



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 07:19 pm BST

PDB ID : 9QYW / pdb\_00009qyw  
Title : MINPP1 from Bacteroides thetaiotaomicron R275W mutant complex with myo-inositol hexakisulfate  
Authors : Shang, X.Y.; Salmon, M.; Hemmings, A.M.  
Deposited on : 2025-04-22  
Resolution : 1.76 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

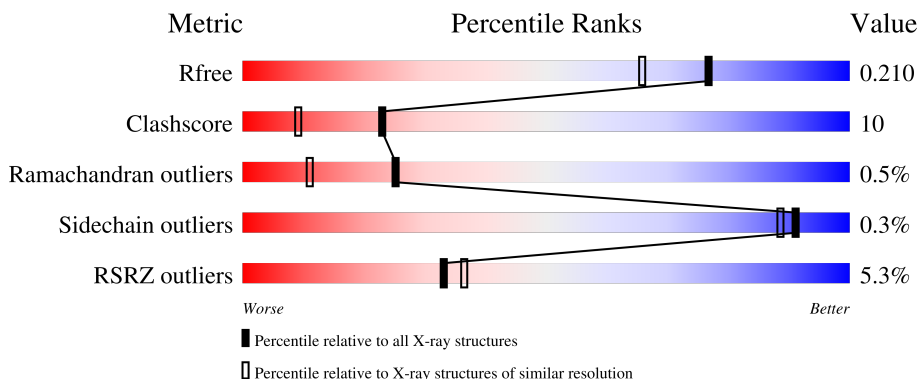
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	B	426	<div> <div>6%</div> <div>74%</div> <div>19%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7415 atoms, of which 46 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 Multiple inositol polyphosphate phosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	8	0
			3313	2145	561	588	19			
1	B	398	Total	C	N	O	S	3	8	0
			3294	2133	558	584	19			

There are 44 discrepancies between the modelled and reference sequences:

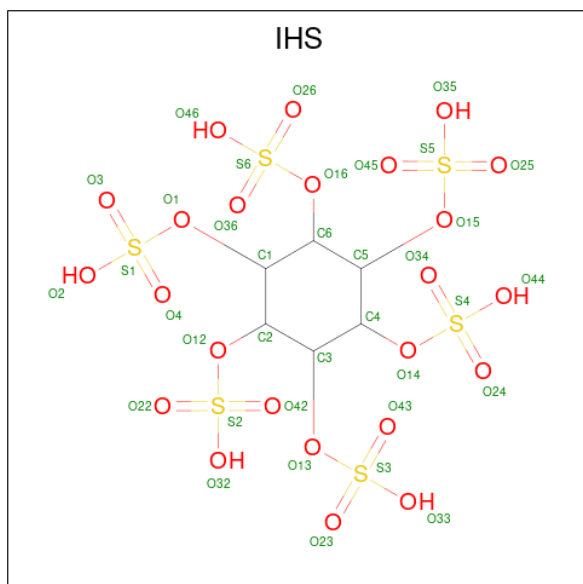
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q89YI8
A	1	GLY	-	expression tag	UNP Q89YI8
A	2	SER	-	expression tag	UNP Q89YI8
A	3	SER	-	expression tag	UNP Q89YI8
A	4	HIS	-	expression tag	UNP Q89YI8
A	5	HIS	-	expression tag	UNP Q89YI8
A	6	HIS	-	expression tag	UNP Q89YI8
A	7	HIS	-	expression tag	UNP Q89YI8
A	8	HIS	-	expression tag	UNP Q89YI8
A	9	HIS	-	expression tag	UNP Q89YI8
A	10	SER	-	expression tag	UNP Q89YI8
A	11	SER	-	expression tag	UNP Q89YI8
A	12	GLY	-	expression tag	UNP Q89YI8
A	13	LEU	-	expression tag	UNP Q89YI8
A	14	VAL	-	expression tag	UNP Q89YI8
A	15	PRO	-	expression tag	UNP Q89YI8
A	16	ARG	-	expression tag	UNP Q89YI8
A	17	GLY	-	expression tag	UNP Q89YI8
A	18	SER	-	expression tag	UNP Q89YI8
A	19	HIS	-	expression tag	UNP Q89YI8
A	20	MET	-	expression tag	UNP Q89YI8
A	275	TRP	ARG	engineered mutation	UNP Q89YI8
B	0	MET	-	initiating methionine	UNP Q89YI8
B	1	GLY	-	expression tag	UNP Q89YI8
B	2	SER	-	expression tag	UNP Q89YI8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP Q89YI8
B	4	HIS	-	expression tag	UNP Q89YI8
B	5	HIS	-	expression tag	UNP Q89YI8
B	6	HIS	-	expression tag	UNP Q89YI8
B	7	HIS	-	expression tag	UNP Q89YI8
B	8	HIS	-	expression tag	UNP Q89YI8
B	9	HIS	-	expression tag	UNP Q89YI8
B	10	SER	-	expression tag	UNP Q89YI8
B	11	SER	-	expression tag	UNP Q89YI8
B	12	GLY	-	expression tag	UNP Q89YI8
B	13	LEU	-	expression tag	UNP Q89YI8
B	14	VAL	-	expression tag	UNP Q89YI8
B	15	PRO	-	expression tag	UNP Q89YI8
B	16	ARG	-	expression tag	UNP Q89YI8
B	17	GLY	-	expression tag	UNP Q89YI8
B	18	SER	-	expression tag	UNP Q89YI8
B	19	HIS	-	expression tag	UNP Q89YI8
B	20	MET	-	expression tag	UNP Q89YI8
B	275	TRP	ARG	engineered mutation	UNP Q89YI8

- Molecule 2 is D-MYO-INOSITOL-HEXASULPHATE (CCD ID: IHS) (formula:  $C_6H_{12}O_{24}S_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			48	6	12	24	6		

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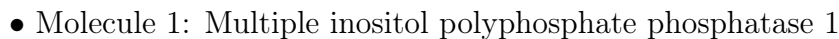
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			46	6	10	24	6		
2	B	1	Total	C	H	O	S	0	0
			48	6	12	24	6		
2	B	1	Total	C	H	O	S	0	0
			48	6	12	24	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	329	Total	O	0	0
			329	329		
3	B	289	Total	O	0	0
			289	289		



- Molecule 1: Multiple inositol polyphosphate phosphatase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.92Å 119.01Å 75.31Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	71.80 – 1.76 71.80 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.80-1.76) 92.5 (71.80-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.179 , 0.209 0.180 , 0.210	Depositor DCC
$R_{free}$ test set	4347 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: IHS

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	0.33	0/3426	0.52	0/4636
1	B	0.32	0/3403	0.52	0/4606
All	All	0.32	0/6829	0.52	0/9242

There are no bond length outliers.

There are no bond angle outliers.

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	3313	0	3324	52	0
1	B	3294	0	3303	78	1
2	A	72	22	24	6	0
2	B	72	24	24	5	1
3	A	329	0	0	14	1
3	B	289	0	0	15	1
All	All	7369	46	6675	137	2

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 10.

