



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 11:05 AM EDT

PDB ID : 2O5K  
Title : Crystal Structure of GSK3beta in complex with a benzoimidazol inhibitor  
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Deposited on : 2006-12-06  
Resolution : 3.20 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](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 : 4.02b-467  
Mogul : 1.8.5 (274361), 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

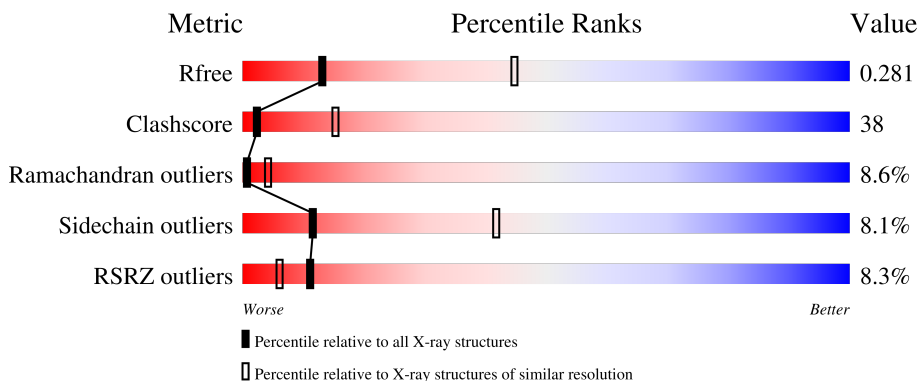
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	372	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2824 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.

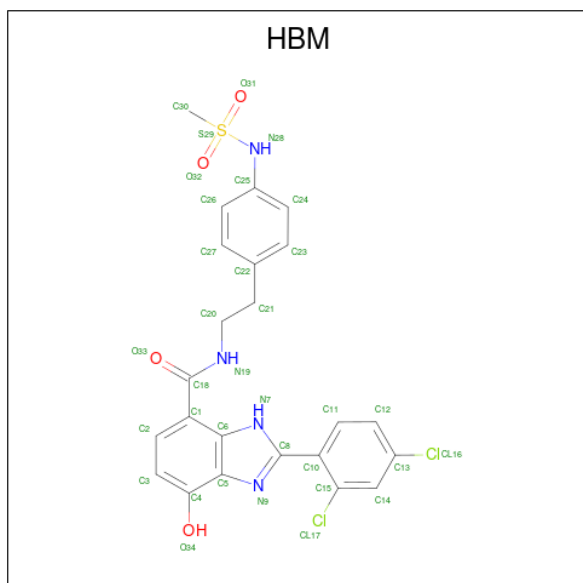
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2790	1796	477	506	11	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	expression tag	UNP P49841
A	23	HIS	-	expression tag	UNP P49841
A	24	HIS	-	expression tag	UNP P49841
A	25	HIS	-	expression tag	UNP P49841
A	26	HIS	-	expression tag	UNP P49841
A	27	HIS	-	expression tag	UNP P49841
A	28	HIS	-	expression tag	UNP P49841

- Molecule 2 is 2-(2,4-DICHLORO-PHENYL)-7-HYDROXY-1H-BENZOIMIDAZOLE-4-CARBOXYLIC ACID [2-(4-METHANESULFONYLAMINO-PHENYL)-ETHYL]-AMIDE (three-letter code: HBM) (formula: C<sub>23</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub>S).

