wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2024 – 02:33 pm GMT

PDB ID	:	6HWR
Title	:	Red kidney bean purple acid phosphatase in complex with adenosine divanadate
Authors	:	Feder, D.; Gahan, L.R.; McGeary, R.P.; Guddat, L.W.; Schenk, G.
Deposited on	:	2018-10-13
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

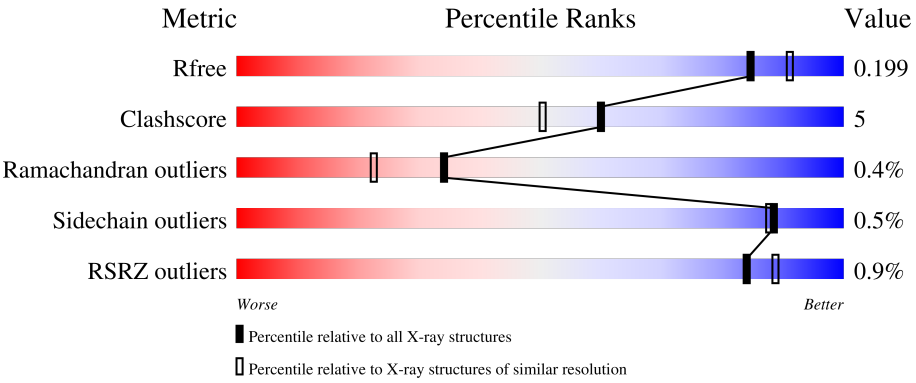
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	426	92% 8%
1	B	426	93% 6%
1	C	426	92% 7%
2	D	426	89% 10%
3	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	3	100%
3	H	3	100%
4	G	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	H1T	C	520	-	-	X	-
17	IPA	D	531	-	-	X	-
7	SO4	A	513	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 17001 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 Fe(3+)-Zn(2+) purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	423	Total	C	N	O	S	0	5	0
			3517	2258	612	637	10			
1	B	425	Total	C	N	O	S	0	4	0
			3529	2265	614	640	10			
1	A	424	Total	C	N	O	S	0	4	0
			3516	2258	608	640	10			

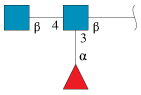
- Molecule 2 is a protein called Fe(3+)-Zn(2+) purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	426	Total	C	N	O	S	0	4	0
			3540	2271	617	641	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	364	ASP	ASN	conflict	UNP P80366

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

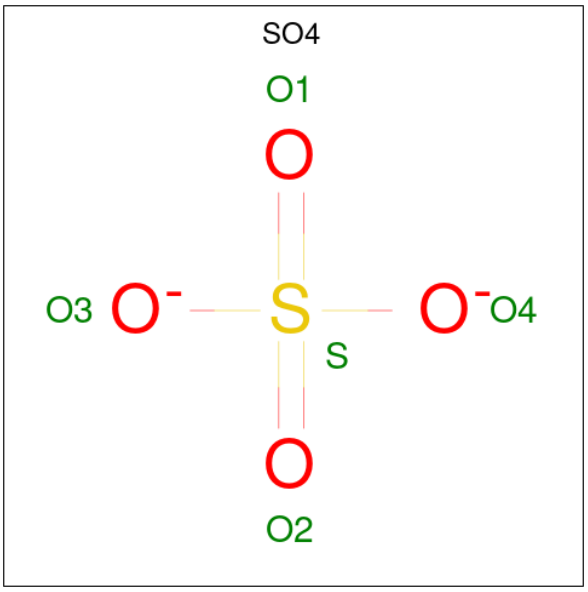
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Fe	0	0
			1	1		
6	B	1	Total	Fe	0	0
			1	1		
6	A	1	Total	Fe	0	0
			1	1		
6	D	1	Total	Fe	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0

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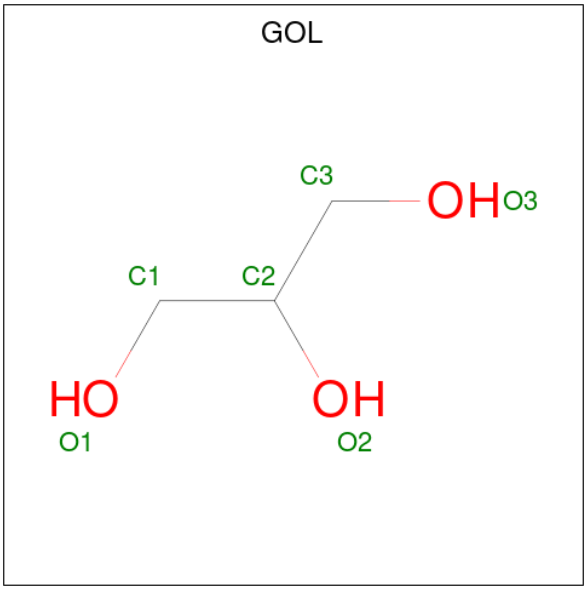
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 10 8 2	0	1
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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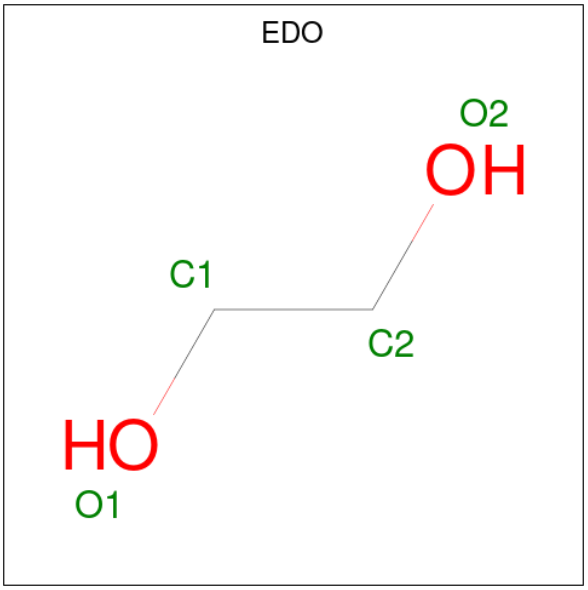
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0

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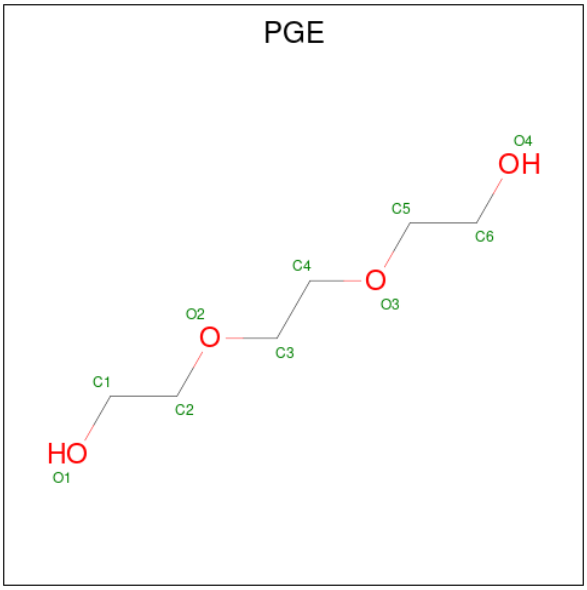
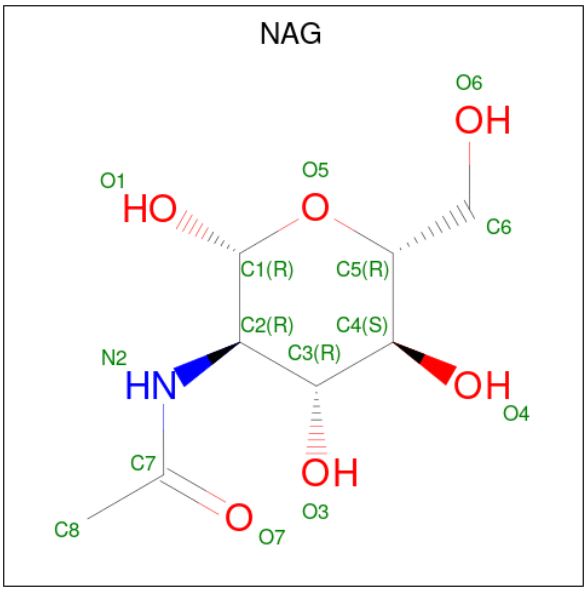
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 7 4 3	0	0
10	D	1	Total C O 7 4 3	0	0
10	D	1	Total C O 7 4 3	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

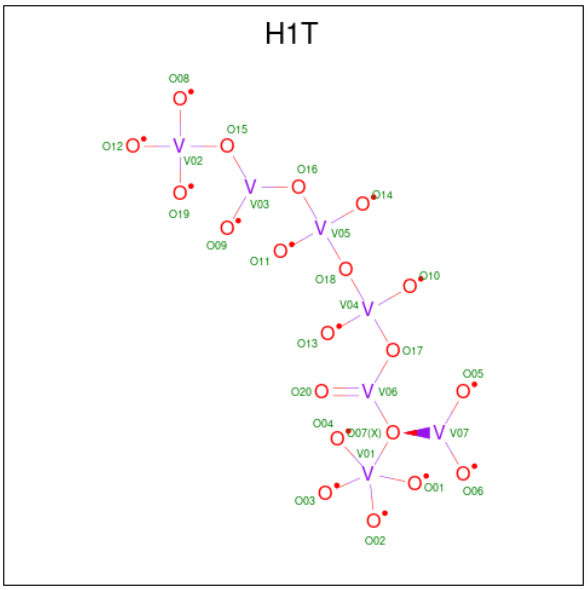


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

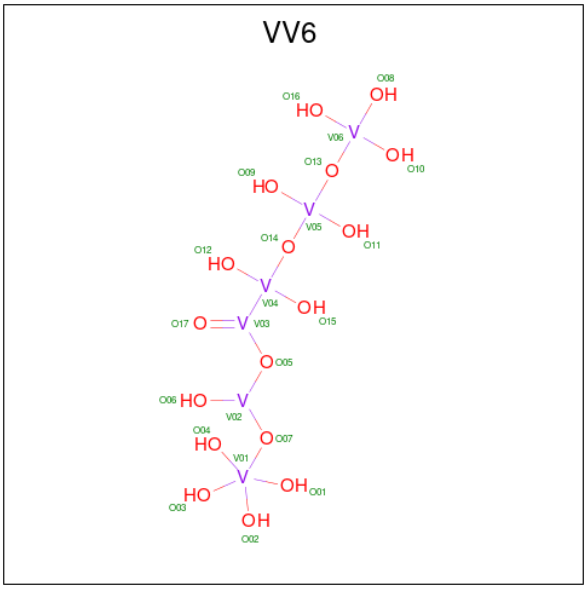
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Na 1 1	0	0
12	B	1	Total Na 1 1	0	0
12	A	2	Total Na 2 2	0	0
12	D	1	Total Na 1 1	0	0

