



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:55 AM UTC

PDB ID : 3K4Q / pdb_00003k4q
Title : Aspergillus niger Phytase in complex with myo-inositol hexakis sulfate
Authors : Oakley, A.J.
Deposited on : 2009-10-06
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

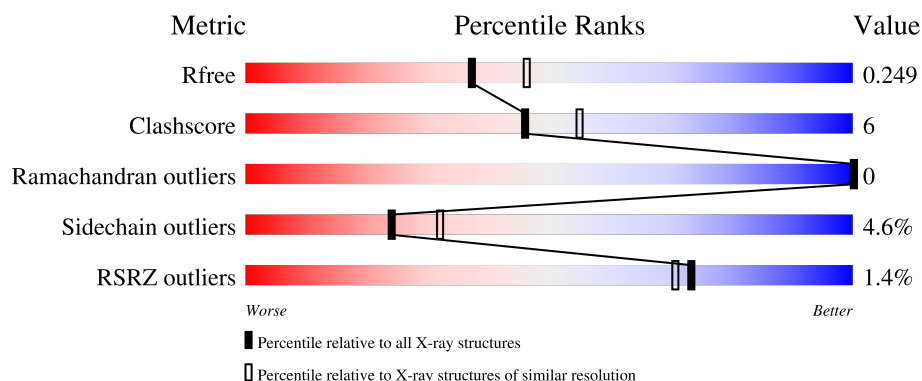
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	444	% 82% 16% ..
1	B	444	2% 81% 15% ..

2 Entry composition [i](#)

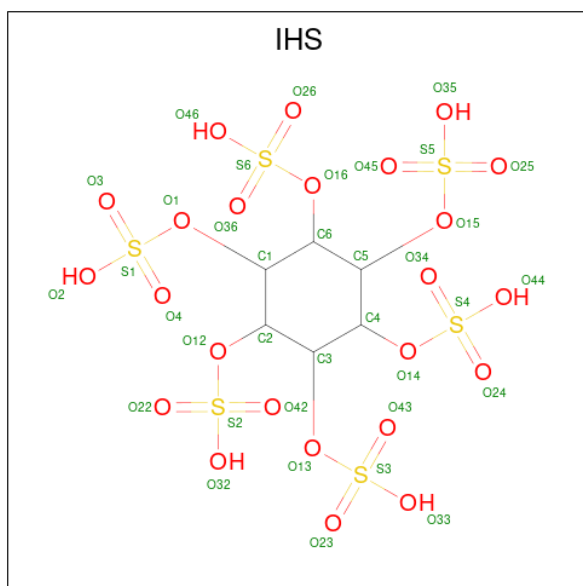
There are 4 unique types of molecules in this entry. The entry contains 7350 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-phytase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	2	0
			3397	2138	567	678	14			
1	B	438	Total	C	N	O	S	0	3	0
			3406	2142	567	683	14			

- Molecule 2 is D-MYO-INOSITOL-HEXASULPHATE (CCD ID: IHS) (formula: $C_6H_{12}O_{24}S_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			36	6	24	6		
2	B	1	Total	C	O	S	0	0
			36	6	24	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

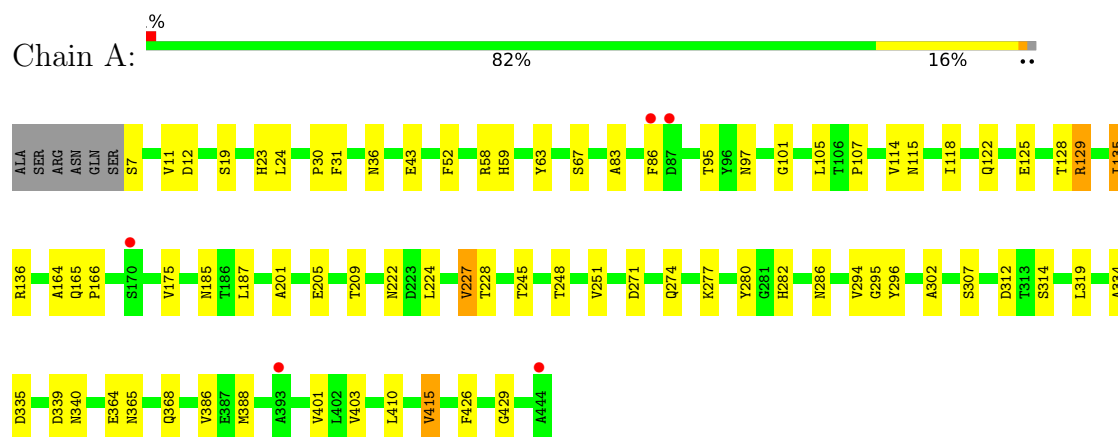
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	178	Total	O	0	0
			178	178		