All (137) 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:B:176:LYS:NZ	3:B:601:HOH:O	1.80	1.14
1:A:68:LYS:HE3	1:A:68:LYS:HA	1.43	0.97
1:A:274:LEU:HG	1:A:278:MET:HE2	1.53	0.90
2:A:501:IHS:S2	3:A:604:HOH:O	2.31	0.89
1:B:48:MET:HG2	1:B:370:TYR:HD2	1.40	0.87
1:A:347:ASP:OD2	3:A:601:HOH:O	1.90	0.86
1:B:337:GLU:O	1:B:338:LYS:HB3	1.77	0.82
1:A:68:LYS:HA	1:A:68:LYS:CE	2.09	0.81
1:B:219:LYS:HG3	1:B:225:PRO:HG3	1.65	0.78
1:A:185:PHE:CD2	1:A:325[A]:GLU:HG3	2.18	0.78
2:B:502:IHS:O34	3:B:603:HOH:O	2.00	0.78
1:B:224:ASN:ND2	1:B:227:GLN:HB2	1.99	0.77
1:B:280:LYS:HE2	1:B:325:GLU:HG3	1.66	0.77
2:A:501:IHS:O32	3:A:604:HOH:O	2.03	0.76
1:B:48:MET:HG2	1:B:370:TYR:CD2	2.20	0.76
1:B:374:ASP:OD2	1:B:376:ARG:NH2	2.20	0.74
1:B:218:MET:HE3	1:B:222:LEU:CD1	2.17	0.74
1:B:48:MET:HG3	1:B:49:THR:N	2.02	0.74
1:B:345:ARG:NH2	3:B:607:HOH:O	2.18	0.74
1:B:287:LYS:HE3	3:B:645:HOH:O	1.88	0.74
1:B:128:ARG:NH2	3:B:608:HOH:O	2.21	0.73
2:A:501:IHS:O23	3:A:605:HOH:O	2.07	0.72
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.55	0.71
1:A:154:MET:HB2	1:A:321:PHE:CD1	2.26	0.70
1:B:20:MET:N	3:B:609:HOH:O	2.22	0.70
1:A:114:LEU:O	1:A:117[A]:THR:HG22	1.90	0.70
1:A:18:SER:O	1:A:22:THR:HG22	1.92	0.69
1:B:218:MET:HE3	1:B:222:LEU:HD12	1.74	0.69
1:A:185:PHE:CG	1:A:325[A]:GLU:HG3	2.28	0.68
1:B:22:THR:HG22	1:B:25:GLN:HG3	1.75	0.67
1:A:96:MET:HE3	1:A:256:LEU:CD2	2.25	0.67
1:A:201:LEU:O	1:A:205:LYS:HG3	1.94	0.67
1:A:49:THR:HB	3:A:636:HOH:O	1.95	0.66
1:B:342:GLN:OE1	3:B:605:HOH:O	2.14	0.65
1:B:231:LYS:O	1:B:235:GLU:HG3	1.96	0.65
1:A:128:ARG:NH2	3:A:602:HOH:O	1.94	0.64
1:B:22:THR:CG2	1:B:25:GLN:HG3	2.28	0.64
1:A:96:MET:HE3	1:A:256:LEU:HD21	1.80	0.64
1:B:338:LYS:HZ1	1:B:354:LYS:H	1.45	0.63
1:A:19:HIS:HA	1:A:22:THR:CG2	2.29	0.62
1:B:201:LEU:O	1:B:205:LYS:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HG23	1:B:25:GLN:H	1.64	0.62
1:B:207:PHE:CZ	1:B:211:LYS:HD2	2.35	0.61
1:B:22:THR:HG22	1:B:25:GLN:CG	2.31	0.60
1:B:20:MET:N	3:B:611:HOH:O	2.34	0.60
1:B:310:SER:OG	1:B:312:LYS:HG3	2.00	0.60
1:B:48:MET:HG3	1:B:49:THR:H	1.67	0.59
1:B:134:PHE:CD1	1:B:161[B]:MET:HE1	2.38	0.59
1:B:114:LEU:HA	1:B:117[A]:THR:HG22	1.84	0.58
1:B:20:MET:CB	1:B:35:PRO:HB3	2.33	0.58
1:B:110[B]:LYS:HG3	1:B:111:LEU:O	2.04	0.58
1:B:22:THR:CG2	1:B:25:GLN:H	2.17	0.58
1:B:224:ASN:HD21	1:B:227:GLN:HB2	1.64	0.57
1:A:280:LYS:HG2	1:A:325[A]:GLU:OE1	2.04	0.57
1:A:303:ARG:NH1	1:A:303:ARG:HG2	2.19	0.57
1:B:134:PHE:CE1	1:B:161[B]:MET:HE1	2.39	0.57
1:A:49:THR:HG22	3:A:860:HOH:O	2.05	0.57
1:B:23:LYS:HD2	2:B:502:IHS:O4	2.06	0.56
1:B:371:ARG:NH1	1:B:377:ILE:HD11	2.21	0.56
1:B:403:GLU:OE1	1:B:406:ARG:NH2	2.40	0.55
1:A:376:ARG:HG3	1:A:376:ARG:NH1	2.22	0.55
1:B:199:ASP:O	1:B:202:PRO:HD2	2.07	0.55
1:B:219:LYS:CG	1:B:225:PRO:HG3	2.36	0.54
1:A:218:MET:HE3	1:A:236:PHE:CD2	2.44	0.53
1:B:146:TYR:CD2	1:B:176:LYS:HG3	2.43	0.53
1:B:231:LYS:HE3	1:B:235:GLU:OE2	2.09	0.53
1:B:419:THR:O	1:B:422:VAL:HG22	2.09	0.53
2:B:502:IHS:O46	2:B:502:IHS:H5	2.09	0.52
1:B:338:LYS:NZ	1:B:354:LYS:H	2.07	0.52
1:B:276:GLN:OE1	1:B:280:LYS:HD2	2.10	0.52
1:B:114:LEU:O	1:B:117[A]:THR:HG22	2.10	0.51
2:B:502:IHS:O46	3:B:606:HOH:O	2.17	0.51
1:B:256:LEU:HB3	1:B:259:LEU:HD12	1.94	0.50
1:A:49:THR:CG2	3:A:860:HOH:O	2.58	0.50
1:B:215:VAL:HG23	3:B:842:HOH:O	2.12	0.50
1:A:114:LEU:HA	1:A:117[A]:THR:HG22	1.94	0.49
1:A:68:LYS:HE3	1:A:68:LYS:CA	2.23	0.49
1:B:40:SER:N	3:B:615:HOH:O	2.46	0.49
1:B:218:MET:CE	1:B:222:LEU:HD12	2.42	0.48
1:A:38:THR:HG22	1:A:39:ASP:N	2.28	0.48
1:A:116:GLU:OE2	3:A:606:HOH:O	2.19	0.48
1:A:396:CYS:HB2	1:B:344[B]:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:CE1	1:A:110[B]:LYS:HE2	2.49	0.47
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.79	0.47
1:B:187:LEU:HD23	1:B:187:LEU:N	2.30	0.47
1:A:197:LYS:HE2	1:A:197:LYS:HB2	1.64	0.47
1:A:303:ARG:NH1	1:A:307:GLU:OE1	2.44	0.46
1:A:229:LEU:HB2	1:A:232:GLU:HG2	1.98	0.46
1:A:123:ALA:O	1:A:127[A]:ILE:HG13	2.16	0.46
1:A:113:LYS:O	1:A:117[B]:THR:HG23	2.16	0.46
1:A:19:HIS:HA	1:A:22:THR:HG22	1.97	0.46
1:B:22:THR:HG22	1:B:25:GLN:HB2	1.98	0.46
1:B:415:MET:HE2	3:B:876:HOH:O	2.16	0.45
1:B:186:ASP:C	1:B:187:LEU:HD23	2.41	0.45
1:B:256:LEU:HB3	1:B:259:LEU:CD1	2.47	0.45
1:B:219:LYS:HG3	1:B:225:PRO:CG	2.39	0.45
1:B:22:THR:HG22	1:B:25:GLN:CB	2.46	0.45
1:B:280:LYS:HE2	1:B:325:GLU:CG	2.43	0.45
1:B:87:THR:HG22	1:B:223:LEU:HD23	1.99	0.45
1:A:397:PHE:CG	1:A:398:PRO:HA	2.52	0.45
1:B:62:ARG:HH21	2:B:501:IHS:HO46	1.64	0.45
1:B:338:LYS:HE2	1:B:357:GLU:OE1	2.16	0.45
1:A:192:VAL:O	1:A:196:GLU:HG3	2.17	0.44
1:B:68:LYS:HB3	1:B:68:LYS:HE3	1.81	0.44
1:B:79:SER:O	1:B:83:GLU:HG2	2.17	0.44
1:A:62:ARG:HE	2:A:501:IHS:HO46	1.66	0.44
1:A:397:PHE:CD1	1:A:398:PRO:HA	2.53	0.44
1:B:143:ILE:HA	1:B:173:SER:O	2.18	0.44
1:B:303:ARG:NH2	3:B:614:HOH:O	2.42	0.44
1:A:403:GLU:HG3	3:A:777:HOH:O	2.17	0.43
1:A:280:LYS:HE3	3:A:747:HOH:O	2.18	0.43
1:A:374:ASP:O	1:A:375:GLN:HB2	2.19	0.43
1:B:113:LYS:O	1:B:117[B]:THR:HG23	2.19	0.43
1:B:295:TRP:CG	1:B:296:PRO:HD3	2.54	0.43
1:B:359:SER:HA	1:B:363:ALA:HB2	2.01	0.43
1:A:371:ARG:HG3	1:A:377:ILE:HD13	2.02	0.42
1:A:161[B]:MET:HE2	1:A:161[B]:MET:HB3	1.96	0.42
1:B:397:PHE:CG	1:B:398:PRO:HA	2.54	0.42
1:B:397:PHE:CD1	1:B:398:PRO:HA	2.55	0.42
1:B:334:MET:HE3	1:B:409:PHE:CZ	2.55	0.42
2:A:501:IHS:C2	3:A:604:HOH:O	2.68	0.42
2:A:501:IHS:H2	3:A:604:HOH:O	2.19	0.41
1:A:26:LYS:HD3	1:A:356:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HD2	3:A:879:HOH:O	2.21	0.41
1:B:195:LYS:NZ	3:B:604:HOH:O	2.11	0.41
1:A:201:LEU:HB3	1:A:202:PRO:HD3	2.02	0.41
1:B:48:MET:CG	1:B:49:THR:N	2.80	0.41
1:B:96:MET:HG2	1:B:256:LEU:HD21	2.02	0.41
1:A:96:MET:HG2	1:A:256:LEU:HD21	2.02	0.41
1:B:247:LEU:HB3	1:B:248:PRO:HD3	2.02	0.41
1:B:274:LEU:HG	1:B:278:MET:HE2	2.02	0.41
1:B:406:ARG:NH1	3:B:602:HOH:O	1.99	0.41
1:A:218:MET:HE2	1:A:222:LEU:CD1	2.51	0.41
1:A:331:VAL:HG13	1:A:336:ILE:HD12	2.03	0.41
1:B:310:SER:OG	1:B:312:LYS:HD2	2.21	0.40
1:A:91:MET:HE2	1:A:91:MET:HB2	1.88	0.40
1:A:134:PHE:CD1	1:A:161[B]:MET:HE1	2.56	0.40