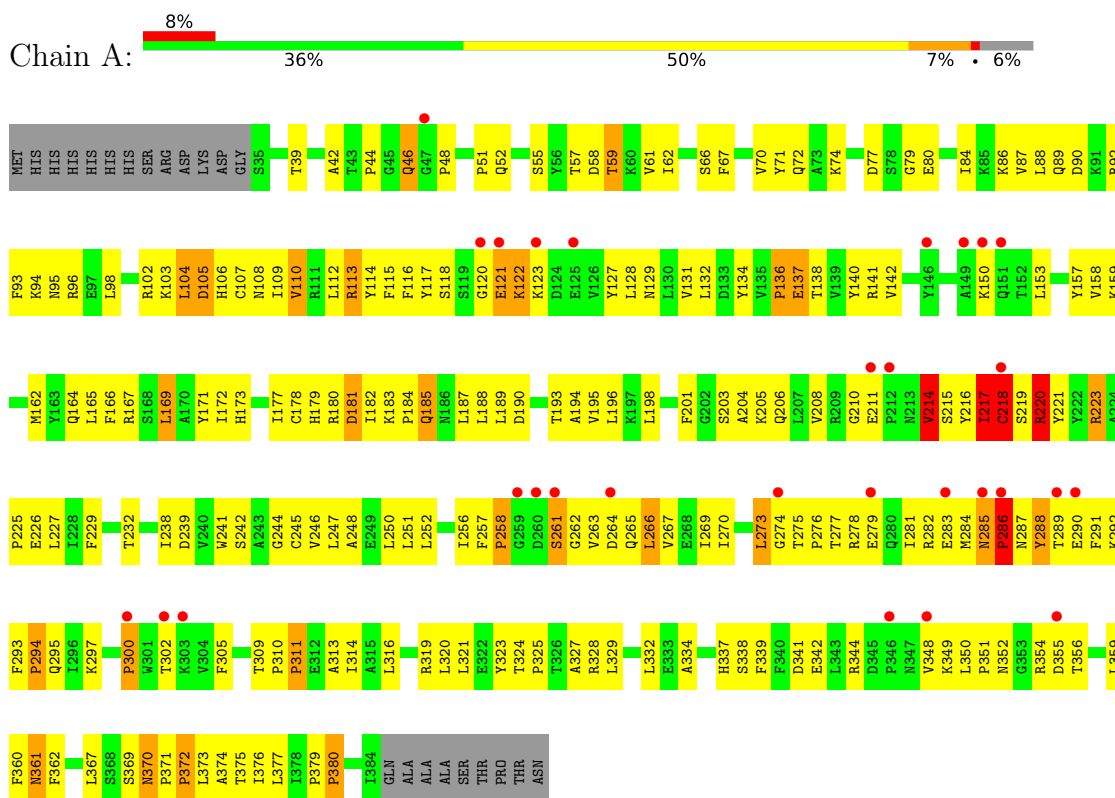


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	34	23	2	4	4	1	0	0

### 3 Residue-property plots

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: Glycogen synthase kinase-3 beta



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.94Å 72.63Å 81.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.53 – 3.20 25.53 – 3.01	Depositor EDS
% Data completeness (in resolution range)	89.5 (25.53-3.20) 88.1 (25.53-3.01)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.99Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.240 , 0.309 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	207 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtrriage
Anisotropy	0.484	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 104.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HBM