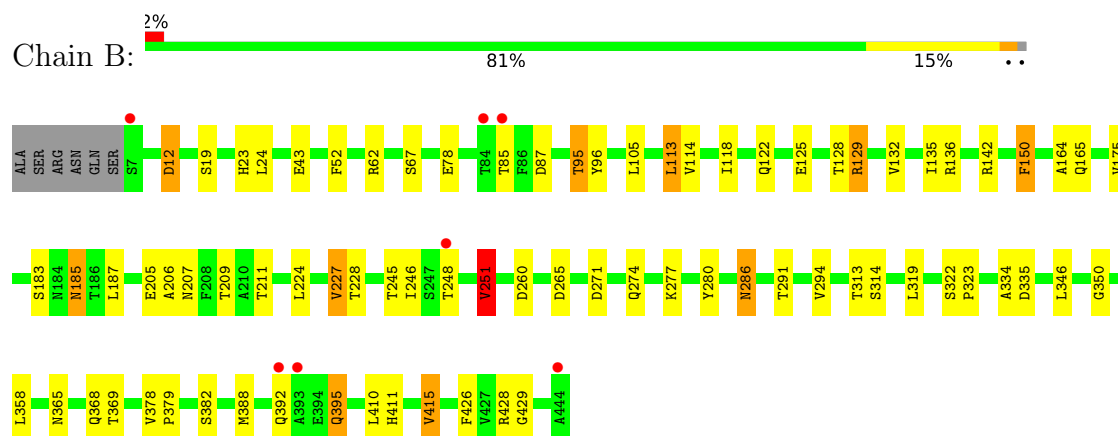
3 Residue-property plots [i](#)

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: 3-phytase A



• Molecule 1: 3-phytase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.70Å 87.57Å 81.77Å 90.00° 110.61° 90.00°	Depositor
Resolution (Å)	62.01 – 2.20 62.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (62.01-2.20) 98.5 (62.01-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.197 , 0.254 0.195 , 0.249	Depositor DCC
R_{free} test set	2377 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7350	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, 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	1.13	3/3484 (0.1%)	1.13	6/4742 (0.1%)
1	B	1.13	3/3496 (0.1%)	1.15	12/4759 (0.3%)
All	All	1.13	6/6980 (0.1%)	1.14	18/9501 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	TYR	N-CA	-6.30	1.38	1.46
1	B	132	VAL	CA-CB	5.89	1.59	1.53
1	A	403	VAL	CA-CB	5.40	1.60	1.53
1	B	334	ALA	C-O	5.05	1.29	1.23
1	A	201	ALA	CA-CB	5.04	1.61	1.53
1	B	346	LEU	CA-C	5.03	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	VAL	CB-CA-C	-7.99	101.58	112.04
1	B	114	VAL	N-CA-C	-7.32	103.54	110.42
1	A	415	VAL	CB-CA-C	-7.07	100.51	111.26
1	B	415	VAL	CB-CA-C	-7.05	100.54	111.26
1	B	165	GLN	CA-C-N	6.57	126.52	120.21
1	B	165	GLN	C-N-CA	6.57	126.52	120.21
1	A	135	ILE	N-CA-C	6.23	116.83	108.11
1	A	114	VAL	N-CA-C	-6.10	104.57	110.42
1	B	150	PHE	N-CA-C	-6.02	104.80	111.36
1	B	87	ASP	N-CA-C	5.70	118.08	109.41
1	A	129	ARG	CB-CG-CD	-5.67	98.26	111.30
1	B	135	ILE	N-CA-C	5.58	116.16	108.12
1	B	183	SER	N-CA-C	5.47	117.64	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLN	CA-C-N	5.29	125.28	120.21
1	A	165	GLN	C-N-CA	5.29	125.28	120.21
1	B	129	ARG	CB-CG-CD	-5.26	99.20	111.30
1	B	286	ASN	CA-C-N	-5.03	114.43	119.56
1	B	286	ASN	C-N-CA	-5.03	114.43	119.56

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	3397	0	3231	37	0
1	B	3406	0	3234	40	0
2	A	36	0	8	0	0
2	B	36	0	8	0	0
3	A	56	0	52	1	0
3	B	56	0	52	3	0
4	A	185	0	0	5	0
4	B	178	0	0	7	0
All	All	7350	0	6585	79	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 6.