All (2) 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)
1:B:303:ARG:NH1	2:B:502:IHS:O26[1_655]	1.30	0.90
3:A:633:HOH:O	3:B:817:HOH:O[1_554]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	404/426 (95%)	395 (98%)	8 (2%)	1 (0%)	44 28
1	B	402/426 (94%)	390 (97%)	9 (2%)	3 (1%)	19 7
All	All	806/852 (95%)	785 (97%)	17 (2%)	4 (0%)	25 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	GLN
1	B	338	LYS
1	A	322	ALA
1	B	322	ALA

### 5.3.2 Protein sidechains

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	362/376 (96%)	361 (100%)	1 (0%)	91	88
1	B	359/376 (96%)	358 (100%)	1 (0%)	91	88
All	All	721/752 (96%)	719 (100%)	2 (0%)	91	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	B	422	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	164	HIS
1	A	318	ASN
1	B	25	GLN
1	B	36	ASN
1	B	81	GLN
1	B	107	GLN
1	B	132	GLN
1	B	224	ASN
1	B	227	GLN
1	B	270	GLN
1	B	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	IHS	A	502	-	36,36,36	1.37	10 (27%)	42,60,60	4.13	27 (64%)
2	IHS	B	502	-	36,36,36	1.25	9 (25%)	42,60,60	2.62	14 (33%)
2	IHS	A	501	-	36,36,36	1.22	6 (16%)	42,60,60	1.17	4 (9%)
2	IHS	B	501	-	36,36,36	1.19	5 (13%)	42,60,60	1.37	6 (14%)

