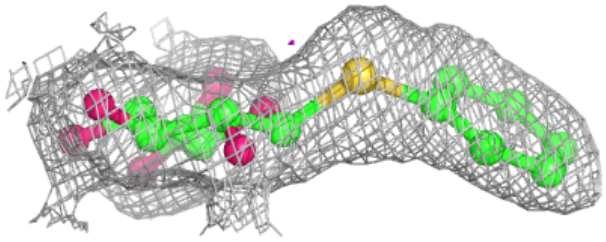
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	702	6/6	0.93	0.13	28,36,42,44	0
3	GOL	A	702	6/6	0.94	0.12	33,37,42,43	0
3	GOL	B	702	6/6	0.95	0.13	34,37,38,41	0
3	GOL	D	702	6/6	0.95	0.11	34,36,43,46	0
3	GOL	E	702	6/6	0.95	0.10	34,42,44,44	0
3	GOL	F	702	6/6	0.95	0.10	35,38,40,45	0
2	FYJ	E	701	19/19	0.96	0.12	27,33,37,38	0
2	FYJ	B	701	19/19	0.97	0.15	23,27,31,31	0
2	FYJ	F	701	19/19	0.97	0.11	25,32,38,39	0
2	FYJ	C	701	19/19	0.97	0.09	21,26,33,34	0
2	FYJ	D	701	19/19	0.97	0.10	21,25,38,41	0
2	FYJ	A	701	19/19	0.98	0.12	22,25,36,37	0

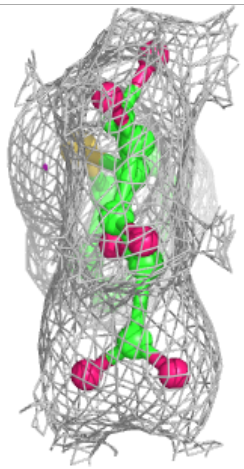
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FYJ E 701:

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

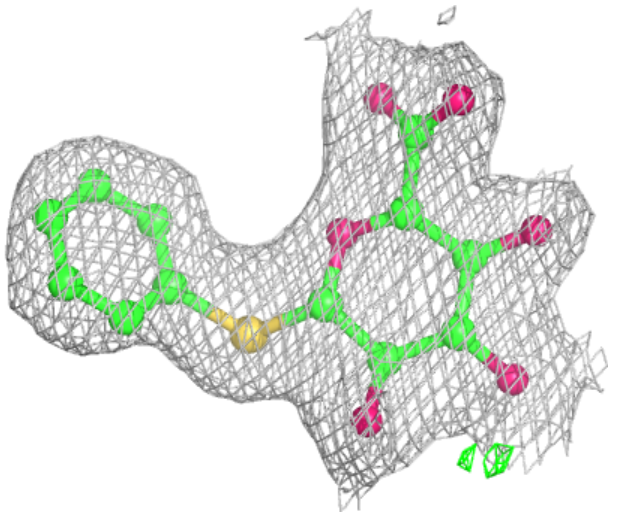


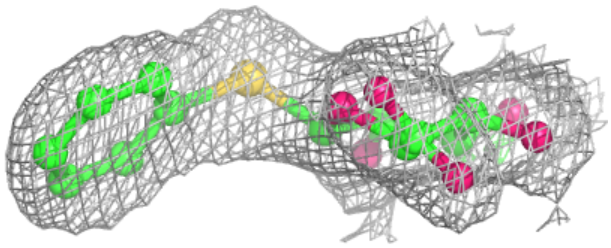


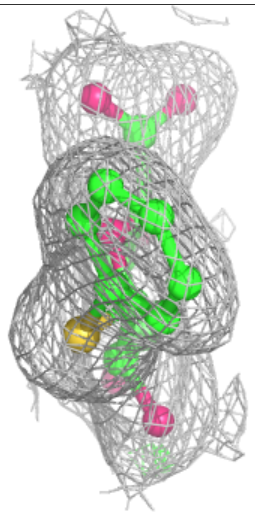


Electron density around FYJ B 701:

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

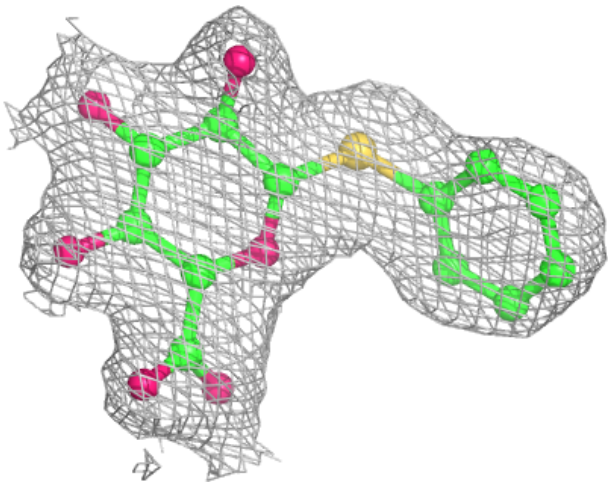


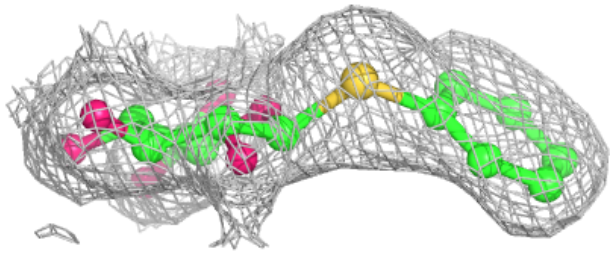


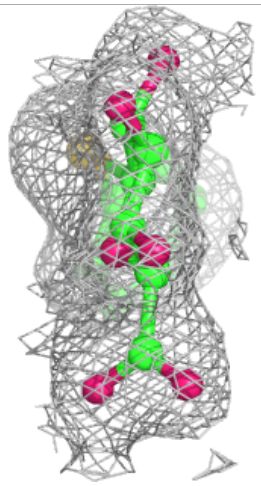


Electron density around FYJ F 701:

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

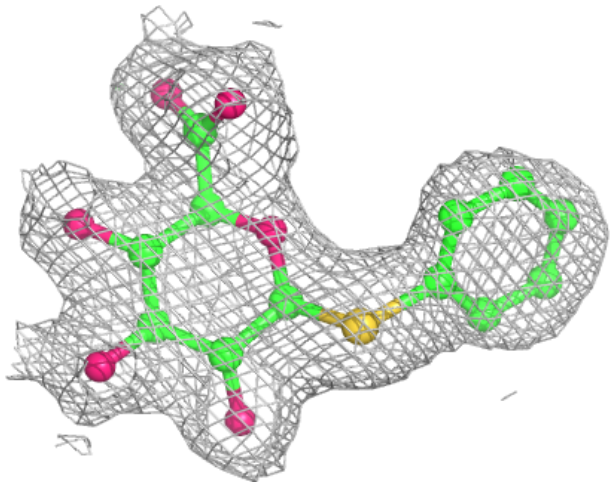


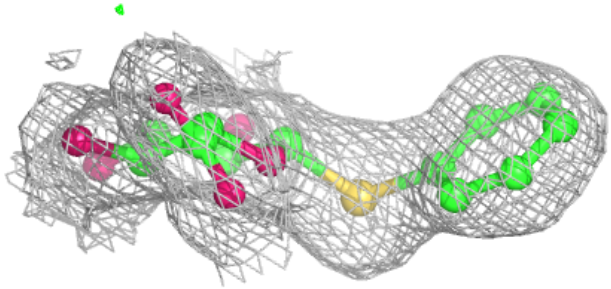


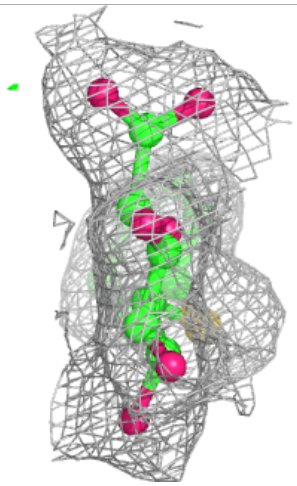


Electron density around FYJ C 701:

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

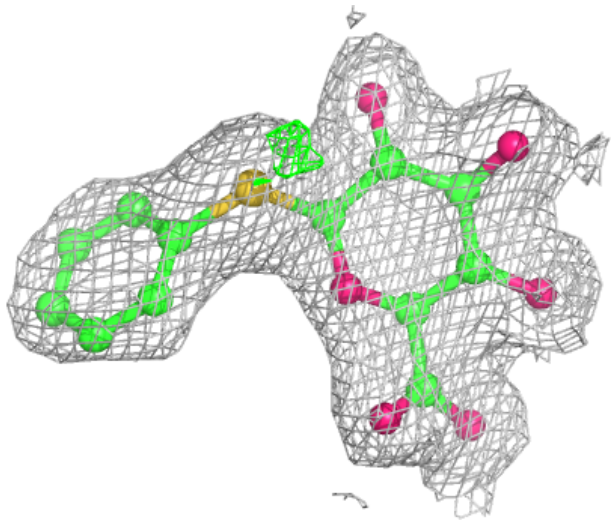


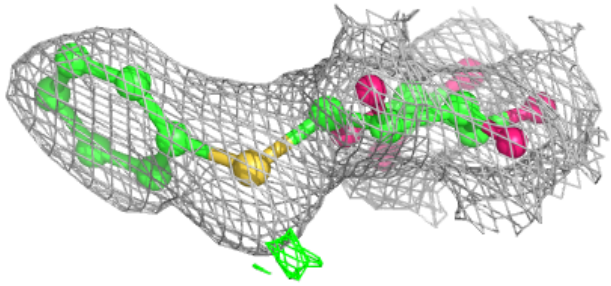


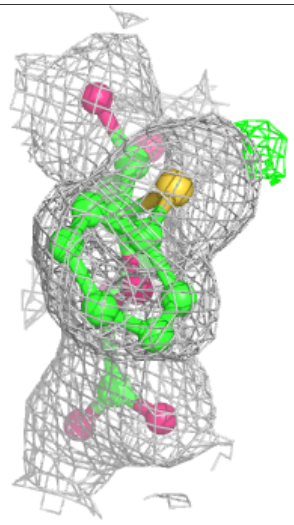


Electron density around FYJ D 701:

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

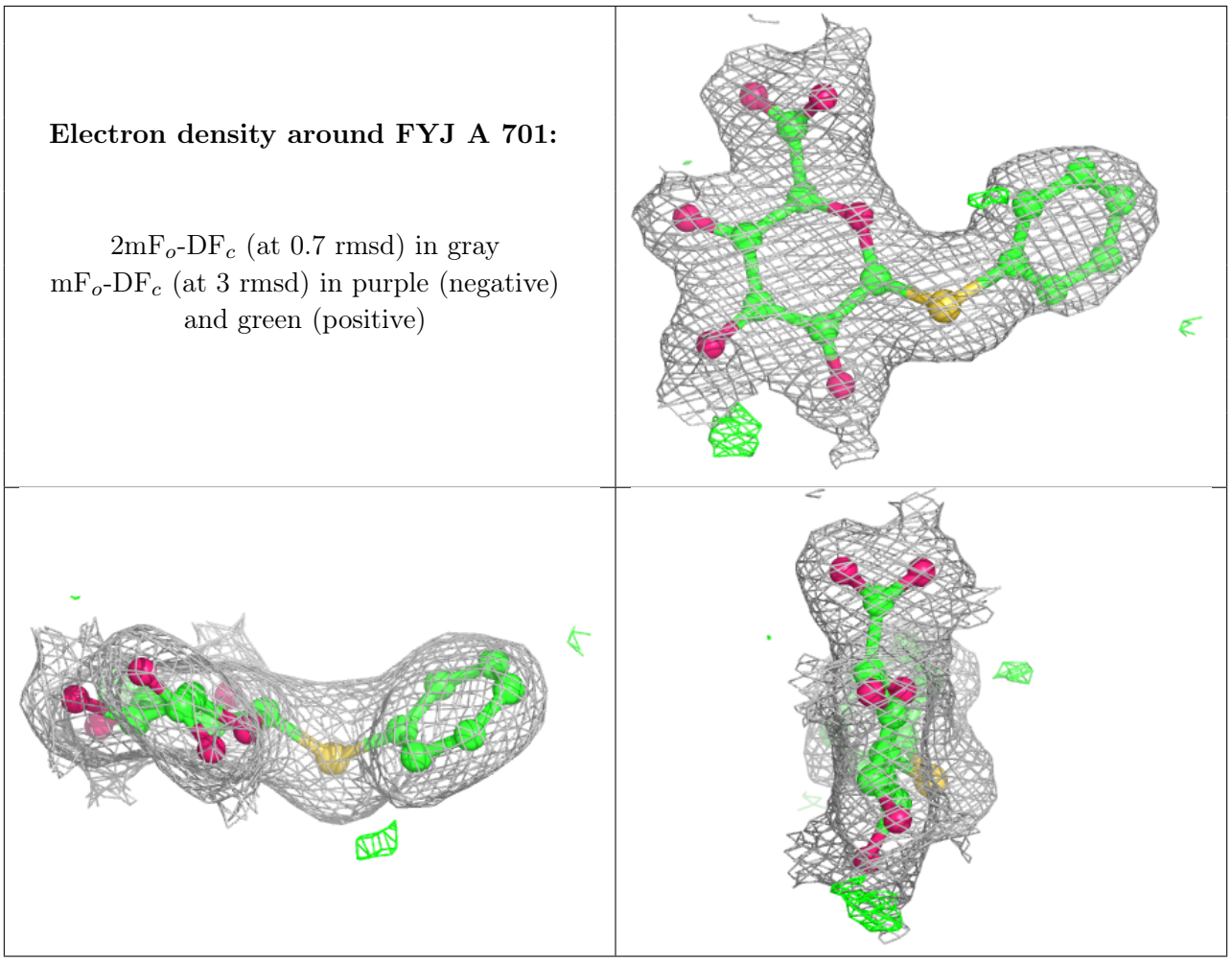






Electron density around FYJ A 701:

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



6.5 Other polymers

There are no such residues in this entry.