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	0.43	0/2861	0.70	0/3894

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 [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	2790	0	2808	216	0
2	A	34	0	20	1	0
All	All	2824	0	2828	216	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 38.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:HD21	1:A:354:ARG:HG2	1.09	1.08
1:A:217:ILE:HD12	1:A:223:ARG:NH2	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:HD2	1:A:141:ARG:HD3	1.34	0.92
1:A:214:VAL:HG21	1:A:216:TYR:CZ	2.03	0.92
1:A:319:ARG:HB3	1:A:329:LEU:HD13	1.56	0.88
1:A:46:GLN:HA	1:A:46:GLN:NE2	1.89	0.88
1:A:352:ASN:ND2	1:A:354:ARG:HG2	1.90	0.86
1:A:138:THR:OG1	1:A:141:ARG:HG2	1.75	0.86
1:A:244:GLY:HA2	1:A:320:LEU:HD23	1.60	0.83
1:A:350:LEU:HD12	1:A:356:THR:HA	1.59	0.82
1:A:46:GLN:HA	1:A:46:GLN:HE21	1.43	0.80
1:A:217:ILE:H	1:A:223:ARG:HH21	1.30	0.80
1:A:162:MET:CE	1:A:247:LEU:HB2	2.12	0.78
1:A:218:CYS:HB3	1:A:223:ARG:HG3	1.66	0.78
1:A:164:GLN:NE2	1:A:196:LEU:H	1.83	0.77
1:A:162:MET:HE1	1:A:247:LEU:HB2	1.66	0.77
1:A:216:TYR:O	1:A:217:ILE:HG23	1.85	0.77
1:A:183:LYS:HG2	1:A:185:GLN:H	1.50	0.76
1:A:329:LEU:HD23	1:A:334:ALA:HA	1.70	0.74
1:A:140:TYR:CD2	1:A:141:ARG:HD3	2.22	0.72
1:A:362:PHE:CE1	1:A:377:LEU:HB3	2.26	0.69
1:A:284:MET:O	1:A:285:ASN:HB3	1.92	0.69
1:A:352:ASN:HD21	1:A:354:ARG:CG	1.97	0.68
1:A:165:LEU:HD22	1:A:187:LEU:HD21	1.75	0.67
1:A:183:LYS:HG3	1:A:184:PRO:HD2	1.77	0.66
1:A:215:SER:O	1:A:217:ILE:HG13	1.95	0.66
1:A:263:VAL:O	1:A:267:VAL:HG23	1.96	0.65
1:A:80:GLU:CD	1:A:113:ARG:HH22	1.99	0.65
1:A:166:PHE:CZ	1:A:320:LEU:HD11	2.32	0.65
1:A:219:SER:O	1:A:223:ARG:HD2	1.96	0.65
1:A:179:HIS:HD2	1:A:198:LEU:HD21	1.62	0.65
1:A:179:HIS:CD2	1:A:198:LEU:HD21	2.32	0.64
1:A:205:LYS:HG2	1:A:206:GLN:N	2.12	0.64
1:A:178:CYS:SG	1:A:238:ILE:HD11	2.39	0.63
1:A:286:PRO:HB3	1:A:288:TYR:CD1	2.34	0.63
1:A:350:LEU:HD22	1:A:352:ASN:OD1	1.99	0.62
1:A:96:ARG:HD3	1:A:204:ALA:O	1.99	0.62
1:A:218:CYS:CB	1:A:223:ARG:HG3	2.30	0.62
1:A:92:ARG:O	1:A:93:PHE:HD1	1.83	0.62
1:A:223:ARG:HG2	1:A:227:LEU:HD23	1.81	0.62
1:A:371:PRO:HB2	1:A:372:PRO:HD3	1.82	0.61
1:A:362:PHE:CZ	1:A:377:LEU:HD13	2.35	0.61
1:A:270:ILE:HG23	1:A:275:THR:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:N	1:A:223:ARG:HH21	1.99	0.60
1:A:116:PHE:O	1:A:129:ASN:HB2	2.02	0.59
1:A:172:ILE:HG13	1:A:173:HIS:N	2.18	0.59
1:A:180:ARG:HG2	1:A:238:ILE:HD11	1.83	0.59
1:A:166:PHE:HZ	1:A:320:LEU:HD11	1.67	0.59