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	IHS	A	502	-	-	10/30/54/54	0/1/1/1
2	IHS	B	502	-	-	7/30/54/54	0/1/1/1
2	IHS	A	501	-	-	6/30/54/54	0/1/1/1
2	IHS	B	501	-	-	3/30/54/54	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	IHS	O13-C3	-2.63	1.40	1.46
2	B	501	IHS	O14-C4	-2.62	1.41	1.46
2	A	502	IHS	O44-S4	2.52	1.65	1.50
2	A	502	IHS	O12-C2	-2.51	1.41	1.46
2	B	502	IHS	O46-S6	2.48	1.65	1.50
2	A	502	IHS	O2-S1	2.44	1.65	1.50
2	A	502	IHS	O1-C1	-2.41	1.41	1.46
2	A	502	IHS	O35-S5	2.40	1.65	1.50
2	A	502	IHS	O33-S3	2.33	1.64	1.50
2	A	502	IHS	O32-S2	2.33	1.64	1.50
2	B	502	IHS	C4-C3	2.30	1.57	1.52
2	B	502	IHS	O32-S2	2.30	1.64	1.50
2	B	502	IHS	O35-S5	2.27	1.64	1.50
2	A	501	IHS	O15-C5	-2.25	1.41	1.46
2	A	501	IHS	O13-C3	-2.25	1.41	1.46
2	B	502	IHS	O2-S1	2.25	1.64	1.50
2	B	502	IHS	O33-S3	2.24	1.64	1.50
2	A	502	IHS	O46-S6	2.23	1.64	1.50
2	B	502	IHS	O44-S4	2.19	1.63	1.50
2	B	502	IHS	O13-C3	-2.19	1.41	1.46
2	A	501	IHS	O1-C1	-2.18	1.41	1.46
2	A	501	IHS	O33-S3	2.14	1.63	1.50
2	B	501	IHS	O33-S3	2.09	1.63	1.50
2	B	502	IHS	C5-C4	2.09	1.56	1.52
2	B	501	IHS	O32-S2	2.07	1.63	1.50
2	A	501	IHS	O44-S4	2.06	1.63	1.50
2	A	502	IHS	O15-C5	-2.04	1.42	1.46
2	A	501	IHS	O35-S5	2.02	1.62	1.50
2	B	501	IHS	O35-S5	2.01	1.62	1.50
2	B	501	IHS	O44-S4	2.01	1.62	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	IHS	O2-S1-O4	-8.38	79.36	108.49
2	A	502	IHS	O43-S3-O23	-7.54	81.97	112.22
2	B	502	IHS	O15-C5-C6	7.45	124.83	108.48
2	A	502	IHS	O33-S3-O43	-7.28	83.18	108.49
2	A	502	IHS	O42-S2-O22	-7.21	83.27	112.22
2	A	502	IHS	O45-S5-O25	-6.82	84.84	112.22
2	A	502	IHS	O35-S5-O45	-6.64	85.43	108.49
2	A	502	IHS	O44-S4-O34	-6.57	85.66	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	IHS	O12-C2-C3	6.54	122.83	108.48
2	A	502	IHS	O32-S2-O42	-6.42	86.17	108.49
2	B	502	IHS	O16-C6-C1	6.09	121.86	108.48
2	A	502	IHS	O44-S4-O24	-6.01	87.59	108.49
2	A	502	IHS	O4-S1-O3	-5.60	89.74	112.22
2	A	502	IHS	O1-C1-C2	5.48	120.52	108.48
2	A	502	IHS	O16-C6-C1	4.90	119.23	108.48
2	A	502	IHS	O14-C4-C3	4.75	118.91	108.48
2	B	502	IHS	C1-O1-S1	4.62	127.80	118.88
2	A	502	IHS	O16-C6-C5	-4.22	99.21	108.48
2	B	502	IHS	O13-C3-C4	4.07	117.41	108.48
2	B	502	IHS	O1-C1-C6	-3.99	99.71	108.48
2	A	502	IHS	O32-S2-O22	3.88	121.97	108.49
2	B	502	IHS	O16-C6-C5	-3.84	100.04	108.48
2	B	501	IHS	O12-C2-C3	3.67	116.55	108.48
2	A	502	IHS	C3-O13-S3	3.61	125.86	118.88
2	A	502	IHS	C5-O15-S5	3.53	125.70	118.88
2	B	502	IHS	O14-C4-C5	3.52	116.21	108.48
2	A	502	IHS	O33-S3-O23	3.48	120.60	108.49
2	A	502	IHS	C6-C1-C2	-3.48	102.80	110.41
2	A	501	IHS	O12-C2-C3	3.40	115.95	108.48
2	B	501	IHS	O13-C3-C4	3.38	115.90	108.48
2	B	502	IHS	O15-C5-C4	-3.33	101.16	108.48
2	A	502	IHS	O2-S1-O3	3.26	119.81	108.49
2	B	502	IHS	C2-O12-S2	-3.25	112.59	118.88
2	B	501	IHS	O15-C5-C4	3.21	115.52	108.48
2	A	502	IHS	C6-C5-C4	3.18	117.37	110.41
2	B	502	IHS	O14-C4-C3	-3.14	101.58	108.48
2	A	502	IHS	O35-S5-O25	3.02	118.99	108.49
2	A	502	IHS	C4-O14-S4	-3.02	113.04	118.88
2	B	502	IHS	C5-C4-C3	2.97	116.92	110.41
2	A	502	IHS	C4-C3-C2	-2.76	104.36	110.41
2	B	501	IHS	C6-C5-C4	-2.71	104.47	110.41
2	A	502	IHS	C3-C2-C1	2.63	116.17	110.41
2	A	502	IHS	C6-O16-S6	2.49	123.69	118.88
2	A	501	IHS	O15-C5-C4	2.46	113.88	108.48
2	A	501	IHS	C3-C2-C1	-2.25	105.48	110.41
2	A	502	IHS	C5-C6-C1	2.13	115.08	110.41
2	A	501	IHS	C5-C4-C3	-2.13	105.76	110.41
2	B	502	IHS	C4-O14-S4	2.11	122.95	118.88
2	B	502	IHS	C3-C2-C1	-2.07	105.88	110.41
2	B	501	IHS	O15-C5-C6	2.03	112.93	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	IHS	C5-O15-S5	-2.02	114.97	118.88

There are no chirality outliers.

All (26) torsion outliers are listed below:

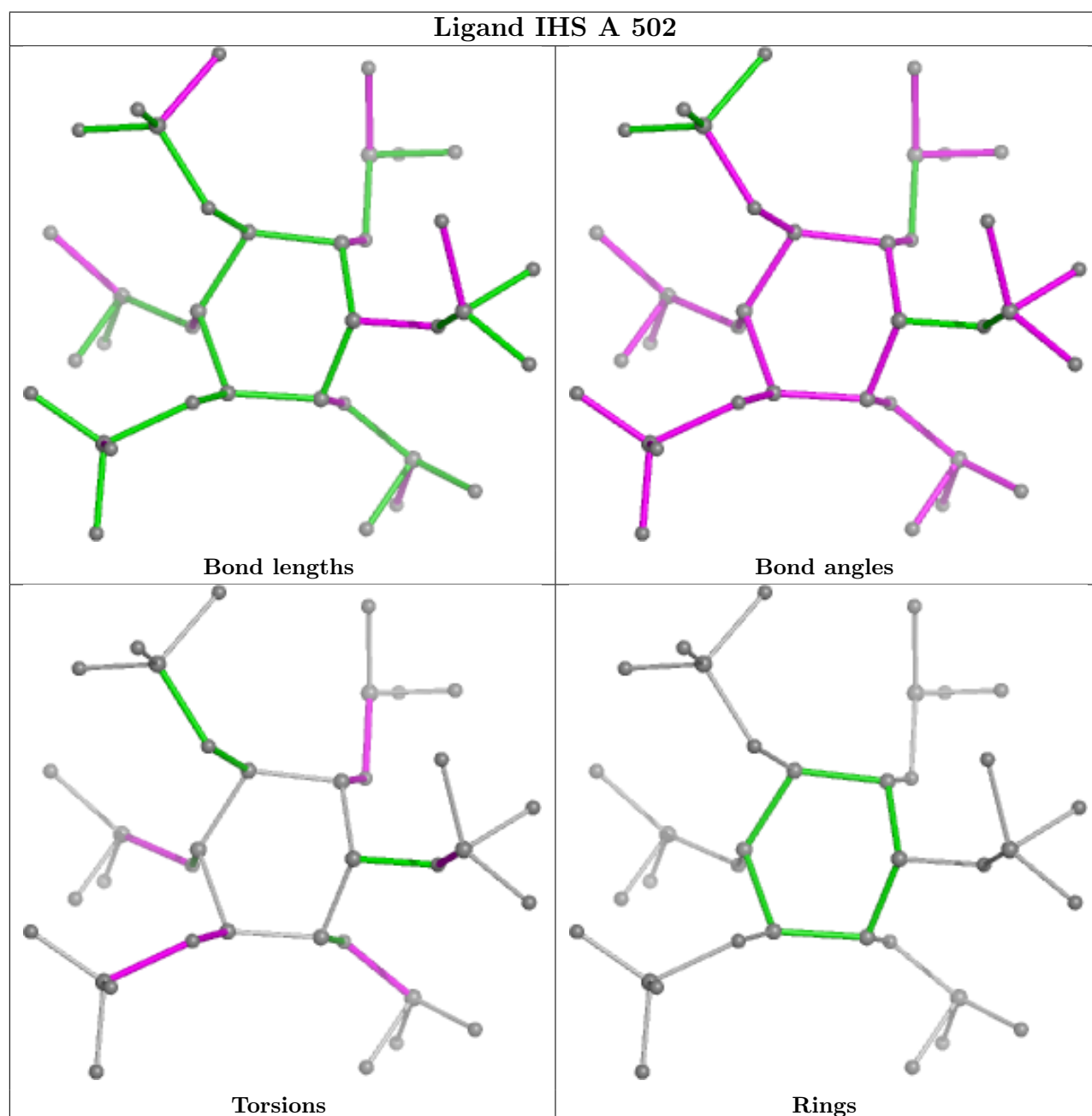
Mol	Chain	Res	Type	Atoms
2	A	501	IHS	C3-O13-S3-O33
2	A	502	IHS	C2-C1-O1-S1
2	A	502	IHS	C6-C1-O1-S1
2	A	502	IHS	C1-O1-S1-O2
2	A	502	IHS	C2-O12-S2-O22
2	A	502	IHS	C2-O12-S2-O42
2	A	502	IHS	C3-O13-S3-O23
2	A	502	IHS	C3-O13-S3-O33
2	A	502	IHS	C4-O14-S4-O34
2	A	502	IHS	C5-O15-S5-O35
2	B	502	IHS	C2-C1-O1-S1
2	B	502	IHS	C6-C1-O1-S1
2	B	502	IHS	C5-O15-S5-O25
2	B	502	IHS	C5-O15-S5-O35
2	B	502	IHS	C5-O15-S5-O45
2	A	501	IHS	C2-O12-S2-O22
2	A	501	IHS	C2-O12-S2-O42
2	A	501	IHS	C3-O13-S3-O23
2	A	501	IHS	C3-O13-S3-O43
2	B	501	IHS	C2-O12-S2-O22
2	B	501	IHS	C2-O12-S2-O42
2	A	501	IHS	C2-O12-S2-O32
2	B	501	IHS	C2-O12-S2-O32
2	A	502	IHS	C5-C4-O14-S4
2	B	502	IHS	C1-C6-O16-S6
2	B	502	IHS	C5-C6-O16-S6

There are no ring outliers.

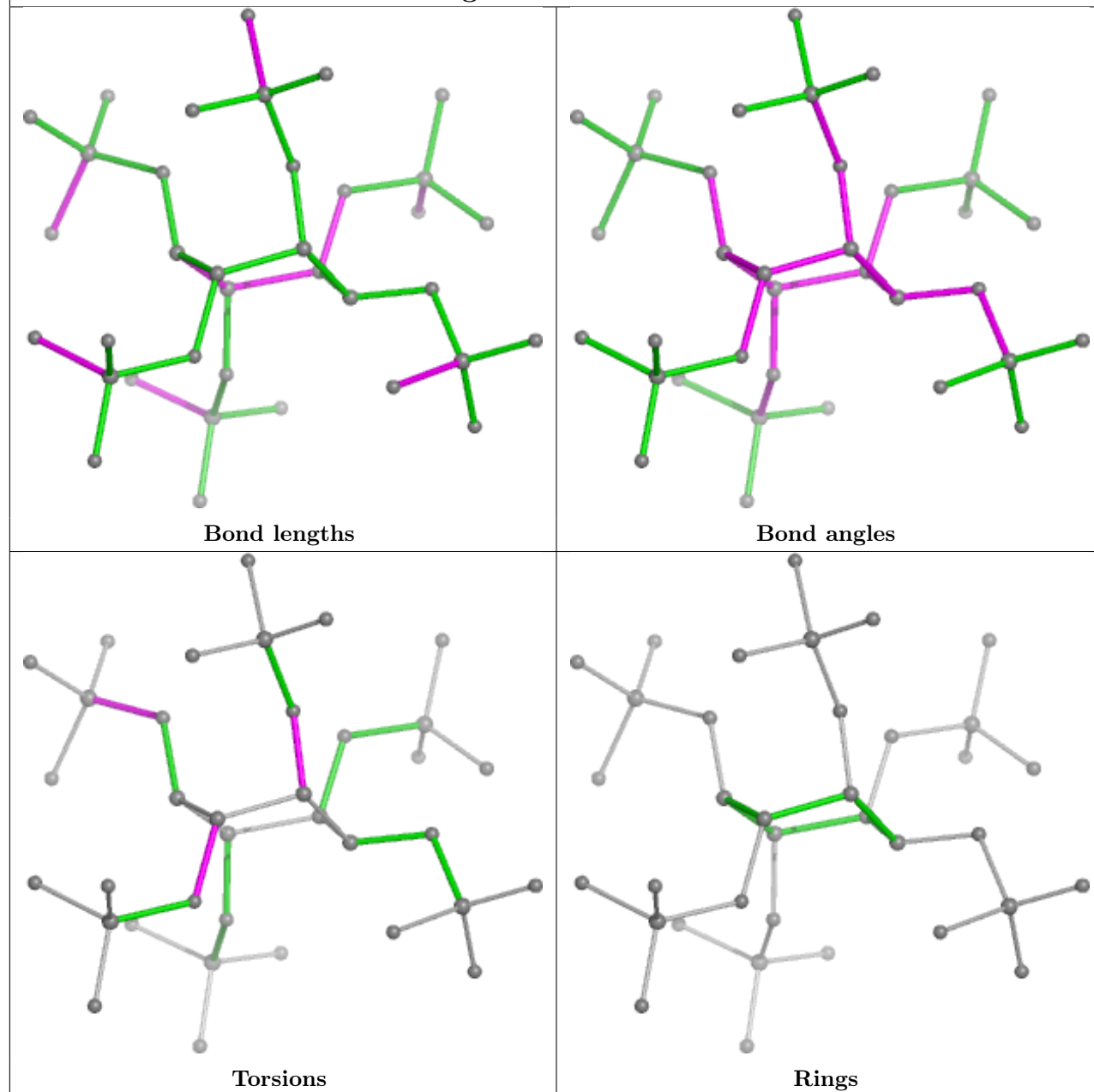
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	IHS	4	1
2	A	501	IHS	6	0
2	B	501	IHS	1	0