All (79) 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:205:GLU:O	1:B:209:THR:HG23	1.82	0.80
1:A:205:GLU:O	1:A:209:THR:HG23	1.82	0.80
1:A:125:GLU:HA	1:A:128:THR:OG1	1.95	0.66
1:B:246:ILE:HG13	4:B:489:HOH:O	1.94	0.66
1:B:260:ASP:OD1	4:B:558:HOH:O	2.14	0.65
1:B:185:ASN:HD22	1:B:187:LEU:H	1.44	0.64
1:A:52:PHE:HB3	1:A:388:MET:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HD22	1:B:185:ASN:C	2.07	0.62
1:B:395:GLN:H	1:B:395:GLN:HE21	1.47	0.61
1:B:125:GLU:HA	1:B:128:THR:OG1	2.01	0.61
1:B:185:ASN:HD21	1:B:187:LEU:HB2	1.66	0.61
1:B:411:HIS:HE1	4:B:557:HOH:O	1.83	0.60
1:B:136:ARG:HB2	1:B:335:ASP:OD1	2.02	0.60
1:A:185:ASN:HD22	1:A:185:ASN:C	2.11	0.58
1:B:12:ASP:HB3	4:B:554:HOH:O	2.05	0.57
1:A:280:TYR:O	1:A:286:ASN:HB2	2.04	0.56
1:B:52:PHE:HB3	1:B:388:MET:HB3	1.87	0.56
1:B:185:ASN:ND2	1:B:187:LEU:H	2.03	0.55
1:A:364:GLU:OE1	4:A:554:HOH:O	2.18	0.55
3:A:1184:NAG:H82	3:A:1316:NAG:H82	1.90	0.54
1:B:429:GLY:HA3	4:B:498:HOH:O	2.07	0.54
1:A:245:THR:O	1:A:248:THR:HG22	2.08	0.53
1:A:24:LEU:HB3	1:A:271:ASP:HB2	1.91	0.53
1:A:185:ASN:ND2	1:A:187:LEU:H	2.07	0.52
1:A:410:LEU:HD13	1:A:426:PHE:CD1	2.45	0.52
1:A:185:ASN:HD22	1:A:187:LEU:H	1.58	0.52
1:B:358:LEU:HD22	1:B:369:THR:HG22	1.92	0.52
1:B:24:LEU:HB3	1:B:271:ASP:HB2	1.92	0.51
1:B:118:ILE:O	1:B:122:GLN:HG3	2.11	0.51
1:B:129:ARG:HB2	1:B:164:ALA:HA	1.93	0.51
1:B:365:ASN:OD1	1:B:368:GLN:HG3	2.10	0.51
1:B:246:ILE:CG1	4:B:489:HOH:O	2.56	0.51
1:B:410:LEU:HD13	1:B:426:PHE:CD1	2.46	0.51
1:B:245:THR:O	1:B:248:THR:HG22	2.11	0.50
1:A:365:ASN:OD1	1:A:368:GLN:HG3	2.11	0.50
1:A:52:PHE:HB3	1:A:388:MET:CB	2.42	0.49
1:A:136:ARG:HG2	1:A:175:VAL:HB	1.93	0.49
1:A:185:ASN:HD21	1:A:187:LEU:HB2	1.76	0.49
1:A:295:GLY:HA3	1:A:314:SER:OG	2.13	0.48
1:B:248:THR:HG21	4:B:559:HOH:O	2.14	0.48
1:B:95:THR:O	1:B:96:TYR:C	2.56	0.48
1:B:379:PRO:HD2	1:B:382:SER:HB3	1.96	0.48
1:A:118:ILE:O	1:A:122:GLN:HG3	2.14	0.48
1:A:429:GLY:HA3	4:A:481:HOH:O	2.13	0.48
1:B:274:GLN:OE1	1:B:277:LYS:HE3	2.14	0.48
1:B:136:ARG:HG2	1:B:175:VAL:HB	1.97	0.47
1:A:135:ILE:HG12	1:A:334:ALA:HB3	1.97	0.46
1:A:274:GLN:OE1	1:A:277:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HA	1:B:251:VAL:HG13	1.97	0.46
1:A:388:MET:HE3	4:A:569:HOH:O	2.15	0.46
1:A:136:ARG:HB2	1:A:335:ASP:OD1	2.15	0.46
1:B:78:GLU:HB3	3:B:1082:NAG:H82	1.97	0.45
1:A:164:ALA:O	1:A:166:PRO:HD3	2.17	0.45
1:B:280:TYR:O	1:B:286:ASN:HB2	2.17	0.45
1:A:282:HIS:CE1	1:A:340:ASN:HB3	2.52	0.44
1:A:339:ASP:OD1	1:A:340:ASN:N	2.51	0.44
1:B:113:LEU:O	1:B:150:PHE:HA	2.18	0.44
1:B:224:LEU:O	1:B:227:VAL:HB	2.18	0.43
1:A:19:SER:O	1:A:23:HIS:HB2	2.18	0.43
1:B:350:GLY:HA3	3:B:1353:NAG:H82	2.00	0.43
1:B:62:ARG:HD3	1:B:142:ARG:CD	2.49	0.43
1:B:313:THR:OG1	1:B:314:SER:N	2.52	0.43
1:A:63:TYR:HB3	1:A:101:GLY:O	2.18	0.42
1:A:224:LEU:O	1:A:227:VAL:HB	2.19	0.42
1:A:58:ARG:HG2	1:A:59:HIS:N	2.34	0.42
1:A:83:ALA:HB3	1:A:86:PHE:CZ	2.54	0.42
1:A:386:VAL:HG22	1:A:401:VAL:HG22	2.02	0.42
1:B:52:PHE:HB3	1:B:388:MET:CB	2.48	0.42
3:B:1184:NAG:HO4	3:B:1184:NAG:HO6	1.57	0.42
1:A:11:VAL:HG22	1:A:115:ASN:CG	2.45	0.41
1:A:129:ARG:HB2	1:A:164:ALA:HA	2.02	0.41
1:A:97:ASN:ND2	4:A:513:HOH:O	2.53	0.41
1:A:30:PRO:O	1:A:31:PHE:C	2.64	0.41
1:B:322:SER:HA	1:B:323:PRO:HD3	1.97	0.41
1:A:302:ALA:HB1	1:A:307:SER:O	2.21	0.40
1:B:378:VAL:O	1:B:378:VAL:HG23	2.21	0.40
1:B:19:SER:O	1:B:23:HIS:HB2	2.21	0.40
1:A:36[A]:ASN:ND2	4:A:618:HOH:O	2.54	0.40
1:B:206:ALA:O	1:B:207:ASN:C	2.64	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	438/444 (99%)	417 (95%)	21 (5%)	0	100	100
1	B	439/444 (99%)	415 (94%)	24 (6%)	0	100	100
All	All	877/888 (99%)	832 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	379/385 (98%)	364 (96%)	15 (4%)	28	38
1	B	381/385 (99%)	361 (95%)	20 (5%)	21	26
All	All	760/770 (99%)	725 (95%)	35 (5%)	24	32