- Molecule 13 is [[[[bis($l^{1}-oxidanyl)-[$l^{1}-oxidanyl-[tris($l^{1}-oxidanyl)vanadiooxy]vanadio]oxy-vanadio]oxy-bis($l^{1}-oxidanyl)vanadio]oxy-oxidanylidene-vanadio]-[bis($l^{1}-oxidanyl)vanadio]-$l^{3}-oxidanyl]-tetrakis($l^{1}-oxidanyl)vanadium (three-letter code: H1T) (formula: $O_{20}V_{7}$).



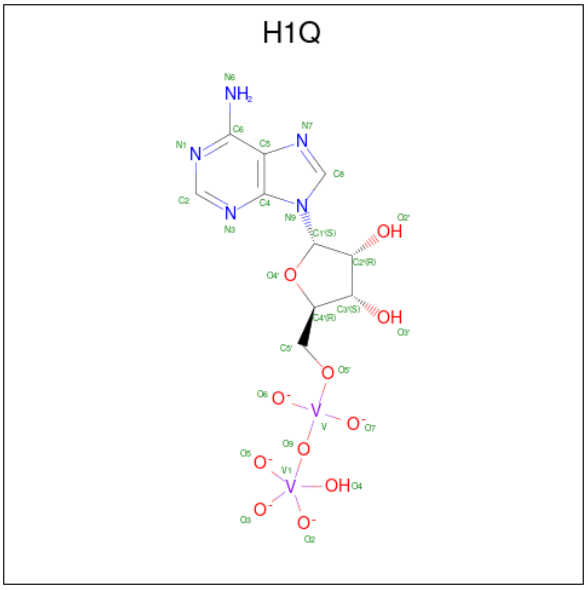
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total O V 27 20 7	0	0

- Molecule 14 is [[[[bis(oxidanyl)-[tris(oxidanyl)vanadiooxy]vanadio]oxy-bis(oxidanyl)vanadio]-oxidanylidene-vanadio]oxy-oxidanyl-vanadio]oxy-tetrakis(oxidanyl)vanadium (three-letter code: VV6) (formula: $H_{12}O_{17}V_{6}$).



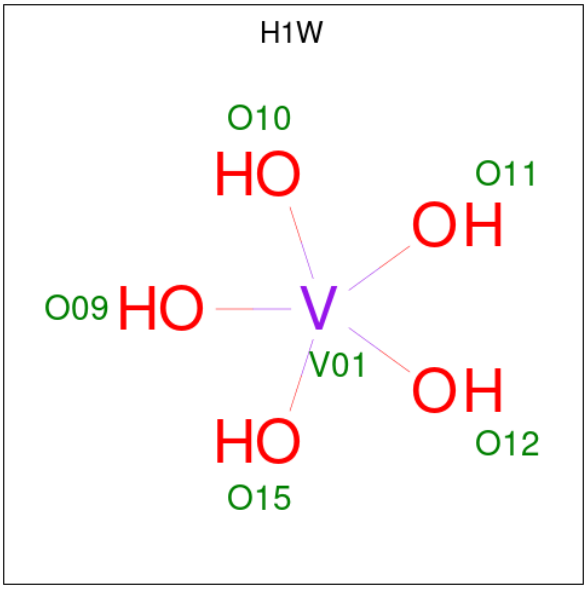
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total O V 23 17 6	0	0

- Molecule 15 is adenosine divanadate (three-letter code: H1Q) (formula: $C_{10}H_{13}N_5O_{11}V_2$).



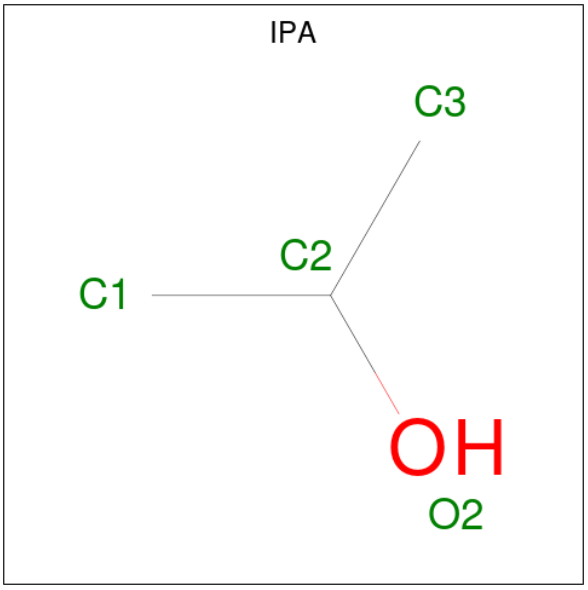
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O V 18 5 11 2	0	0

- Molecule 16 is pentakis(oxidanyl)vanadium (three-letter code: H1W) (formula: H_5O_5V).



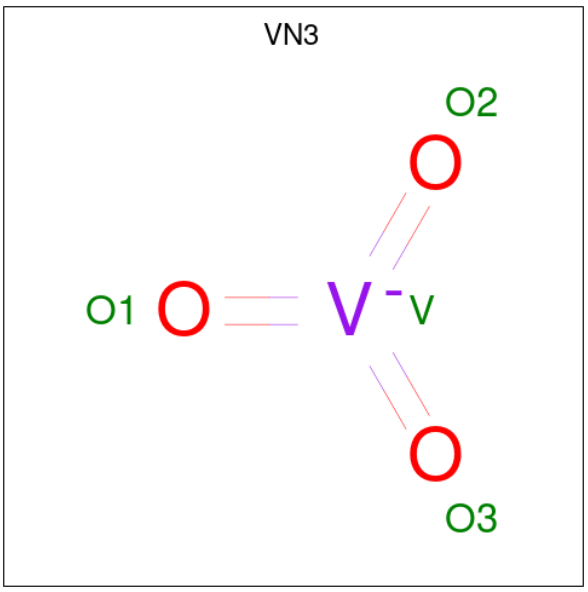
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total O V 12 10 2	0	1

- Molecule 17 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

- Molecule 18 is VANADATE ION (three-letter code: VN3) (formula: O_3V).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total O V 4 3 1	0	0

- Molecule 19 is water.

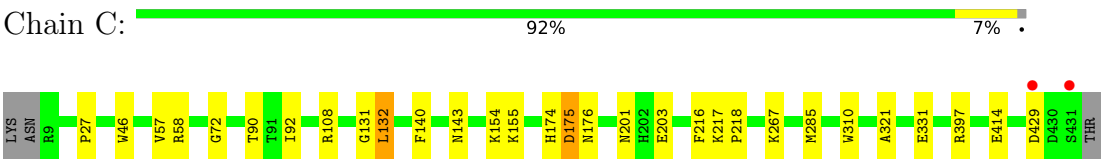
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	C	598	Total O 599 599	0	1
19	B	562	Total O 563 563	0	1
19	A	558	Total O 558 558	0	0
19	D	508	Total O 510 510	0	2

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.

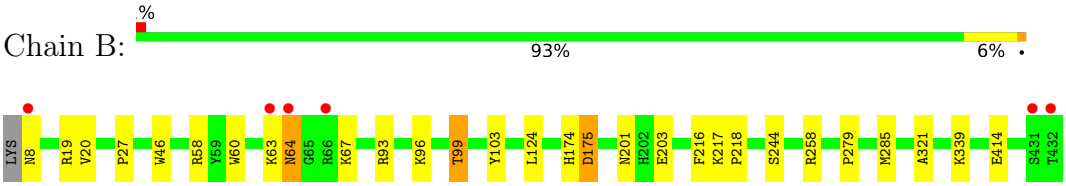
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain C:



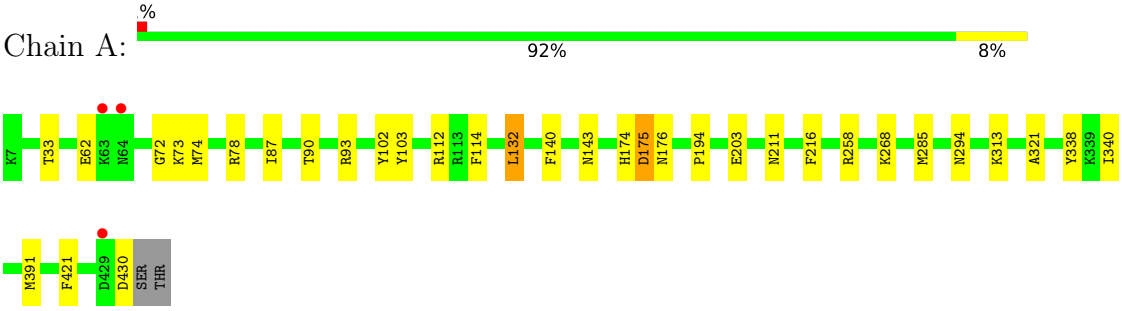
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain B:



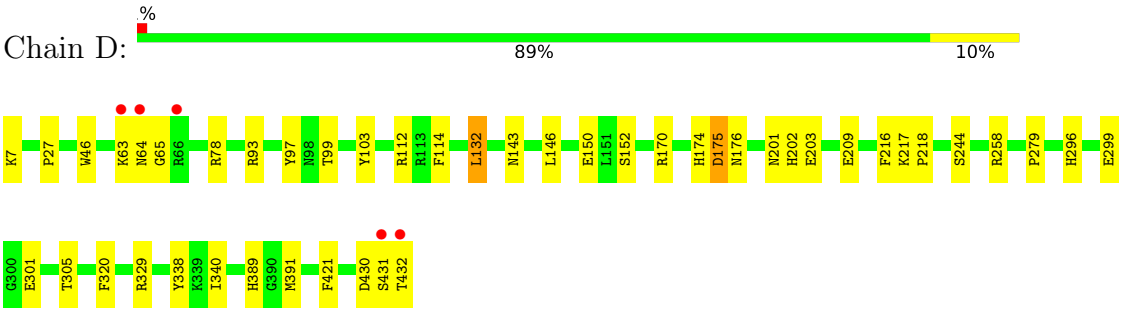
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain A:



• Molecule 2: Fe(3+)-Zn(2+) purple acid phosphatase

Chain D:

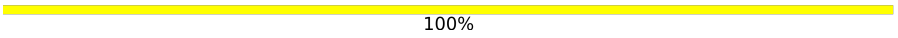


• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

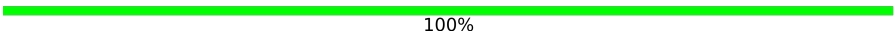
• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.24Å 126.24Å 296.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 1.95 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-1.95) 100.0 (19.97-1.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.163 , 0.199 0.163 , 0.199	Depositor DCC
R_{free} test set	2001 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17001	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, GOL, FUC, EDO, NAG, PGE, SO4, H1T, VN3, VV6, H1W, ZN, IPA, NA, H1Q

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	0.38	0/3644	0.56	1/4955 (0.0%)
1	B	0.38	0/3654	0.55	0/4968
1	C	0.39	0/3648	0.58	1/4958 (0.0%)
2	D	0.38	0/3665	0.57	1/4980 (0.0%)
All	All	0.38	0/14611	0.56	3/19861 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	132	LEU	CA-CB-CG	-8.47	95.81	115.30
2	D	132	LEU	CA-CB-CG	-6.74	99.80	115.30
1	A	132	LEU	CA-CB-CG	-6.32	100.76	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3516	0	3329	29	0
1	B	3529	0	3351	20	0
1	C	3517	0	3344	22	0
2	D	3540	0	3365	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	38	0	34	2	0
3	F	38	0	34	2	0
3	H	38	0	34	0	0
4	G	28	0	25	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	65	0	0	2	0
7	B	40	0	0	1	0
7	C	35	0	0	1	0
7	D	75	0	0	0	0
8	A	6	0	8	1	0
8	B	18	0	24	1	0
8	C	6	0	8	0	0
9	A	16	0	24	3	0
9	B	4	0	6	0	0
9	C	8	0	12	3	0
9	D	20	0	30	4	0
10	C	7	0	9	1	0
10	D	14	0	18	3	0
11	A	28	0	26	2	0
11	B	28	0	26	0	0
11	C	28	0	26	4	0
11	D	28	0	26	1	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	C	27	0	0	9	0
14	B	23	0	0	3	0
15	A	18	0	0	3	0
16	D	12	0	0	4	0
17	D	4	0	8	6	0
18	D	4	0	0	0	0
19	A	558	0	0	14	0
19	B	563	0	0	9	1
19	C	599	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	510	0	0	3	0
All	All	17001	0	13767	130	1

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.

The worst 5 of 130 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ARG:HH12	9:C:512:EDO:H12	1.37	0.88
2:D:112:ARG:HE	10:D:523:PGE:H4	1.45	0.80
1:C:143:ASN:HD22	11:C:517:NAG:H83	1.48	0.77
1:B:124:LEU:HD12	1:B:279:PRO:HG3	1.66	0.76
2:D:329:ARG:HH12	2:D:432:THR:HB	1.52	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:974:HOH:O	19:B:840:HOH:O[6_445]	2.17	0.03

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	426/426 (100%)	406 (95%)	19 (4%)	1 (0%)	47	38
1	B	427/426 (100%)	406 (95%)	19 (4%)	2 (0%)	29	17
1	C	426/426 (100%)	406 (95%)	17 (4%)	3 (1%)	22	11
2	D	428/426 (100%)	410 (96%)	17 (4%)	1 (0%)	47	38
All	All	1707/1704 (100%)	1628 (95%)	72 (4%)	7 (0%)	34	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	C	175	ASP
1	B	175	ASP
2	D	175	ASP
1	C	155	LYS

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	376/375 (100%)	374 (100%)	2 (0%)	88	88
1	B	378/375 (101%)	376 (100%)	2 (0%)	88	88
1	C	377/375 (100%)	376 (100%)	1 (0%)	92	92
2	D	379/375 (101%)	377 (100%)	2 (0%)	88	88
All	All	1510/1500 (101%)	1503 (100%)	7 (0%)	88	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	176	ASN
2	D	176	ASN
2	D	7	LYS
1	B	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

11 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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.48	0	17,19,21	0.68	0
3	FUC	E	2	3	10,10,11	0.78	0	14,14,16	0.81	0
3	NAG	E	3	3	14,14,15	0.50	0	17,19,21	0.45	0
3	NAG	F	1	3,1	14,14,15	0.32	0	17,19,21	0.64	1 (5%)
3	FUC	F	2	3	10,10,11	0.84	1 (10%)	14,14,16	0.98	1 (7%)
3	NAG	F	3	3	14,14,15	0.43	0	17,19,21	0.46	0
4	NAG	G	1	1,4	14,14,15	0.47	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.37	0
3	NAG	H	1	2,3	14,14,15	0.49	0	17,19,21	0.67	0
3	FUC	H	2	3	10,10,11	0.65	0	14,14,16	0.82	0
3	NAG	H	3	3	14,14,15	0.46	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	2/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	FUC	O5-C1	-2.09	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	FUC	C1-O5-C5	2.16	117.67	112.78
3	F	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	3	NAG	C8-C7-N2-C2
3	E	3	NAG	O7-C7-N2-C2
3	F	3	NAG	C8-C7-N2-C2

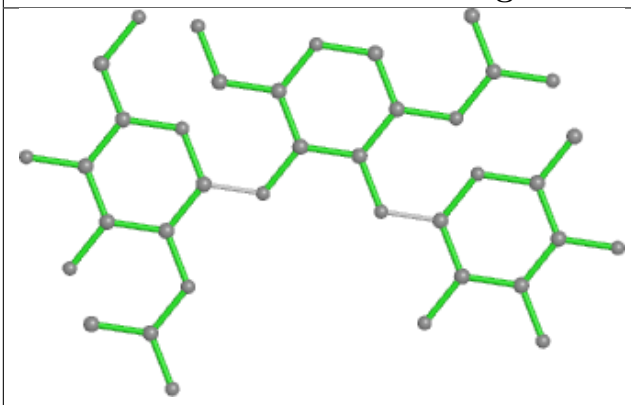
There are no ring outliers.

4 monomers are involved in 5 short contacts:

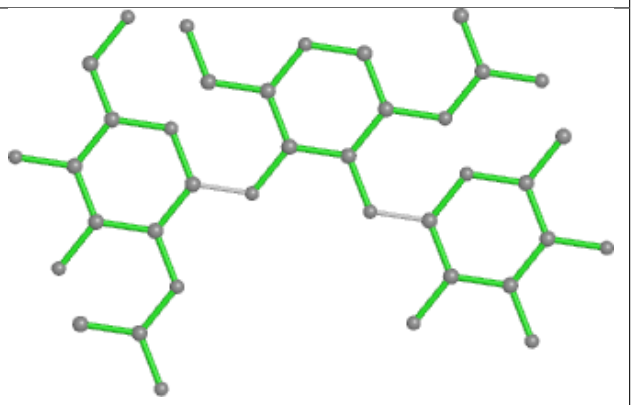
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	NAG	2	0
3	E	3	NAG	1	0
3	E	1	NAG	1	0
4	G	2	NAG	1	0