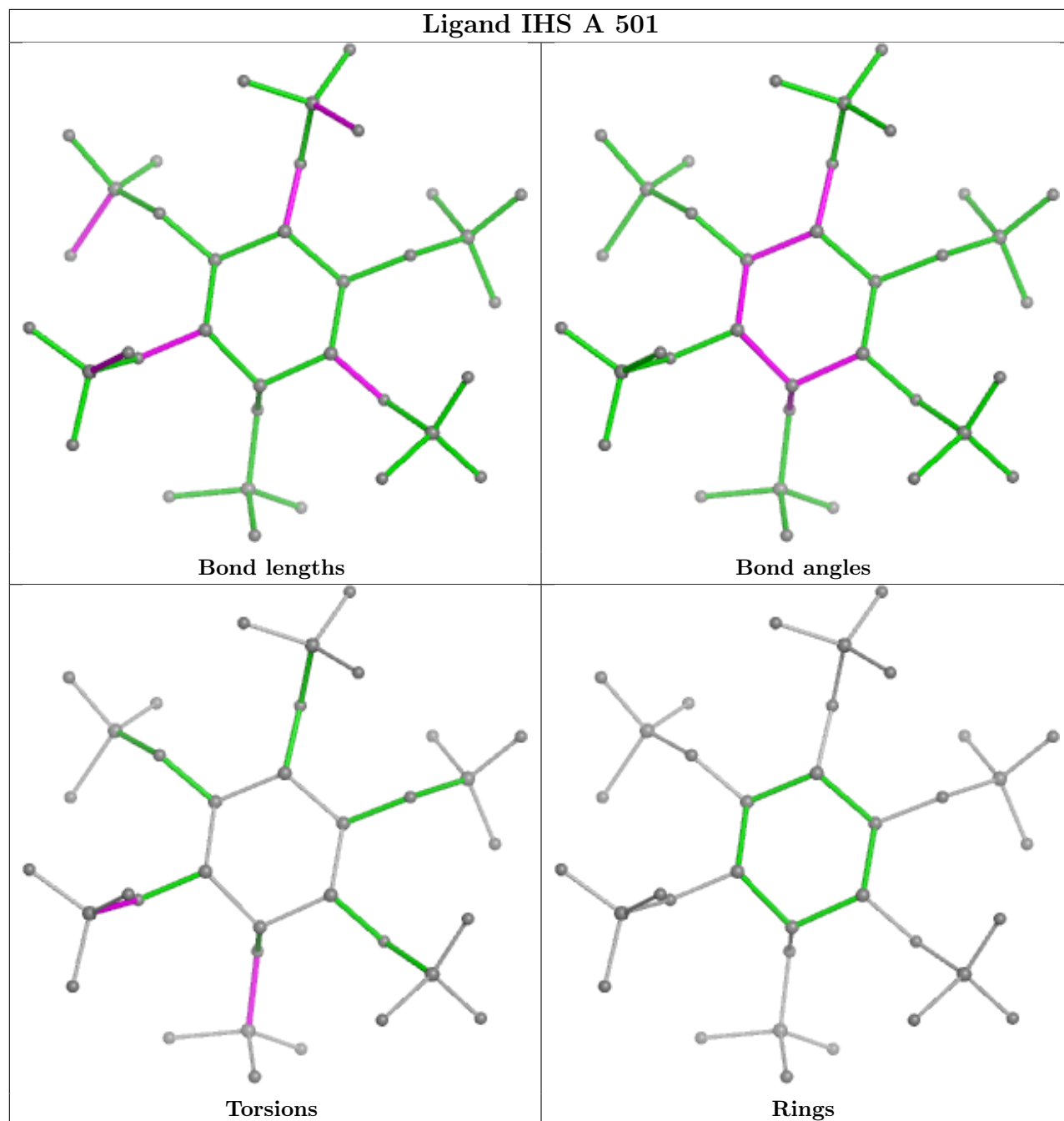
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