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	12	ASP
1	A	43	GLU
1	A	67	SER
1	A	95	THR
1	A	105	LEU
1	A	107	PRO
1	A	222	ASN
1	A	227	VAL
1	A	228	THR
1	A	251	VAL
1	A	294	VAL
1	A	312	ASP
1	A	319	LEU
1	A	415	VAL

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Mol	Chain	Res	Type
1	B	12	ASP
1	B	43	GLU
1	B	67	SER
1	B	85	THR
1	B	95	THR
1	B	105	LEU
1	B	113	LEU
1	B	185	ASN
1	B	211	THR
1	B	227	VAL
1	B	228	THR
1	B	251	VAL
1	B	265	ASP
1	B	291	THR
1	B	294	VAL
1	B	319	LEU
1	B	392	GLN
1	B	395	GLN
1	B	415	VAL
1	B	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	185	ASN
1	A	329	ASN
1	A	390	GLN
1	A	411	HIS
1	B	185	ASN
1	B	292	GLN
1	B	306	HIS
1	B	390	GLN
1	B	395	GLN
1	B	411	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	500	-	36,36,36	1.25	3 (8%)	48,60,60	2.05	13 (27%)
3	NAG	B	1316	1	14,14,15	0.89	0	17,19,21	2.17	5 (29%)
3	NAG	B	1353	1	14,14,15	0.77	0	17,19,21	1.39	1 (5%)
3	NAG	B	1184	1	14,14,15	1.07	1 (7%)	17,19,21	3.58	9 (52%)
3	NAG	A	1353	1	14,14,15	0.68	0	17,19,21	1.96	6 (35%)
3	NAG	A	1082	1	14,14,15	0.54	0	17,19,21	1.73	4 (23%)
2	IHS	B	500	-	36,36,36	1.22	5 (13%)	48,60,60	2.43	18 (37%)
3	NAG	A	1184	1	14,14,15	0.77	0	17,19,21	1.50	5 (29%)
3	NAG	B	1082	1	14,14,15	0.65	0	17,19,21	1.35	3 (17%)
3	NAG	A	1316	1	14,14,15	0.89	1 (7%)	17,19,21	1.82	4 (23%)

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	500	-	-	6/30/54/54	0/1/1/1
3	NAG	B	1316	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1184	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1353	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1082	1	-	0/6/23/26	0/1/1/1
2	IHS	B	500	-	-	9/30/54/54	0/1/1/1
3	NAG	A	1184	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1082	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1316	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	IHS	O1-C1	-4.24	1.36	1.46
2	B	500	IHS	O1-C1	-3.49	1.38	1.46
2	B	500	IHS	O12-C2	-2.98	1.39	1.46
2	A	500	IHS	O14-C4	-2.68	1.40	1.46
3	B	1184	NAG	O5-C5	2.51	1.48	1.43
2	B	500	IHS	O15-C5	-2.31	1.41	1.46
2	B	500	IHS	O14-C4	-2.31	1.41	1.46
2	A	500	IHS	O14-S4	-2.13	1.50	1.57
3	A	1316	NAG	C1-C2	2.09	1.55	1.52
2	B	500	IHS	O1-S1	-2.04	1.51	1.57