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

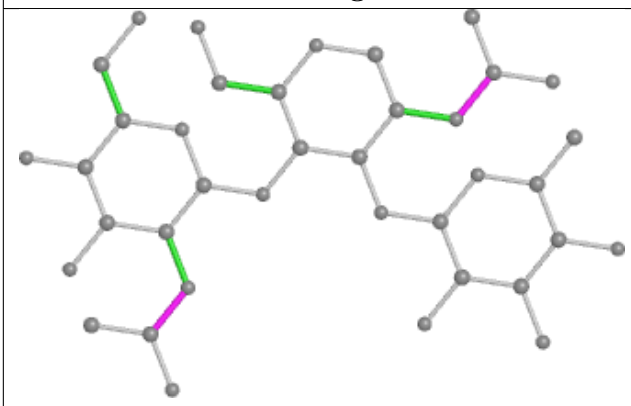
Oligosaccharide Chain E



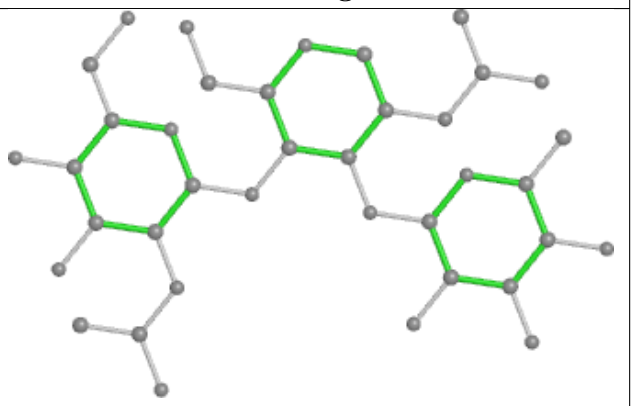
Bond lengths



Bond angles

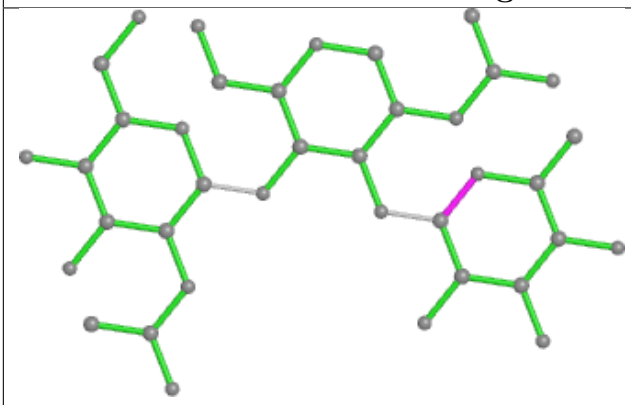


Torsions

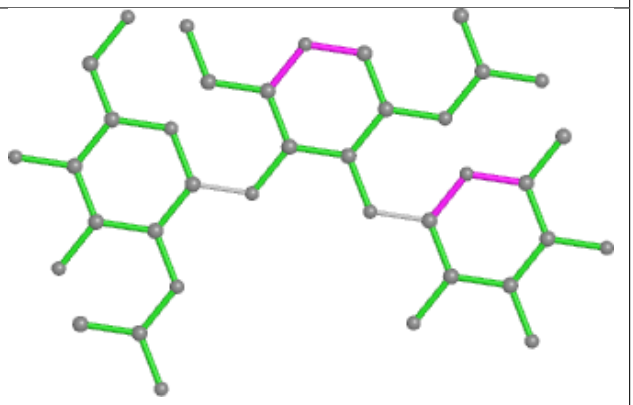


Rings

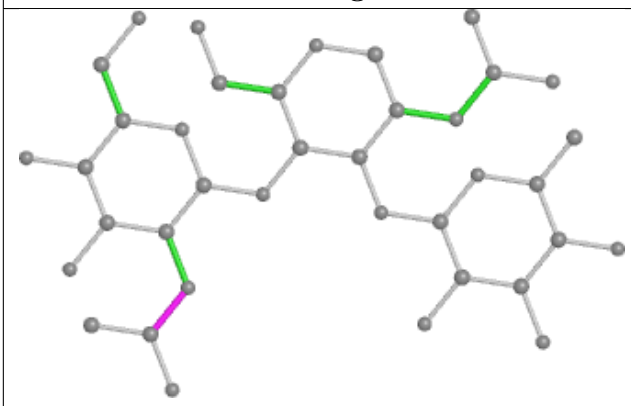
Oligosaccharide Chain F



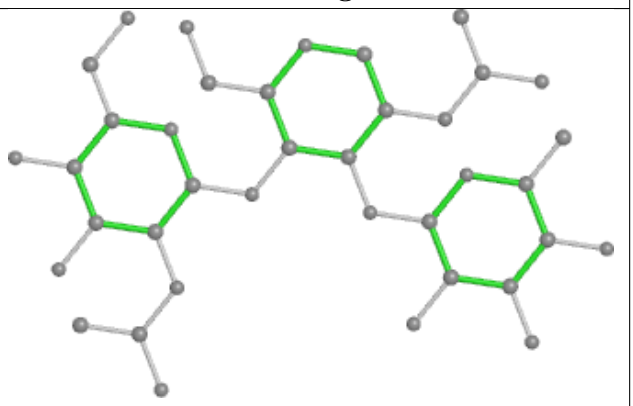
Bond lengths



Bond angles

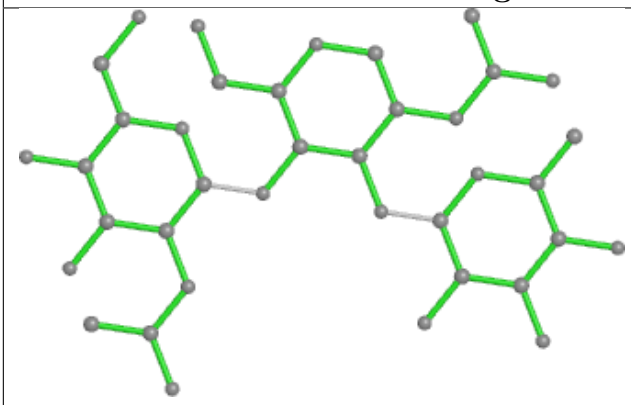


Torsions

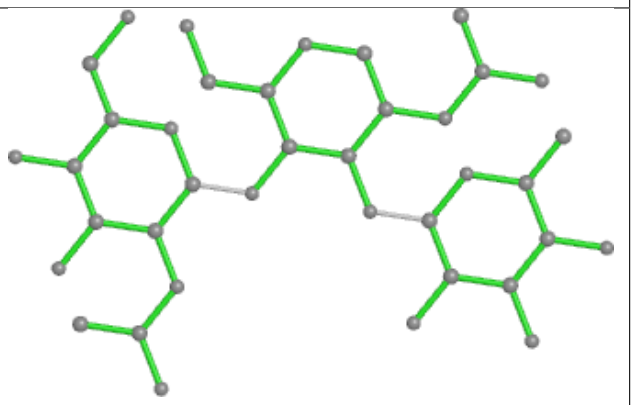


Rings

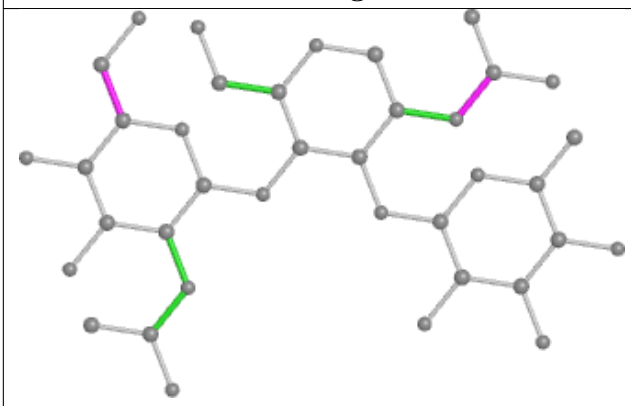
Oligosaccharide Chain H



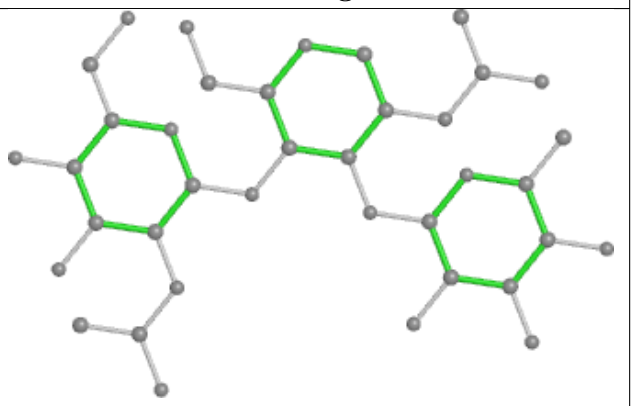
Bond lengths



Bond angles

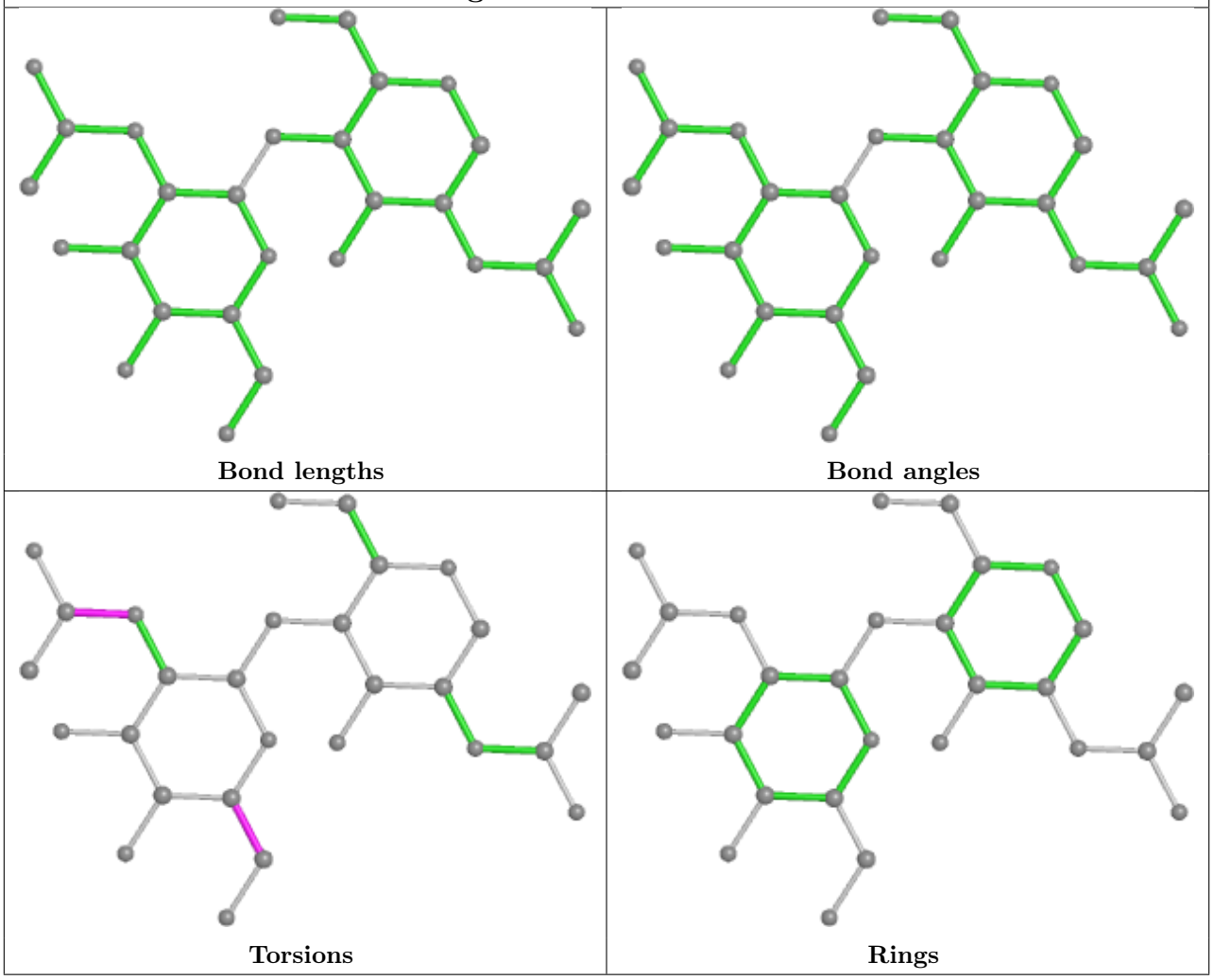


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 91 ligands modelled in this entry, 13 are monoatomic - leaving 78 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	$\#\|Z\| > 2$
9	EDO	D	521	-	3,3,3	0.46	0	2,2,2	0.34	0
7	SO4	D	510	-	4,4,4	0.16	0	6,6,6	0.21	0
7	SO4	A	504	-	4,4,4	0.11	0	6,6,6	0.29	0
7	SO4	C	503	-	4,4,4	0.20	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GOL	B	511	-	5,5,5	0.89	0	5,5,5	1.03	0
7	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.11	0
7	SO4	A	510	-	4,4,4	0.11	0	6,6,6	0.07	0
17	IPA	D	531	-	3,3,3	0.50	0	3,3,3	0.32	0
7	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.20	0
7	SO4	C	506	-	4,4,4	0.07	0	6,6,6	0.20	0
9	EDO	D	517	-	3,3,3	0.44	0	2,2,2	0.53	0
7	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.12	0
7	SO4	A	512	-	4,4,4	0.12	0	6,6,6	0.16	0
9	EDO	C	511	-	3,3,3	0.38	0	2,2,2	0.75	0
7	SO4	B	508	-	4,4,4	0.13	0	6,6,6	0.13	0
9	EDO	A	520	-	3,3,3	0.52	0	2,2,2	0.24	0
14	VV6	B	521	5,6	1,22,22	1.95	0	-		
11	NAG	B	518	1	14,14,15	0.45	0	17,19,21	0.46	0
7	SO4	D	509	-	4,4,4	0.17	0	6,6,6	0.09	0
7	SO4	D	513[A]	-	4,4,4	0.15	0	6,6,6	0.21	0
8	GOL	B	513	-	5,5,5	0.97	0	5,5,5	1.02	0
9	EDO	C	512	-	3,3,3	0.54	0	2,2,2	0.17	0
11	NAG	A	524	1	14,14,15	0.44	0	17,19,21	0.51	0
7	SO4	D	513[B]	-	4,4,4	0.16	0	6,6,6	0.22	0
9	EDO	A	518	-	3,3,3	0.47	0	2,2,2	0.40	0
7	SO4	A	511	-	4,4,4	0.21	0	6,6,6	0.17	0
7	SO4	D	512	-	4,4,4	0.11	0	6,6,6	0.22	0
7	SO4	D	516	-	4,4,4	0.16	0	6,6,6	0.09	0
7	SO4	B	507	-	4,4,4	0.12	0	6,6,6	0.17	0
11	NAG	D	527	2	14,14,15	0.42	0	17,19,21	0.48	0
7	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.05	0
10	PGE	D	522	-	6,6,9	0.18	0	5,5,8	1.64	1 (20%)
11	NAG	D	528	2	14,14,15	0.52	0	17,19,21	0.51	0
9	EDO	D	518	-	3,3,3	0.47	0	2,2,2	0.38	0
10	PGE	C	513	-	6,6,9	0.15	0	5,5,8	1.40	0
7	SO4	A	513	-	4,4,4	0.19	0	6,6,6	0.47	0
7	SO4	B	509	-	4,4,4	0.10	0	6,6,6	0.14	0
7	SO4	D	511	-	4,4,4	0.14	0	6,6,6	0.16	0
7	SO4	D	508	-	4,4,4	0.09	0	6,6,6	0.26	0
16	H1W	D	530[A]	5,6	0,5,5	-	-	-		
7	SO4	C	504	-	4,4,4	0.09	0	6,6,6	0.15	0
7	SO4	A	507	-	4,4,4	0.19	0	6,6,6	0.15	0
7	SO4	D	506	-	4,4,4	0.11	0	6,6,6	0.21	0
9	EDO	D	520	-	3,3,3	0.48	0	2,2,2	0.29	0
7	SO4	D	515	-	4,4,4	0.17	0	6,6,6	0.23	0