1:A:360:PHE:O	1:A:362:PHE:N	2.34	0.58
1:A:348:VAL:O	1:A:348:VAL:HG13	2.03	0.58
1:A:98:LEU:O	1:A:102:ARG:HG3	2.04	0.57
1:A:238:ILE:HG13	1:A:239:ASP:N	2.20	0.57
1:A:262:GLY:O	1:A:265:GLN:HB3	2.05	0.57
1:A:89:GLN:HE22	1:A:95:ASN:HB2	1.70	0.56
1:A:220:ARG:HD3	1:A:221:TYR:CD1	2.39	0.56
1:A:164:GLN:HE22	1:A:196:LEU:H	1.52	0.56
1:A:167:ARG:NH2	1:A:361:ASN:OD1	2.37	0.56
1:A:159:LYS:NZ	1:A:342:GLU:CB	2.69	0.56
1:A:217:ILE:H	1:A:223:ARG:NH2	2.00	0.56
1:A:104:LEU:HD21	1:A:172:ILE:HG22	1.88	0.55
1:A:324:THR:HB	1:A:327:ALA:HB3	1.89	0.55
1:A:226:GLU:HG2	1:A:227:LEU:N	2.22	0.55
1:A:341:ASP:O	1:A:344:ARG:N	2.38	0.55
1:A:220:ARG:HD3	1:A:221:TYR:HD1	1.72	0.54
1:A:324:THR:HB	1:A:327:ALA:CB	2.38	0.54
1:A:278:ARG:O	1:A:282:ARG:HB2	2.08	0.54
1:A:350:LEU:CD2	1:A:352:ASN:H	2.20	0.54
1:A:106:HIS:CD2	1:A:108:ASN:HB2	2.44	0.53
1:A:184:PRO:HD3	1:A:246:VAL:HG22	1.91	0.53
1:A:362:PHE:CE2	1:A:377:LEU:HD13	2.43	0.53
1:A:190:ASP:HB3	1:A:193:THR:OG1	2.09	0.53
1:A:261:SER:HB2	1:A:264:ASP:CB	2.39	0.52
1:A:114:TYR:H	1:A:131:VAL:HB	1.74	0.52
1:A:286:PRO:C	1:A:288:TYR:H	2.12	0.52
1:A:247:LEU:O	1:A:251:LEU:HG	2.09	0.51
1:A:264:ASP:O	1:A:267:VAL:HB	2.11	0.51
1:A:157:TYR:OH	1:A:351:PRO:HB2	2.11	0.51
1:A:98:LEU:O	1:A:98:LEU:HD12	2.09	0.51
1:A:159:LYS:NZ	1:A:342:GLU:HB2	2.25	0.51
1:A:245:CYS:O	1:A:248:ALA:N	2.43	0.51
1:A:217:ILE:HD13	1:A:227:LEU:HD21	1.92	0.51
1:A:162:MET:HG3	1:A:247:LEU:HD13	1.92	0.50
1:A:256:ILE:HG23	1:A:257:PHE:CG	2.47	0.50
1:A:94:LYS:HD2	1:A:94:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:HIS:NE2	1:A:108:ASN:HB2	2.26	0.50
1:A:182:ILE:O	1:A:242:SER:HB3	2.11	0.50
1:A:284:MET:C	1:A:286:PRO:HD2	2.32	0.50
1:A:293:PHE:HB3	1:A:294:PRO:HD2	1.93	0.50
1:A:216:TYR:C	1:A:217:ILE:HG13	2.32	0.50
1:A:183:LYS:HD2	1:A:185:GLN:OE1	2.12	0.50
1:A:214:VAL:HG23	1:A:215:SER:H	1.77	0.50
1:A:319:ARG:NH2	1:A:327:ALA:O	2.45	0.49
1:A:193:THR:HB	1:A:195:VAL:HG23	1.93	0.49
1:A:217:ILE:HD12	1:A:223:ARG:HH21	1.73	0.49
1:A:252:LEU:HD21	1:A:305:PHE:HA	1.94	0.49
1:A:291:PHE:CE2	1:A:293:PHE:HB2	2.48	0.49
1:A:362:PHE:HB3	1:A:367:LEU:HD11	1.95	0.49
1:A:118:SER:CB	1:A:129:ASN:HD21	2.25	0.49
1:A:183:LYS:HE2	1:A:185:GLN:HB2	1.95	0.49
1:A:220:ARG:N	1:A:220:ARG:HD2	2.28	0.49
1:A:261:SER:HB2	1:A:264:ASP:HB2	1.95	0.49
1:A:181:ASP:HB2	1:A:203:SER:OG	2.13	0.49
1:A:184:PRO:HG3	1:A:246:VAL:HG13	1.95	0.49
1:A:257:PHE:O	1:A:258:PRO:O	2.30	0.48
1:A:277:THR:O	1:A:281:ILE:HG13	2.13	0.48