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1184	NAG	C1-C2-N2	8.94	124.52	110.43
2	B	500	IHS	C5-C6-C1	-7.48	94.01	110.43
2	B	500	IHS	C2-O12-S2	6.64	134.97	119.04
2	B	500	IHS	O32-S2-O12	6.62	121.59	106.37
3	B	1316	NAG	C1-O5-C5	6.37	120.72	112.19
2	A	500	IHS	C5-C6-C1	-5.76	97.79	110.43
3	B	1184	NAG	O5-C5-C6	5.43	118.23	107.66
3	B	1184	NAG	C2-N2-C7	-4.84	116.42	122.90
3	B	1184	NAG	C4-C3-C2	-4.78	104.02	111.02
2	A	500	IHS	O14-C4-C3	-4.50	98.74	108.56
2	A	500	IHS	O12-C2-C1	4.49	118.35	108.56
2	B	500	IHS	O15-C5-C4	4.27	117.88	108.56
3	B	1353	NAG	C1-O5-C5	3.79	117.27	112.19
3	A	1082	NAG	O5-C1-C2	-3.77	105.45	111.29
3	A	1316	NAG	O3-C3-C2	-3.72	101.67	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1184	NAG	C3-C4-C5	-3.72	103.48	110.23
3	A	1316	NAG	C1-O5-C5	3.71	117.15	112.19
3	A	1353	NAG	C2-N2-C7	-3.66	118.00	122.90
3	A	1316	NAG	O4-C4-C5	3.60	118.20	109.32
2	A	500	IHS	C6-C1-C2	3.58	118.29	110.43
2	A	500	IHS	O44-S4-O14	-3.47	98.39	106.37
2	A	500	IHS	C4-C3-C2	3.44	117.97	110.43
3	B	1184	NAG	O5-C1-C2	-3.43	105.99	111.29
2	A	500	IHS	C3-O13-S3	-3.41	110.87	119.04
2	A	500	IHS	O32-S2-O12	3.38	114.14	106.37
3	A	1082	NAG	C2-N2-C7	3.33	127.36	122.90
2	B	500	IHS	O14-C4-C5	-3.28	101.39	108.56
3	B	1184	NAG	O4-C4-C5	3.23	117.28	109.32
3	B	1316	NAG	O3-C3-C2	-3.21	102.74	109.40
3	B	1184	NAG	C6-C5-C4	-3.16	105.25	113.02
2	B	500	IHS	O13-C3-C4	3.05	115.22	108.56
2	A	500	IHS	C6-O16-S6	3.04	126.34	119.04
3	A	1353	NAG	C6-C5-C4	3.02	120.42	113.02
3	B	1082	NAG	O5-C1-C2	-2.97	106.70	111.29
3	A	1082	NAG	C3-C4-C5	-2.94	104.90	110.23
2	B	500	IHS	O46-S6-O16	2.91	113.06	106.37
2	B	500	IHS	C4-C3-C2	2.91	116.81	110.43
3	B	1184	NAG	C1-O5-C5	2.87	116.03	112.19
2	B	500	IHS	O43-S3-O23	-2.86	101.22	112.24
3	A	1353	NAG	O5-C1-C2	-2.80	106.96	111.29
2	A	500	IHS	O13-C3-C4	2.75	114.57	108.56
3	B	1082	NAG	C2-N2-C7	2.71	126.54	122.90
3	A	1353	NAG	O4-C4-C3	-2.68	104.06	110.38
2	B	500	IHS	C6-O16-S6	2.65	125.39	119.04
2	A	500	IHS	O15-C5-C4	2.55	114.13	108.56
2	B	500	IHS	C3-O13-S3	-2.51	113.02	119.04
3	B	1316	NAG	C4-C3-C2	2.46	114.63	111.02
2	B	500	IHS	C6-C1-C2	2.45	115.80	110.43
2	A	500	IHS	C2-O12-S2	2.44	124.90	119.04
2	B	500	IHS	O35-S5-O15	2.44	111.98	106.37
2	B	500	IHS	O32-S2-O42	2.43	117.05	108.56
3	A	1316	NAG	C2-N2-C7	-2.36	119.73	122.90
3	A	1184	NAG	O5-C5-C4	-2.30	105.24	110.83
3	B	1316	NAG	O5-C5-C6	2.28	112.09	107.66
2	B	500	IHS	O33-S3-O23	2.26	116.47	108.56
2	B	500	IHS	O42-S2-O22	-2.25	103.55	112.24
3	A	1184	NAG	O3-C3-C2	2.24	114.06	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1353	NAG	O4-C4-C5	2.24	114.85	109.32
3	A	1184	NAG	O4-C4-C5	2.20	114.73	109.32
3	B	1082	NAG	C1-C2-N2	2.16	113.84	110.43
3	A	1082	NAG	O5-C5-C4	-2.15	105.61	110.83
2	B	500	IHS	O35-S5-O25	2.14	116.05	108.56
3	A	1353	NAG	O5-C5-C6	-2.12	103.54	107.66
3	B	1316	NAG	O7-C7-C8	-2.11	118.31	122.05
2	B	500	IHS	O12-C2-C3	2.07	113.07	108.56
2	A	500	IHS	O32-S2-O42	2.06	115.78	108.56
3	A	1184	NAG	C3-C4-C5	-2.03	106.54	110.23
3	A	1184	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	IHS	C1-C2-O12-S2
2	B	500	IHS	C4-O14-S4-O34
2	B	500	IHS	C4-O14-S4-O44
3	A	1353	NAG	O5-C5-C6-O6
3	B	1184	NAG	O5-C5-C6-O6
3	A	1353	NAG	C4-C5-C6-O6
2	B	500	IHS	C2-O12-S2-O22
2	B	500	IHS	C2-O12-S2-O42
2	B	500	IHS	C4-O14-S4-O24
3	B	1082	NAG	C4-C5-C6-O6
2	B	500	IHS	C1-O1-S1-O2
2	B	500	IHS	C1-O1-S1-O3
2	B	500	IHS	C2-O12-S2-O32
3	B	1082	NAG	O5-C5-C6-O6
3	B	1184	NAG	C4-C5-C6-O6
2	A	500	IHS	C1-O1-S1-O2
2	A	500	IHS	C2-O12-S2-O32
2	A	500	IHS	C4-O14-S4-O44
2	A	500	IHS	C4-O14-S4-O34
2	A	500	IHS	C2-C3-O13-S3
2	B	500	IHS	C1-O1-S1-O4