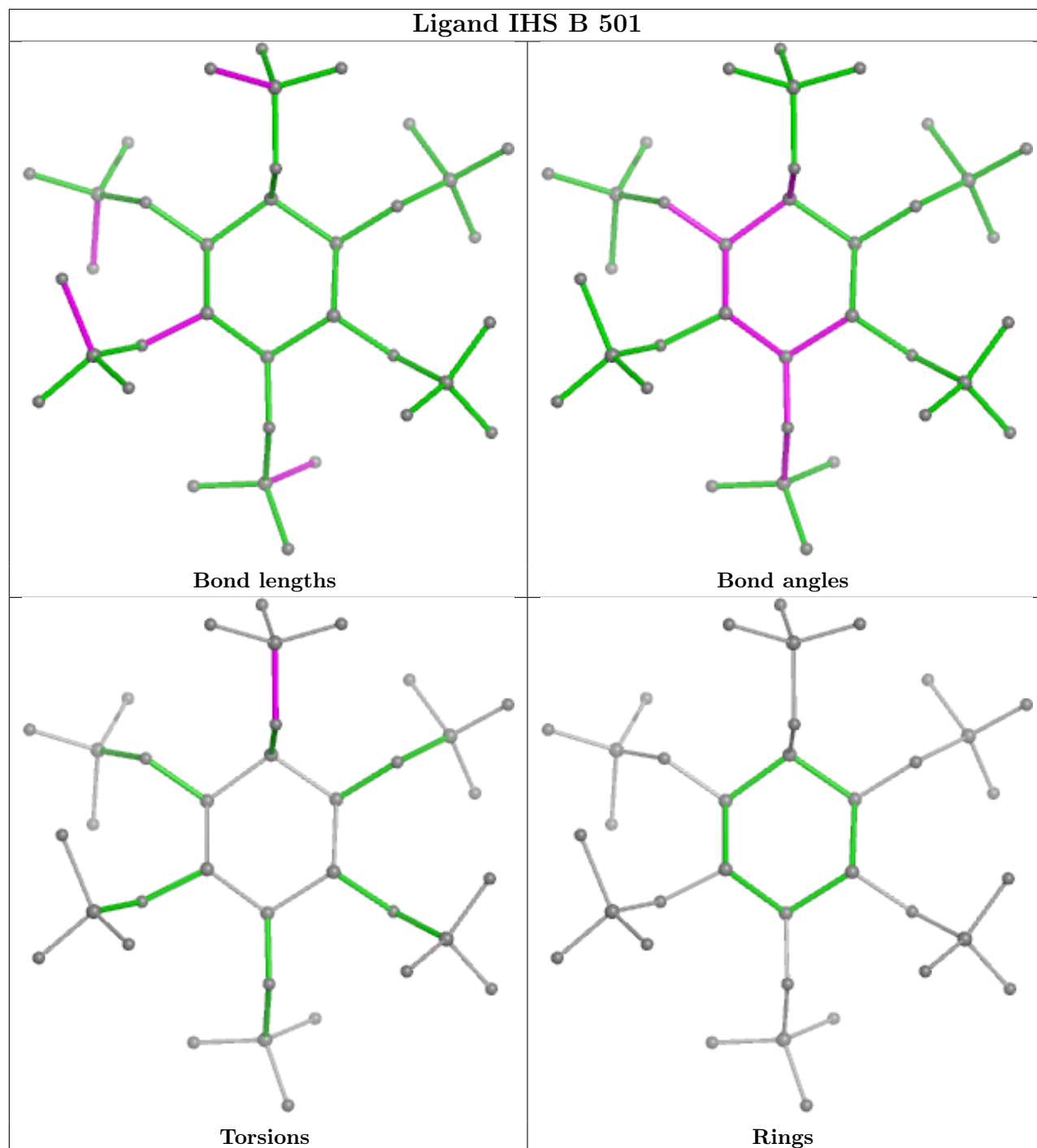


## Ligand IHS B 502



## Ligand IHS A 501





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/426 (93%)	0.13	16 (4%) 43 48	13, 27, 46, 61	8 (2%)
1	B	398/426 (93%)	0.28	26 (6%) 26 29	13, 28, 51, 73	8 (2%)
All	All	798/852 (93%)	0.21	42 (5%) 33 36	13, 27, 50, 73	16 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	ASN	4.6
1	A	38	THR	4.3
1	B	39	ASP	4.1
1	A	39	ASP	3.9
1	A	40	SER	3.9
1	B	224	ASN	3.8
1	A	423	PHE	3.8
1	B	48	MET	3.7
1	B	20	MET	3.6
1	B	38	THR	3.4
1	A	48	MET	3.3
1	B	226	GLU	3.2
1	B	40	SER	3.1
1	A	344	CYS	3.1
1	B	222	LEU	2.7
1	A	19	HIS	2.7
1	A	259	LEU	2.7
1	B	303	ARG	2.7
1	B	228	TYR	2.7
1	A	338	LYS	2.5
1	B	80	ALA	2.5
1	B	229	LEU	2.5
1	B	421	SER	2.4
1	A	424	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	258	ASP	2.4
1	B	396	CYS	2.3
1	B	217	ILE	2.3
1	A	21	GLN	2.3
1	B	21	GLN	2.3
1	B	49	THR	2.3
1	B	258	ASP	2.2
1	B	209	HIS	2.2
1	B	36	ASN	2.2
1	B	84	ASN	2.2
1	A	82	GLN	2.2
1	A	209	HIS	2.2
1	A	88	SER	2.2
1	B	201	LEU	2.2
1	B	345	ARG	2.1
1	B	230	ASP	2.1
1	B	225	PRO	2.0
1	A	213	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](#)

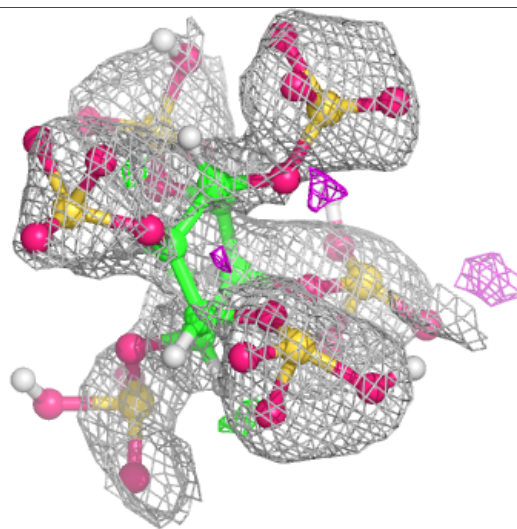
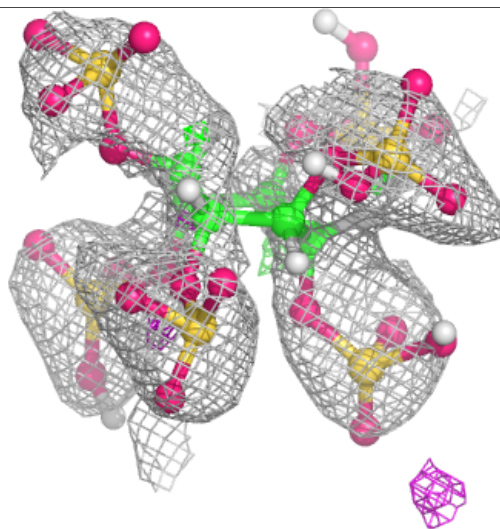
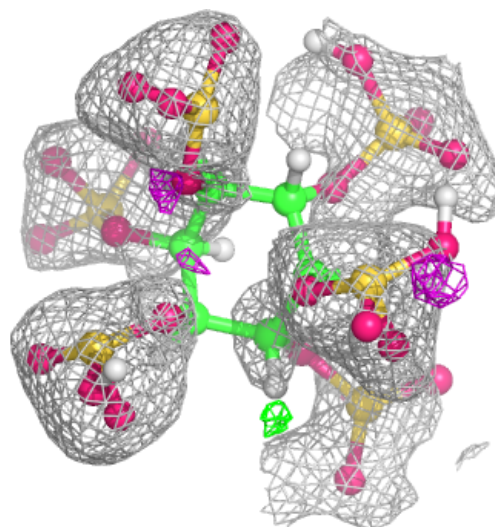
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IHS	A	502	36/36	0.73	0.15	53,66,78,92	46
2	IHS	B	502	36/36	0.78	0.16	43,56,68,71	48
2	IHS	B	501	36/36	0.95	0.09	17,34,49,58	0
2	IHS	A	501	36/36	0.96	0.09	17,29,42,55	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 IHS A 502:**

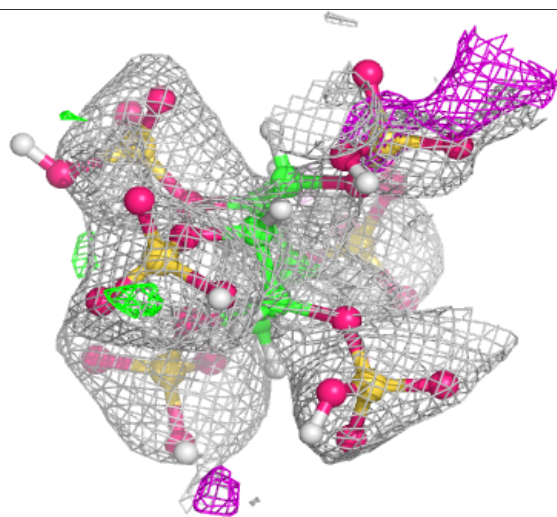
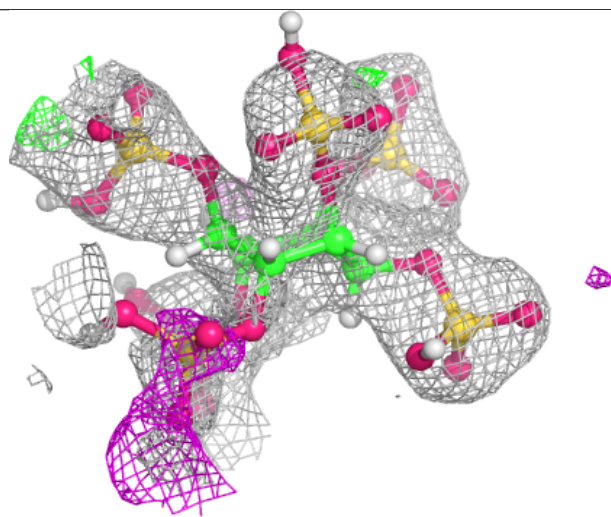
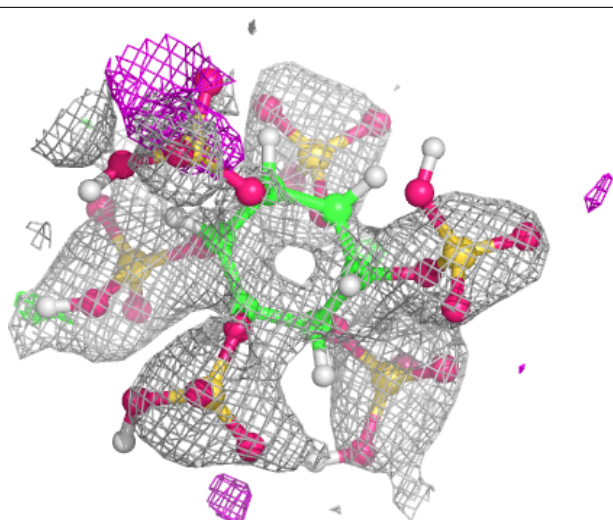
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