1:A:74:LYS:HA	1:A:80:GLU:O	2.13	0.48
1:A:159:LYS:NZ	1:A:342:GLU:HB3	2.29	0.48
1:A:180:ARG:CZ	1:A:217:ILE:HG21	2.43	0.48
1:A:276:PRO:HB3	1:A:323:TYR:CE2	2.49	0.48
1:A:44:PRO:C	1:A:46:GLN:H	2.16	0.48
1:A:284:MET:O	1:A:285:ASN:CB	2.59	0.48
1:A:58:ASP:O	1:A:59:THR:C	2.51	0.48
1:A:115:PHE:HA	1:A:129:ASN:O	2.13	0.48
1:A:104:LEU:HD22	1:A:171:TYR:CE1	2.48	0.48
1:A:136:PRO:O	1:A:137:GLU:O	2.31	0.48
1:A:177:ILE:HD13	1:A:206:GLN:HG3	1.95	0.48
1:A:180:ARG:HG2	1:A:238:ILE:CD1	2.43	0.48
1:A:98:LEU:HD22	1:A:128:LEU:HD11	1.97	0.47
1:A:118:SER:HB2	1:A:129:ASN:HD21	1.80	0.47
1:A:62:ILE:HD13	1:A:72:GLN:HB2	1.96	0.47
1:A:109:ILE:O	1:A:110:VAL:C	2.53	0.47
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.80	0.47
1:A:172:ILE:HG13	1:A:173:HIS:H	1.78	0.47
1:A:355:ASP:OD1	1:A:356:THR:N	2.48	0.47
1:A:214:VAL:HG21	1:A:216:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HB2	1:A:337:HIS:CE1	2.50	0.47
1:A:193:THR:O	1:A:194:ALA:HB3	2.15	0.46
1:A:229:PHE:HB3	1:A:286:PRO:HG2	1.97	0.46
1:A:279:GLU:O	1:A:283:GLU:HG3	2.16	0.46
1:A:51:PRO:C	1:A:52:GLN:HG3	2.35	0.46
1:A:159:LYS:HZ2	1:A:342:GLU:CB	2.29	0.46
1:A:106:HIS:CD2	1:A:108:ASN:H	2.34	0.46
1:A:350:LEU:HD22	1:A:352:ASN:H	1.79	0.46
1:A:44:PRO:C	1:A:46:GLN:N	2.70	0.45
1:A:112:LEU:HD13	1:A:132:LEU:HD21	1.99	0.45
1:A:104:LEU:HD22	1:A:171:TYR:HE1	1.81	0.45
1:A:286:PRO:HB3	1:A:288:TYR:HD1	1.80	0.45
1:A:185:GLN:HE21	1:A:185:GLN:N	2.14	0.45
1:A:316:LEU:HD13	1:A:337:HIS:CG	2.51	0.45
1:A:153:LEU:HD12	1:A:250:LEU:HD11	1.98	0.45
1:A:86:LYS:HG2	1:A:127:TYR:HD2	1.82	0.45
1:A:309:THR:HB	1:A:314:ILE:HD11	1.98	0.45
1:A:281:ILE:HA	1:A:284:MET:HE3	1.99	0.45
1:A:84:ILE:N	1:A:84:ILE:HD12	2.32	0.45
1:A:87:VAL:HG12	1:A:88:LEU:N	2.31	0.44
1:A:187:LEU:HD12	1:A:198:LEU:HD12	1.99	0.44
1:A:284:MET:C	1:A:286:PRO:CD	2.86	0.44
1:A:369:SER:O	1:A:370:ASN:HB2	2.17	0.44
1:A:165:LEU:HD13	1:A:187:LEU:HD11	2.00	0.44
1:A:158:VAL:HG13	1:A:250:LEU:HD23	1.99	0.44
1:A:256:ILE:C	1:A:258:PRO:HD3	2.38	0.44
1:A:270:ILE:O	1:A:274:GLY:N	2.50	0.44
1:A:42:ALA:O	1:A:51:PRO:HA	2.18	0.44
1:A:375:THR:O	1:A:376:ILE:HD13	2.17	0.44
1:A:117:TYR:N	1:A:117:TYR:CD1	2.85	0.44
1:A:131:VAL:O	1:A:132:LEU:HD23	2.18	0.44
1:A:140:TYR:HD2	1:A:141:ARG:CD	2.16	0.44
1:A:220:ARG:HD2	1:A:220:ARG:H	1.82	0.44
1:A:284:MET:O	1:A:286:PRO:HD3	2.17	0.44
1:A:373:LEU:O	1:A:377:LEU:HG	2.18	0.44
1:A:110:VAL:HG12	1:A:198:LEU:O	2.18	0.43
1:A:180:ARG:O	1:A:181:ASP:HB2	2.16	0.43
1:A:217:ILE:HD12	1:A:217:ILE:N	2.33	0.43