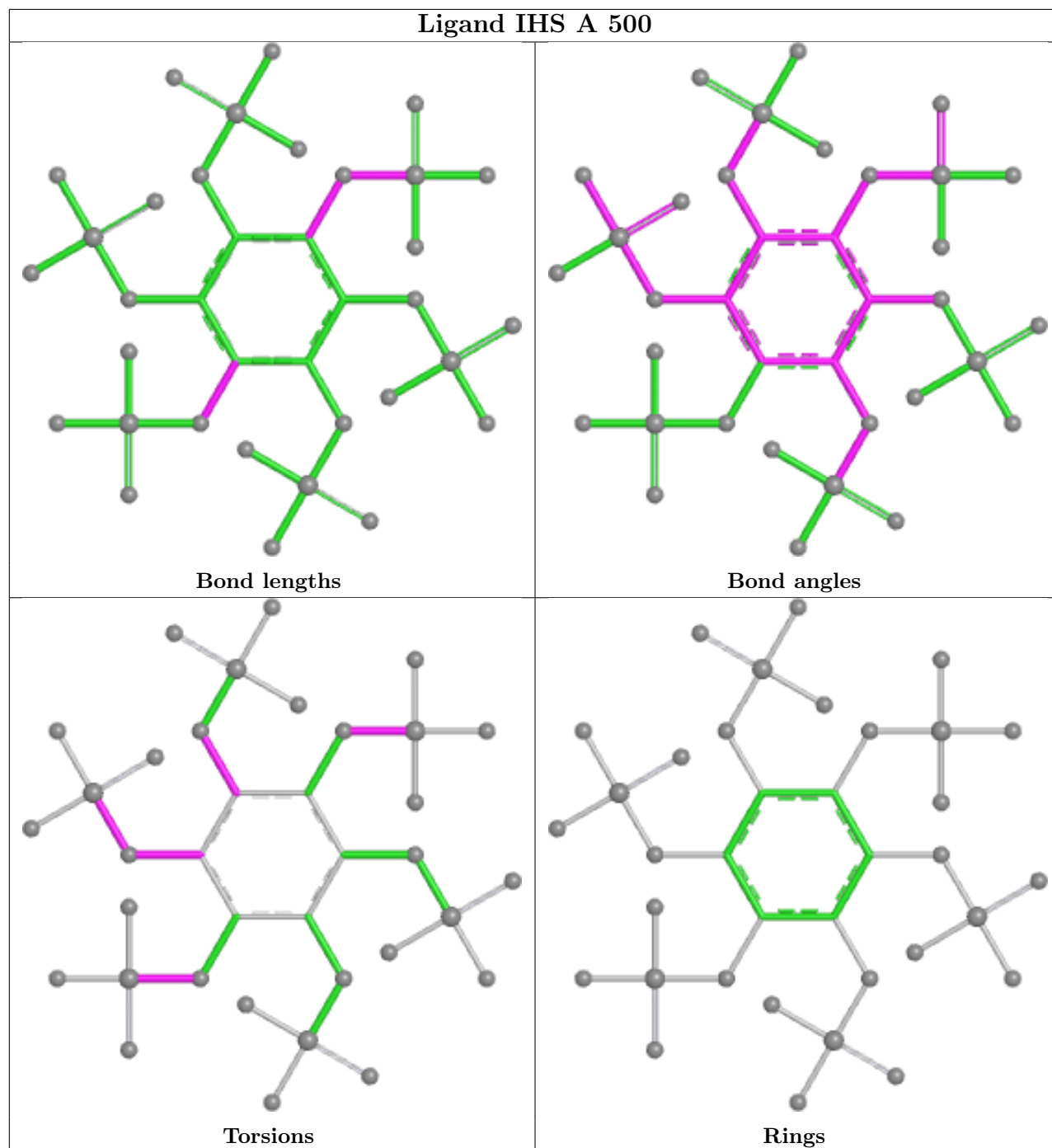
There are no ring outliers.