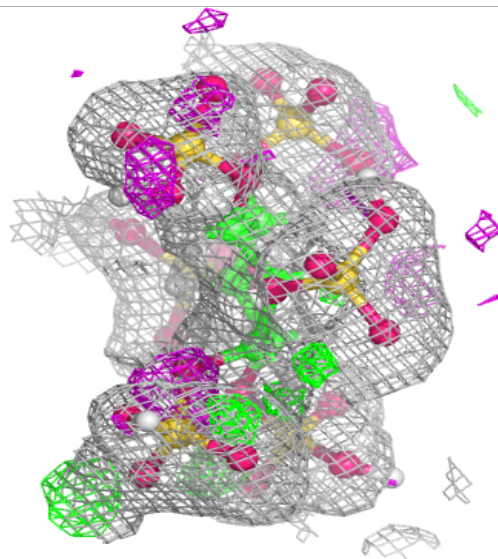
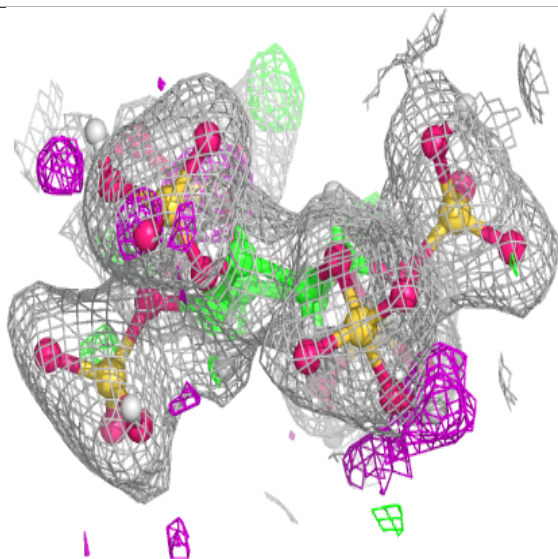
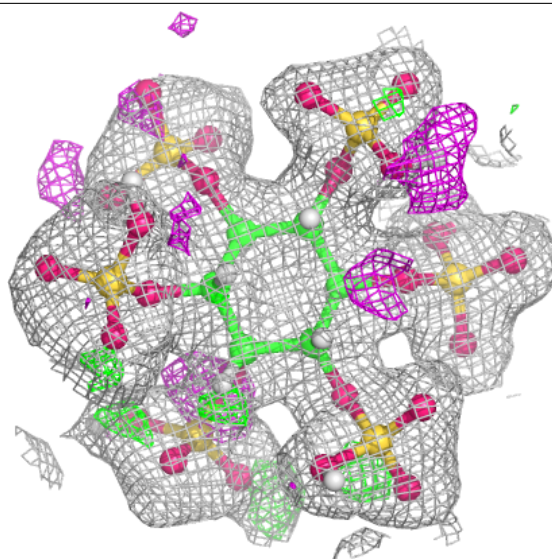
**Electron density around IHS B 502:**

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



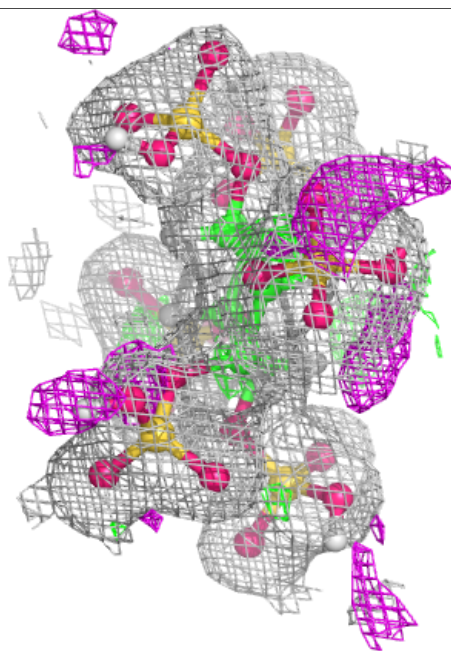
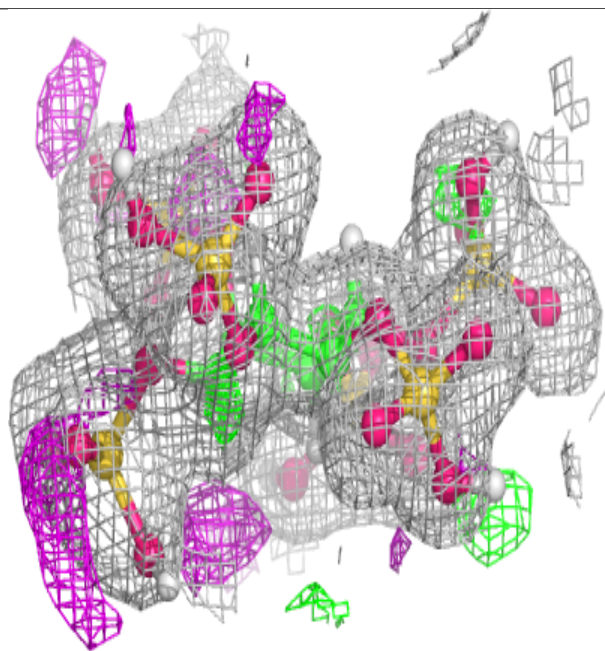
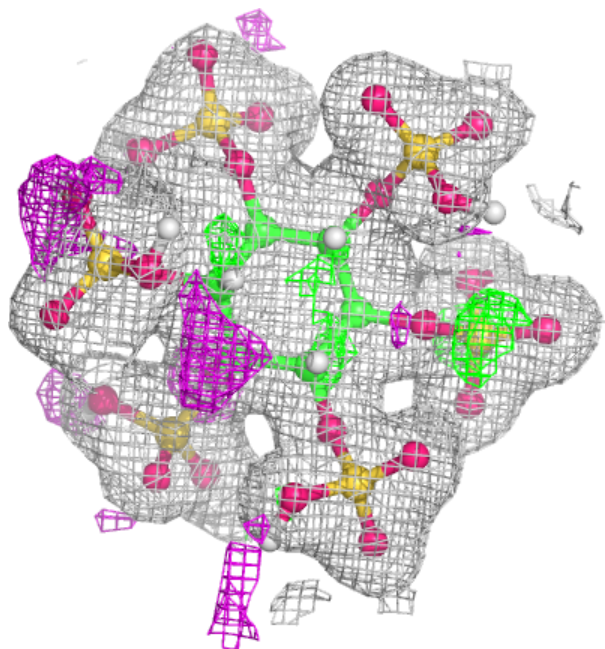
**Electron density around IHS B 501:**

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



**Electron density around IHS A 501:**

$2mF_o-DF_c$  (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.