1:A:229:PHE:HB3	1:A:286:PRO:CG	2.48	0.43
1:A:214:VAL:HG21	1:A:216:TYR:CE1	2.50	0.43
1:A:349:LYS:NZ	1:A:349:LYS:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:58:ASP:HB2	2.19	0.43
1:A:159:LYS:HZ3	1:A:342:GLU:HB3	1.84	0.43
1:A:183:LYS:HG3	1:A:184:PRO:CD	2.47	0.43
1:A:159:LYS:HZ3	1:A:342:GLU:CB	2.31	0.43
1:A:225:PRO:HD3	1:A:241:TRP:CE2	2.54	0.43
1:A:137:GLU:O	1:A:138:THR:CG2	2.67	0.42
1:A:325:PRO:HA	1:A:328:ARG:NH1	2.34	0.42
1:A:39:THR:HG23	1:A:55:SER:HB3	2.01	0.42
1:A:218:CYS:HB3	1:A:219:SER:H	1.70	0.42
1:A:256:ILE:HG23	1:A:257:PHE:CD2	2.54	0.42
1:A:379:PRO:HA	1:A:380:PRO:HD3	1.85	0.42
1:A:289:THR:HB	1:A:290:GLU:OE2	2.19	0.42
1:A:372:PRO:O	1:A:375:THR:HG23	2.19	0.42
1:A:61:VAL:HG22	1:A:71:TYR:CE1	2.54	0.42
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.88	0.42
1:A:95:ASN:ND2	1:A:128:LEU:HD22	2.34	0.42
1:A:242:SER:O	1:A:246:VAL:HG23	2.19	0.42
1:A:313:ALA:HB2	1:A:339:PHE:CE1	2.54	0.42
1:A:137:GLU:O	1:A:138:THR:HG23	2.19	0.42
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.87	0.42
1:A:270:ILE:HG23	1:A:274:GLY:O	2.19	0.42
1:A:138:THR:O	1:A:142:VAL:HG23	2.19	0.42
1:A:74:LYS:HG3	1:A:79:GLY:O	2.20	0.41
1:A:261:SER:HB2	1:A:264:ASP:HB3	2.02	0.41
1:A:138:THR:HG22	1:A:188:LEU:HA	2.01	0.41
1:A:208:VAL:HG21	1:A:211:GLU:OE1	2.20	0.41
1:A:266:LEU:HA	1:A:269:ILE:HG13	2.02	0.41
1:A:309:THR:HA	1:A:310:PRO:HD2	1.93	0.41
1:A:112:LEU:HD13	1:A:132:LEU:CD2	2.50	0.41
1:A:285:ASN:N	1:A:286:PRO:HD2	2.36	0.41
1:A:104:LEU:HD11	1:A:201:PHE:CE2	2.56	0.41
1:A:273:LEU:HD11	1:A:321:LEU:O	2.20	0.41
1:A:122:LYS:HB2	1:A:123:LYS:H	1.52	0.41
1:A:297:LYS:HD3	1:A:297:LYS:C	2.41	0.41
1:A:164:GLN:HE21	1:A:196:LEU:HB3	1.86	0.41
1:A:183:LYS:HD2	1:A:185:GLN:CD	2.42	0.41
1:A:210:GLY:O	1:A:211:GLU:HG3	2.21	0.41
1:A:273:LEU:HD13	1:A:323:TYR:CE1	2.55	0.41
1:A:287:ASN:O	1:A:289:THR:N	2.50	0.41
1:A:216:TYR:O	1:A:217:ILE:HG13	2.20	0.40
1:A:217:ILE:N	1:A:223:ARG:NH2	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HB	1:A:218:CYS:H	1.61	0.40
1:A:58:ASP:OD1	1:A:74:LYS:HE3	2.21	0.40
1:A:291:PHE:CZ	1:A:293:PHE:HB2	2.55	0.40
1:A:104:LEU:O	1:A:105:ASP:HB2	2.21	0.40
1:A:134:TYR:HA	2:A:0:HBM:O34	2.21	0.40
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.86	0.40
1:A:167:ARG:NH1	1:A:359:LEU:HA	2.37	0.40
1:A:288:TYR:C	1:A:290:GLU:N	2.74	0.40
1:A:372:PRO:C	1:A:374:ALA:H	2.24	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	348/372 (94%)	263 (76%)	55 (16%)	30 (9%)	<b>1</b> <b>4</b>