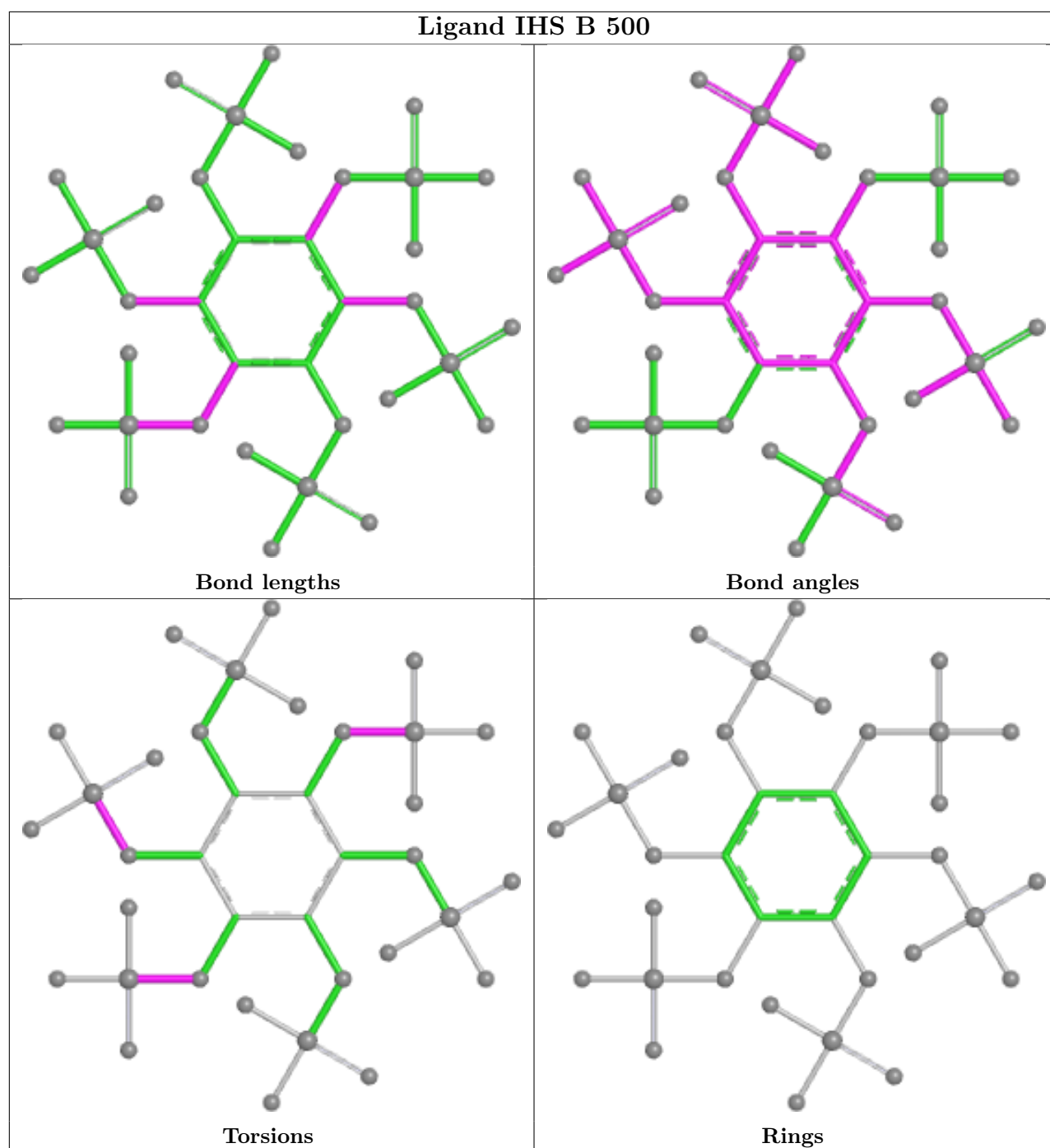
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1353	NAG	1	0
3	B	1184	NAG	1	0
3	A	1184	NAG	1	0
3	B	1082	NAG	1	0
3	A	1316	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 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 A 500





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	438/444 (98%)	-0.22	5 (1%) 78 76	13, 25, 46, 56	2 (0%)
1	B	438/444 (98%)	-0.25	7 (1%) 70 67	13, 25, 46, 55	3 (0%)
All	All	876/888 (98%)	-0.24	12 (1%) 73 71	13, 25, 46, 56	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	ALA	4.0
1	B	393	ALA	3.7
1	A	393	ALA	3.2
1	B	85	THR	3.1
1	B	392	GLN	2.9
1	B	444	ALA	2.3
1	B	84	THR	2.3
1	A	86	PHE	2.3
1	B	7	SER	2.3
1	B	248	THR	2.2
1	A	87	ASP	2.1
1	A	170	SER	2.1

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 oligosaccharides in this entry.