7	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.12	0
16	H1W	D	530[B]	5,6	0,5,5	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	EDO	A	519	-	3,3,3	0.51	0	2,2,2	0.33	0
7	SO4	B	510	-	4,4,4	0.16	0	6,6,6	0.13	0
15	H1Q	A	527	5,12,6	10,18,30	1.05	1 (10%)	9,30,49	0.68	0
7	SO4	A	515	-	4,4,4	0.22	0	6,6,6	0.42	0
11	NAG	C	517	1	14,14,15	0.44	0	17,19,21	0.61	0
11	NAG	A	523	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
7	SO4	C	505	-	4,4,4	0.20	0	6,6,6	0.21	0
8	GOL	A	516	-	5,5,5	1.02	0	5,5,5	1.11	0
7	SO4	D	504	-	4,4,4	0.25	0	6,6,6	0.16	0
7	SO4	C	509	-	4,4,4	0.14	0	6,6,6	0.08	0
7	SO4	A	514	-	4,4,4	0.13	0	6,6,6	0.10	0
9	EDO	A	517	-	3,3,3	0.46	0	2,2,2	0.52	0
7	SO4	D	507	12	4,4,4	0.18	0	6,6,6	0.23	0
7	SO4	A	509	-	4,4,4	0.17	0	6,6,6	0.26	0
7	SO4	A	508	-	4,4,4	0.17	0	6,6,6	0.10	0
10	PGE	D	523	-	6,6,9	0.32	0	5,5,8	0.23	0
7	SO4	D	514	-	4,4,4	0.14	0	6,6,6	0.10	0
7	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.13	0
13	H1T	C	520	5,12,6	0,26,26	-	-	-		
9	EDO	D	519	-	3,3,3	0.46	0	2,2,2	0.39	0
8	GOL	B	512	-	5,5,5	0.86	0	5,5,5	1.20	1 (20%)
7	SO4	A	505	-	4,4,4	0.12	0	6,6,6	0.15	0
18	VN3	D	532	-	0,3,3	-	-	-		
11	NAG	C	518	1	14,14,15	0.46	0	17,19,21	0.61	1 (5%)
7	SO4	C	507	-	4,4,4	0.16	0	6,6,6	0.10	0
9	EDO	B	514	-	3,3,3	0.50	0	2,2,2	0.40	0
7	SO4	C	508	-	4,4,4	0.13	0	6,6,6	0.23	0
7	SO4	B	504	-	4,4,4	0.12	0	6,6,6	0.42	0
7	SO4	B	505	-	4,4,4	0.12	0	6,6,6	0.14	0
8	GOL	C	510	-	5,5,5	1.13	0	5,5,5	0.90	0
11	NAG	B	519	1	14,14,15	0.43	0	17,19,21	0.44	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
9	EDO	D	521	-	-	0/1/1/1	-
8	GOL	B	513	-	-	2/4/4/4	-
9	EDO	C	512	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	524	1	-	0/6/23/26	0/1/1/1
9	EDO	A	518	-	-	0/1/1/1	-
8	GOL	B	511	-	-	0/4/4/4	-
9	EDO	D	520	-	-	0/1/1/1	-
9	EDO	A	517	-	-	0/1/1/1	-
9	EDO	A	519	-	-	0/1/1/1	-
10	PGE	D	523	-	-	3/4/4/7	-
15	H1Q	A	527	5,12,6	-	0/2/26/33	0/1/1/3
11	NAG	C	517	1	-	2/6/23/26	0/1/1/1
11	NAG	A	523	1	-	4/6/23/26	0/1/1/1
9	EDO	D	519	-	-	0/1/1/1	-
11	NAG	D	527	2	-	4/6/23/26	0/1/1/1
9	EDO	D	517	-	-	0/1/1/1	-
8	GOL	B	512	-	-	0/4/4/4	-
9	EDO	C	511	-	-	1/1/1/1	-
9	EDO	A	520	-	-	1/1/1/1	-
11	NAG	C	518	1	-	0/6/23/26	0/1/1/1
8	GOL	A	516	-	-	3/4/4/4	-
9	EDO	B	514	-	-	1/1/1/1	-
10	PGE	D	522	-	-	0/4/4/7	-
11	NAG	D	528	2	-	2/6/23/26	0/1/1/1
9	EDO	D	518	-	-	0/1/1/1	-
10	PGE	C	513	-	-	1/4/4/7	-
11	NAG	B	518	1	-	0/6/23/26	0/1/1/1
8	GOL	C	510	-	-	0/4/4/4	-
11	NAG	B	519	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	527	H1Q	O9-V1	2.45	1.92	1.68

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	523	NAG	C1-O5-C5	2.38	115.42	112.19
8	B	512	GOL	C3-C2-C1	-2.19	103.19	111.70
10	D	522	PGE	O2-C2-C1	-2.18	100.48	110.07
11	C	518	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	513	GOL	O1-C1-C2-C3
8	A	516	GOL	O1-C1-C2-C3
11	C	517	NAG	C8-C7-N2-C2
11	C	517	NAG	O7-C7-N2-C2
11	A	523	NAG	C8-C7-N2-C2

There are no ring outliers.