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	181	ASP
1	A	214	VAL
1	A	217	ILE
1	A	218	CYS
1	A	258	PRO
1	A	285	ASN
1	A	66	SER
1	A	105	ASP
1	A	136	PRO
1	A	232	THR
1	A	300	PRO

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Mol	Chain	Res	Type
1	A	48	PRO
1	A	90	ASP
1	A	121	GLU
1	A	150	LYS
1	A	220	ARG
1	A	286	PRO
1	A	294	PRO
1	A	338	SER
1	A	104	LEU
1	A	288	TYR
1	A	59	THR
1	A	110	VAL
1	A	361	ASN
1	A	380	PRO
1	A	292	LYS
1	A	120	GLY
1	A	70	VAL
1	A	370	ASN

### 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	309/330 (94%)	284 (92%)	25 (8%)	<b>11</b> 42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	67	PHE
1	A	77	ASP
1	A	103	LYS
1	A	107	CYS
1	A	113	ARG
1	A	121	GLU
1	A	122	LYS

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Mol	Chain	Res	Type
1	A	169	LEU
1	A	185	GLN
1	A	189	LEU
1	A	214	VAL
1	A	217	ILE
1	A	218	CYS
1	A	220	ARG
1	A	223	ARG
1	A	261	SER
1	A	266	LEU
1	A	273	LEU
1	A	286	PRO
1	A	295	GLN
1	A	300	PRO
1	A	302	THR
1	A	311	PRO
1	A	372	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	89	GLN
1	A	106	HIS
1	A	129	ASN
1	A	151	GLN
1	A	164	GLN
1	A	185	GLN
1	A	206	GLN
1	A	265	GLN
1	A	365	GLN

### 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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	HBM	A	0	-	36,37,37	3.92	24 (66%)	39,54,54	1.74	11 (28%)

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	HBM	A	0	-	-	5/15/19/19	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	0	HBM	C15-C10	9.35	1.58	1.42
2	A	0	HBM	S29-N28	8.29	1.74	1.63
2	A	0	HBM	C24-C25	6.65	1.50	1.39
2	A	0	HBM	C23-C22	5.92	1.51	1.38
2	A	0	HBM	C26-C25	5.74	1.48	1.39
2	A	0	HBM	C27-C22	5.21	1.50	1.38
2	A	0	HBM	C18-N19	5.05	1.44	1.33
2	A	0	HBM	C12-C13	4.98	1.47	1.38
2	A	0	HBM	C24-C23	4.73	1.47	1.38
2	A	0	HBM	C14-C13	4.31	1.45	1.38
2	A	0	HBM	C11-C10	4.20	1.50	1.42
2	A	0	HBM	C8-N9	4.13	1.42	1.34
2	A	0	HBM	C2-C1	4.07	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	0	HBM	C27-C26	3.97	1.46	1.38
2	A	0	HBM	C30-S29	3.73	1.84	1.75
2	A	0	HBM	C3-C4	3.69	1.44	1.37
2	A	0	HBM	C14-C15	3.40	1.44	1.36
2	A	0	HBM	C3-C2	3.21	1.44	1.38
2	A	0	HBM	O32-S29	2.95	1.48	1.43
2	A	0	HBM	C11-C12	2.77	1.42	1.36
2	A	0	HBM	C8-N7	2.71	1.39	1.34
2	A	0	HBM	C6-C5	2.44	1.52	1.43
2	A	0	HBM	C4-C5	2.15	1.45	1.42
2	A	0	HBM	C21-C22	2.09	1.57	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	0	HBM	O34-C4-C5	4.87	130.96	119.31
2	A	0	HBM	O33-C18-C1	-3.98	116.21	121.72
2	A	0	HBM	O34-C4-C3	-3.48	110.08	122.20
2	A	0	HBM	C10-C15-CL17	2.60	123.97	119.21
2	A	0	HBM	O32-S29-C30	-2.55	104.19	108.28
2	A	0	HBM	O31-S29-C30	-2.33	104.54	108.28
2	A	0	HBM	C14-C15-CL17	-2.23	114.43	118.73
2	A	0	HBM	C20-C21-C22	2.18	117.91	112.87
2	A	0	HBM	C25-N28-S29	-2.15	117.31	123.83
2	A	0	HBM	C2-C1-C6	-2.12	115.77	118.37
2	A	0	HBM	C1-C18-N19	2.12	119.16	116.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