6.4 Ligands

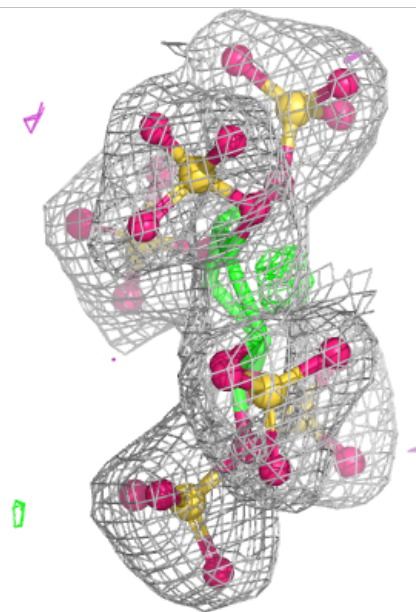
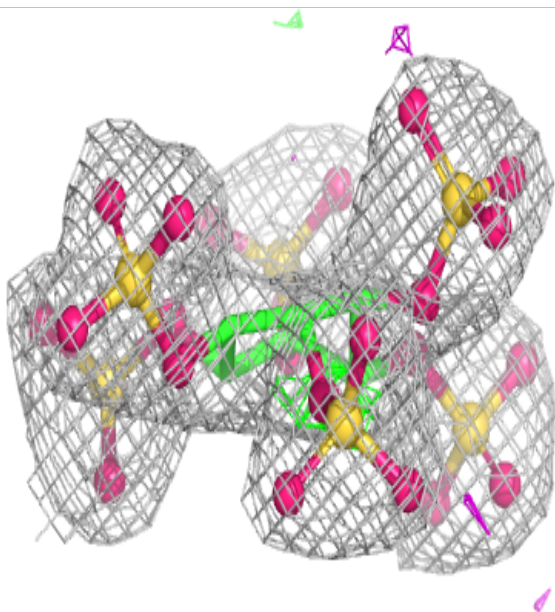
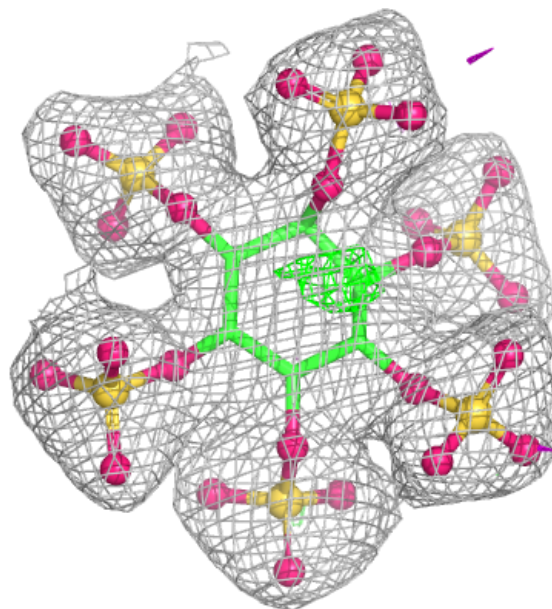
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	1184	14/15	0.82	0.12	32,38,47,48	0
3	NAG	B	1316	14/15	0.83	0.12	35,39,41,41	0
3	NAG	A	1184	14/15	0.87	0.10	27,36,41,45	0
3	NAG	A	1316	14/15	0.90	0.09	31,36,39,39	0
3	NAG	B	1082	14/15	0.91	0.08	30,39,45,46	0
3	NAG	A	1353	14/15	0.92	0.07	22,25,31,32	0
3	NAG	A	1082	14/15	0.93	0.07	26,39,47,51	0
2	IHS	B	500	36/36	0.97	0.06	12,27,30,31	36
2	IHS	A	500	36/36	0.97	0.07	11,27,32,32	36
3	NAG	B	1353	14/15	0.97	0.05	21,23,28,33	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.

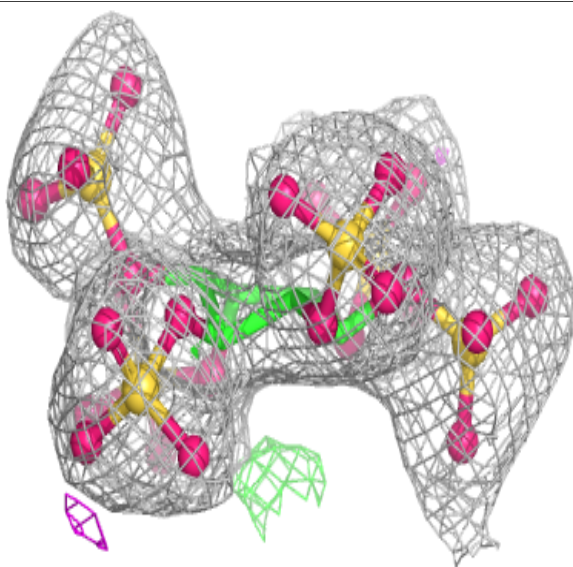
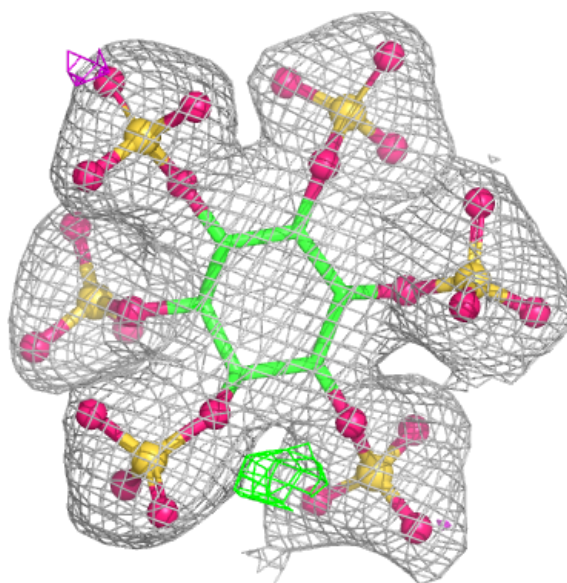
Electron density around IHS B 500:

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



Electron density around IHS A 500:

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.