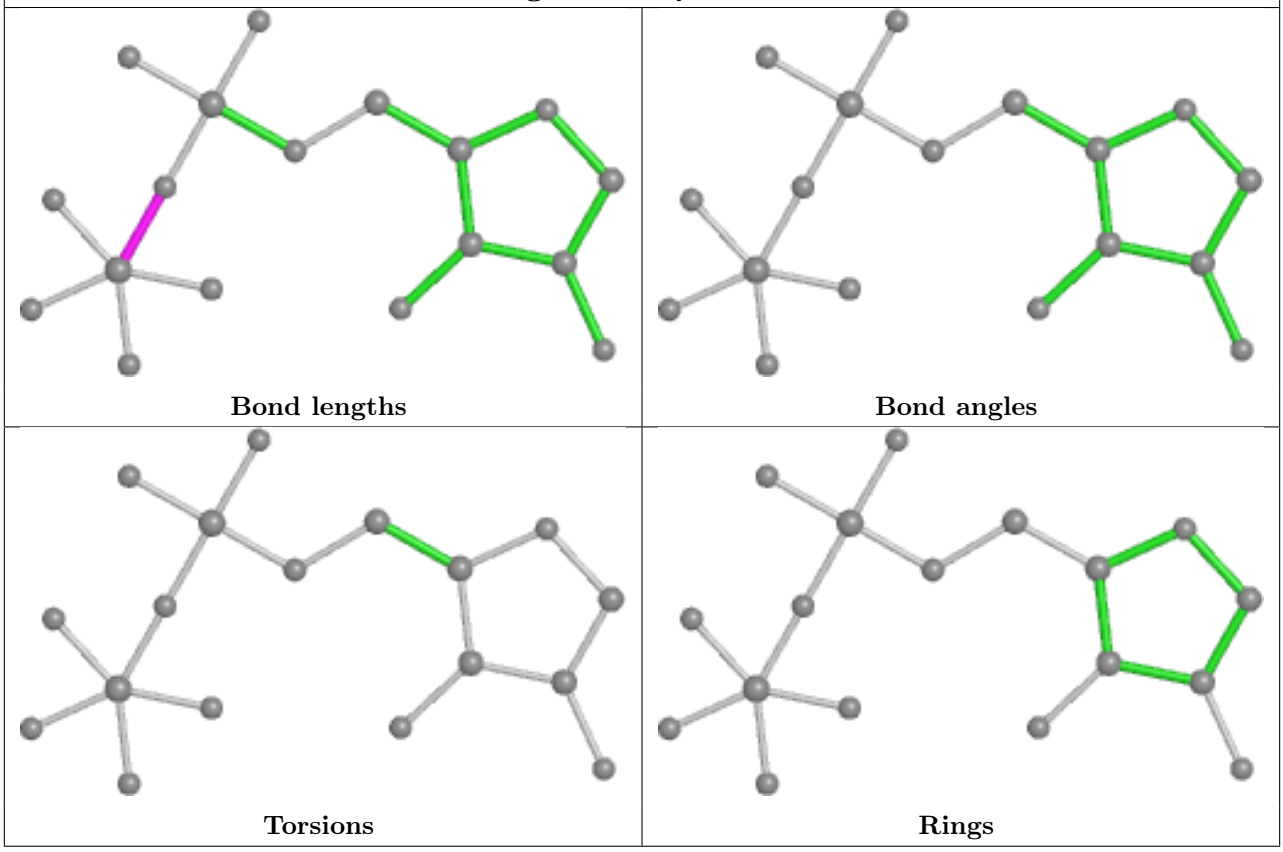
25 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	521	EDO	1	0
17	D	531	IPA	6	0
9	D	517	EDO	1	0
9	C	511	EDO	1	0
9	A	520	EDO	2	0
14	B	521	VV6	3	0
9	C	512	EDO	2	0
11	D	527	NAG	1	0
10	D	522	PGE	1	0
9	D	518	EDO	1	0
10	C	513	PGE	1	0
7	A	513	SO4	2	0
16	D	530[A]	H1W	1	0
7	C	504	SO4	1	0
9	D	520	EDO	1	0
16	D	530[B]	H1W	3	0
15	A	527	H1Q	3	0
11	C	517	NAG	4	0
11	A	523	NAG	2	0
8	A	516	GOL	1	0
9	A	517	EDO	1	0
10	D	523	PGE	2	0
13	C	520	H1T	9	0
8	B	512	GOL	1	0
7	B	504	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 H1Q A 527



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	424/426 (99%)	-0.57	3 (0%)	87	92	11, 18, 31, 61	0
1	B	425/426 (99%)	-0.52	6 (1%)	75	82	11, 19, 32, 61	0
1	C	423/426 (99%)	-0.65	2 (0%)	91	94	11, 16, 29, 54	0
2	D	426/426 (100%)	-0.56	5 (1%)	79	84	11, 17, 33, 59	0
All	All	1698/1704 (99%)	-0.58	16 (0%)	84	89	11, 17, 31, 61	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ASN	5.2
1	A	64	ASN	4.9
2	D	64	ASN	4.8
2	D	431	SER	4.6
1	C	431	SER	4.5

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

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
4	NAG	G	2	14/15	0.84	0.26	26,40,49,56	0
3	FUC	H	2	10/11	0.88	0.22	35,39,46,52	0

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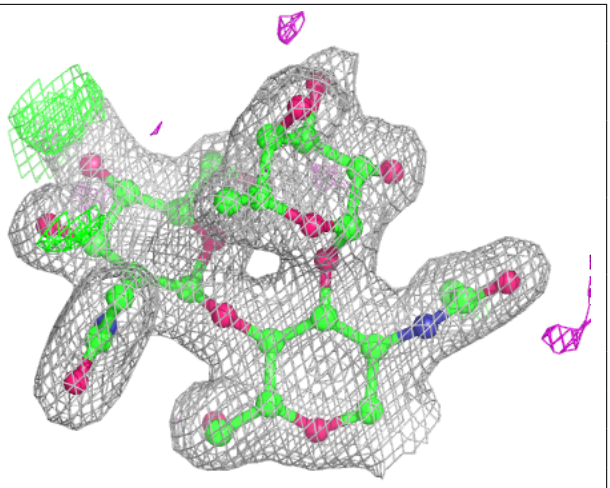
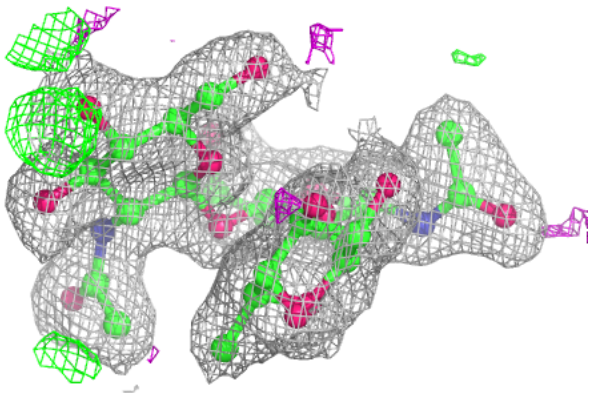
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	3	14/15	0.91	0.24	26,36,48,50	0
3	NAG	F	3	14/15	0.92	0.12	16,27,30,36	0
3	NAG	E	3	14/15	0.93	0.14	16,25,33,34	0
4	NAG	G	1	14/15	0.94	0.11	19,26,34,34	0
3	NAG	H	1	14/15	0.94	0.10	20,26,33,43	0
3	NAG	F	1	14/15	0.95	0.09	17,20,28,29	0
3	FUC	F	2	10/11	0.95	0.10	22,26,35,36	0
3	FUC	E	2	10/11	0.95	0.19	27,29,31,38	0
3	NAG	E	1	14/15	0.95	0.08	17,20,27,32	0

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

Electron density around Chain E:

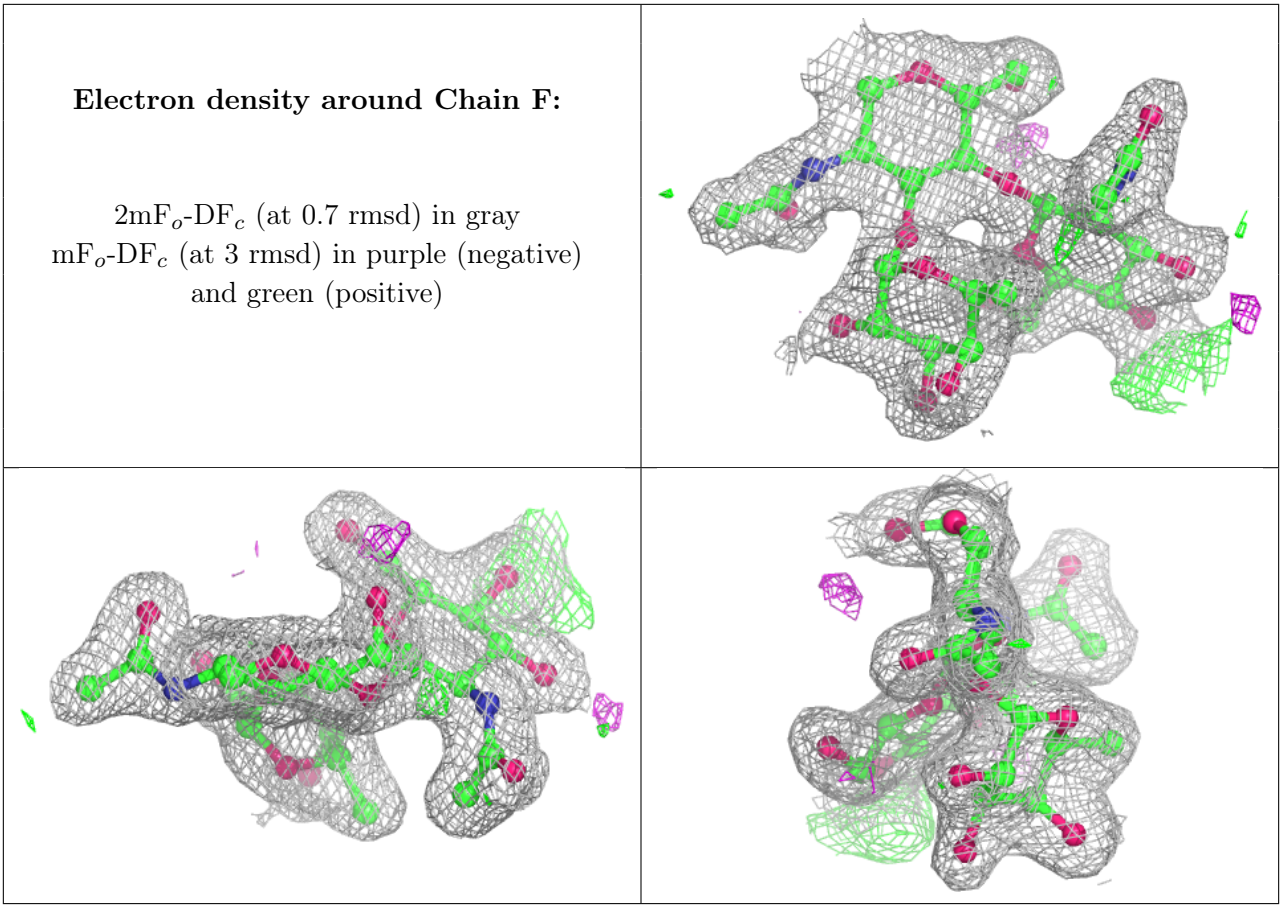
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





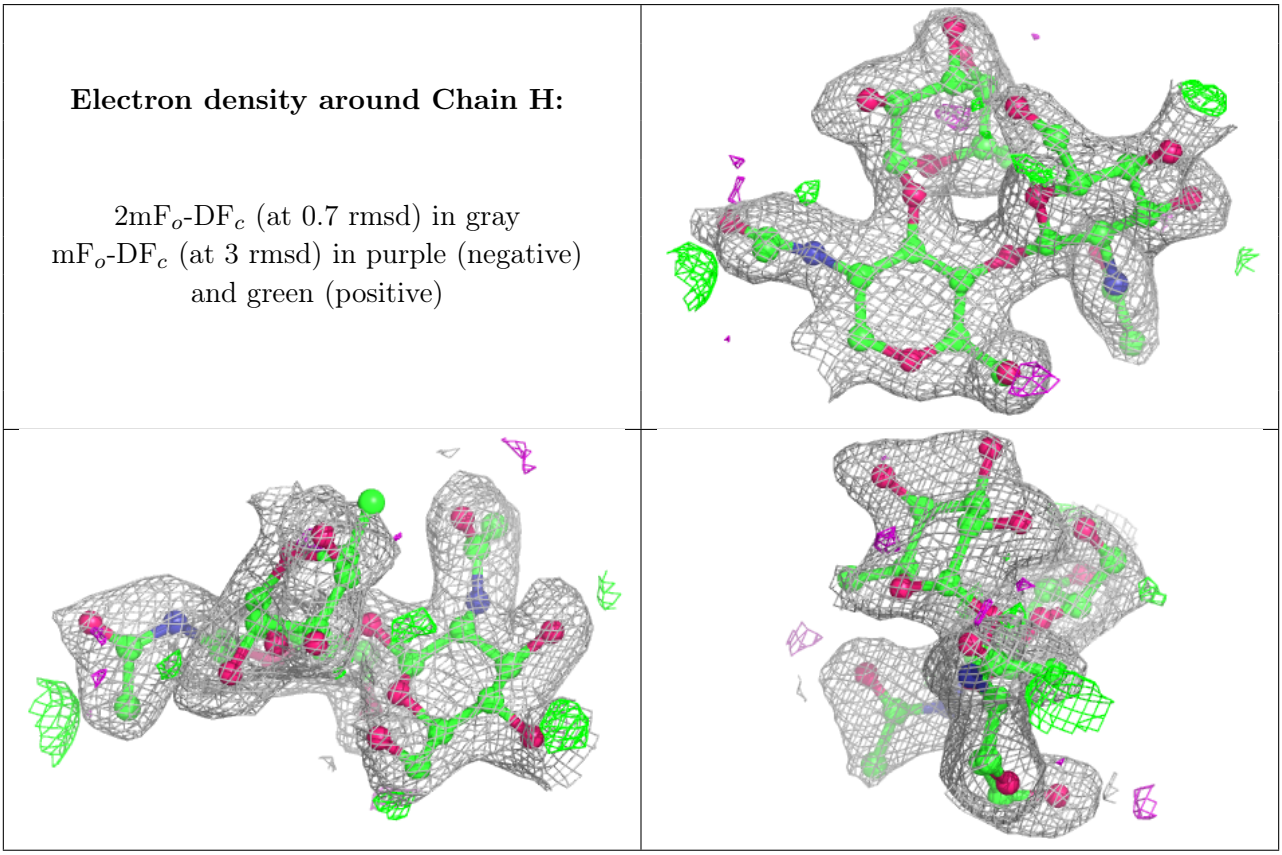
Electron density around Chain F:

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



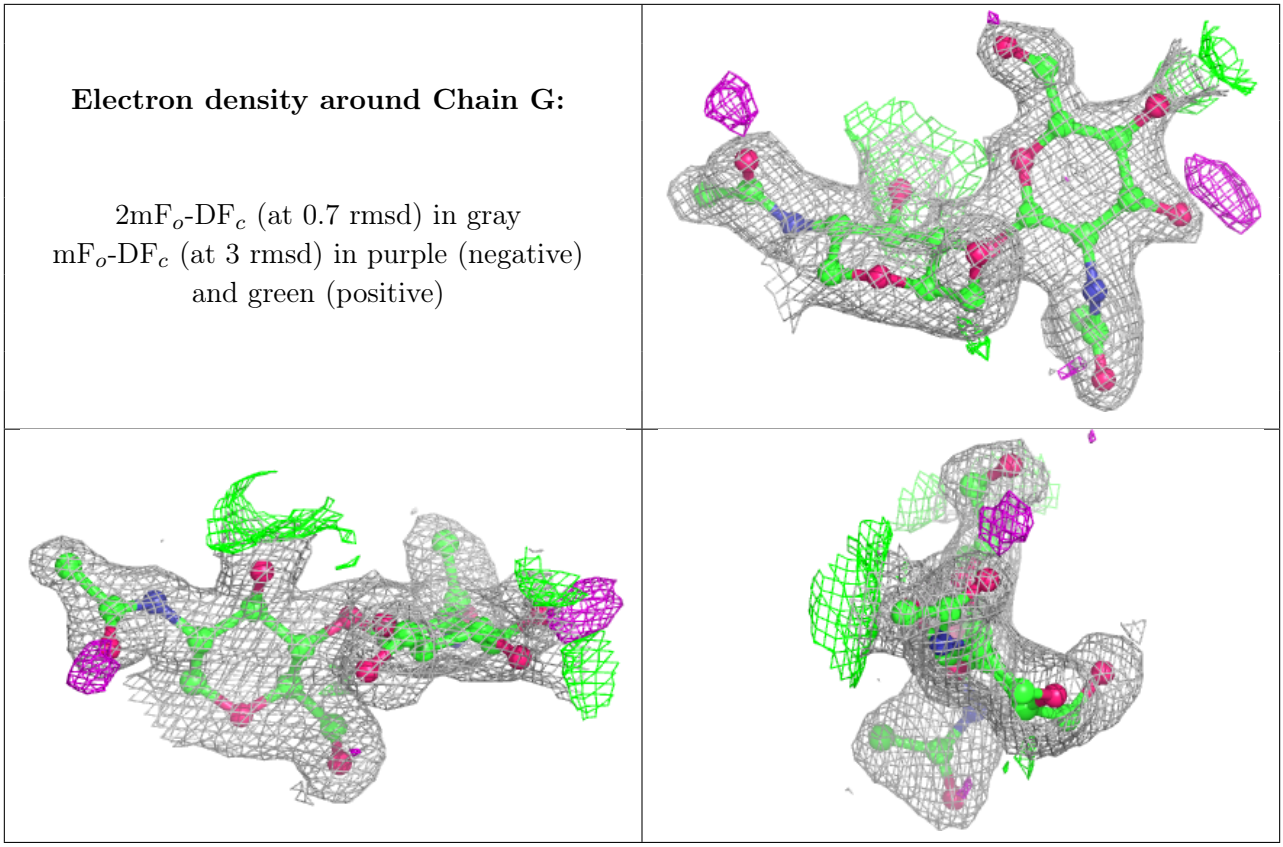
Electron density around Chain H:

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



Electron density around Chain G:

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



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
9	EDO	A	520	4/4	0.76	0.12	40,44,44,51	0
9	EDO	A	517	4/4	0.80	0.16	36,40,47,53	0
9	EDO	D	521	4/4	0.82	0.21	55,55,60,62	0
17	IPA	D	531	4/4	0.82	0.23	17,23,33,41	0
11	NAG	D	528	14/15	0.84	0.15	32,38,45,48	0
14	VV6	B	521	23/23	0.84	0.29	19,47,67,82	23
9	EDO	C	512	4/4	0.84	0.25	37,43,44,44	0
10	PGE	D	523	7/10	0.85	0.20	34,41,48,49	0
12	NA	A	526	1/1	0.86	0.14	44,44,44,44	1
9	EDO	A	518	4/4	0.87	0.13	36,38,40,51	0
13	H1T	C	520	27/27	0.87	0.29	15,43,60,78	27
9	EDO	D	518	4/4	0.88	0.25	44,45,48,61	0
9	EDO	C	511	4/4	0.88	0.18	18,23,33,43	0
18	VN3	D	532	4/4	0.88	0.29	44,50,56,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	A	511	5/5	0.89	0.29	48,48,67,70	0
8	GOL	B	512	6/6	0.89	0.25	36,39,41,47	0
11	NAG	A	524	14/15	0.89	0.21	33,36,46,56	0
7	SO4	D	503	5/5	0.90	0.30	61,64,76,77	0
7	SO4	A	509	5/5	0.90	0.27	46,52,71,76	0
8	GOL	B	513	6/6	0.90	0.30	29,37,40,41	0
7	SO4	C	507	5/5	0.90	0.26	35,41,72,76	0
7	SO4	A	512	5/5	0.90	0.21	29,47,51,52	0
7	SO4	A	514	5/5	0.90	0.36	45,51,74,79	0
9	EDO	A	519	4/4	0.91	0.12	35,39,40,47	0
7	SO4	A	505	5/5	0.91	0.33	47,60,76,77	0
9	EDO	D	517	4/4	0.91	0.21	32,35,36,44	0
7	SO4	D	511	5/5	0.91	0.23	54,59,72,73	0
7	SO4	A	506	5/5	0.91	0.37	46,48,70,76	0
10	PGE	C	513	7/10	0.91	0.13	18,26,35,37	0
7	SO4	A	515	5/5	0.91	0.29	35,39,50,51	0
11	NAG	C	518	14/15	0.92	0.17	28,34,41,44	0
15	H1Q	A	527	18/28	0.92	0.27	22,38,51,70	18
11	NAG	B	518	14/15	0.92	0.18	29,35,43,43	0
9	EDO	D	519	4/4	0.92	0.27	32,45,48,57	0
7	SO4	A	503	5/5	0.93	0.31	69,70,75,83	0
11	NAG	A	523	14/15	0.93	0.14	17,27,35,42	0
7	SO4	A	507	5/5	0.93	0.33	43,51,59,59	0
7	SO4	D	504	5/5	0.93	0.23	35,42,50,58	0
7	SO4	C	509	5/5	0.93	0.34	45,61,71,77	0
9	EDO	D	520	4/4	0.93	0.11	32,39,40,40	0
9	EDO	B	514	4/4	0.93	0.18	26,36,39,42	0
7	SO4	D	514	5/5	0.93	0.36	58,64,70,77	0
7	SO4	D	515	5/5	0.93	0.28	40,45,70,70	0
7	SO4	D	516	5/5	0.93	0.49	51,71,79,85	0
7	SO4	D	513[A]	5/5	0.94	0.15	18,22,28,28	5
11	NAG	D	527	14/15	0.94	0.13	18,24,36,37	0
7	SO4	D	513[B]	5/5	0.94	0.15	15,22,28,30	5
10	PGE	D	522	7/10	0.94	0.13	17,23,36,42	0
7	SO4	A	513	5/5	0.94	0.27	41,41,45,47	0
11	NAG	C	517	14/15	0.94	0.10	13,23,30,34	0
7	SO4	B	510	5/5	0.94	0.26	42,55,62,65	0
7	SO4	D	505	5/5	0.94	0.31	39,46,67,68	0
7	SO4	A	504	5/5	0.94	0.23	30,36,52,58	0
7	SO4	D	512	5/5	0.95	0.41	41,55,59,61	0
7	SO4	B	507	5/5	0.95	0.31	42,59,64,65	0
7	SO4	A	508	5/5	0.95	0.33	55,56,65,68	0

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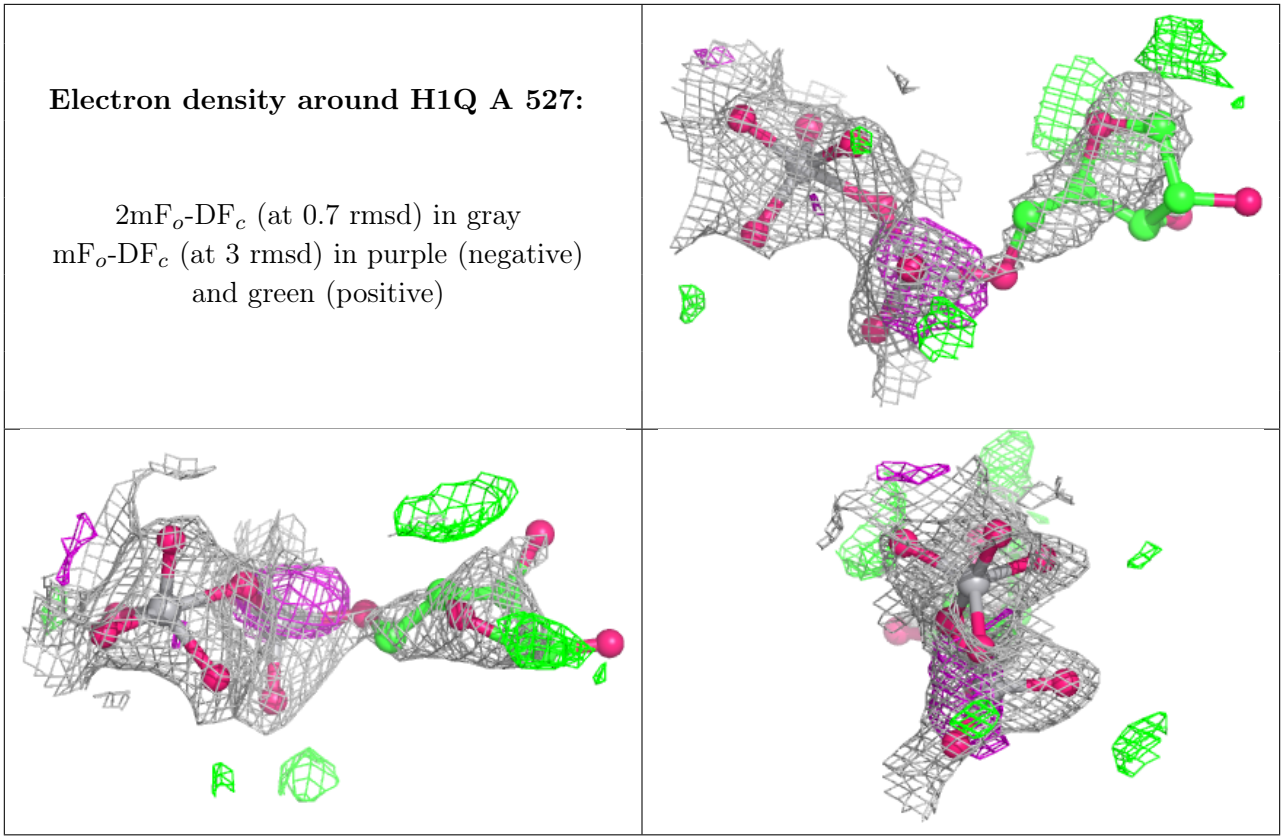
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	C	504	5/5	0.95	0.22	36,41,43,45	0
7	SO4	D	506	5/5	0.95	0.19	24,32,41,46	0
7	SO4	D	508	5/5	0.95	0.17	28,40,43,51	0
8	GOL	B	511	6/6	0.95	0.09	22,34,37,46	0
7	SO4	D	510	5/5	0.95	0.30	44,54,61,71	0
7	SO4	B	504	5/5	0.95	0.21	35,40,47,50	0
11	NAG	B	519	14/15	0.95	0.10	19,25,33,36	0
7	SO4	C	508	5/5	0.96	0.23	44,55,62,69	0
7	SO4	C	506	5/5	0.96	0.25	31,47,51,53	0
7	SO4	B	508	5/5	0.97	0.27	45,49,53,61	0
7	SO4	D	509	5/5	0.97	0.29	44,57,61,62	0
8	GOL	C	510	6/6	0.97	0.06	17,17,21,23	0
16	H1W	D	530[A]	6/6	0.97	0.20	20,22,30,33	6
16	H1W	D	530[B]	6/6	0.97	0.20	22,29,31,46	6
7	SO4	B	505	5/5	0.97	0.19	33,43,49,54	0
7	SO4	C	505	5/5	0.97	0.23	38,41,44,44	0
7	SO4	B	509	5/5	0.98	0.16	30,34,36,42	0
7	SO4	B	503	5/5	0.98	0.18	24,28,39,40	0
7	SO4	B	506	5/5	0.98	0.27	38,39,47,47	0
8	GOL	A	516	6/6	0.98	0.07	20,23,24,25	0
7	SO4	A	510	5/5	0.98	0.29	36,44,48,49	0
12	NA	C	519	1/1	0.99	0.15	32,32,32,32	0
7	SO4	C	503	5/5	0.99	0.05	24,26,27,28	0
7	SO4	D	507	5/5	0.99	0.19	28,39,43,44	0
12	NA	B	520	1/1	1.00	0.15	9,9,9,9	0
12	NA	A	525	1/1	1.00	0.13	9,9,9,9	0
5	ZN	C	501	1/1	1.00	0.02	20,20,20,20	0
12	NA	D	529	1/1	1.00	0.15	10,10,10,10	0
5	ZN	B	501	1/1	1.00	0.02	23,23,23,23	0
5	ZN	A	501	1/1	1.00	0.03	20,20,20,20	1
5	ZN	D	501	1/1	1.00	0.02	19,19,19,19	1
6	FE	C	502	1/1	1.00	0.02	21,21,21,21	1
6	FE	B	502	1/1	1.00	0.05	21,21,21,21	1
6	FE	A	502	1/1	1.00	0.02	19,19,19,19	1
6	FE	D	502	1/1	1.00	0.03	22,22,22,22	1

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 H1Q A 527:

$2mF_o$-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 (i)

There are no such residues in this entry.