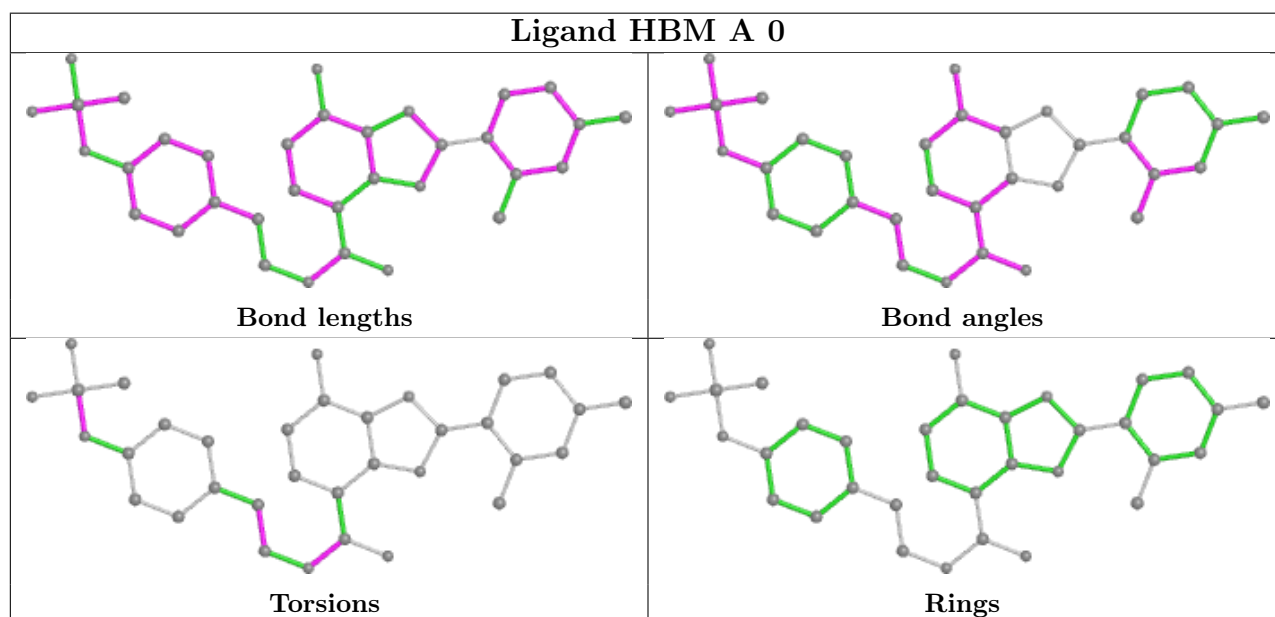
Mol	Chain	Res	Type	Atoms
2	A	0	HBM	N19-C20-C21-C22
2	A	0	HBM	C25-N28-S29-C30
2	A	0	HBM	C25-N28-S29-O32
2	A	0	HBM	C1-C18-N19-C20
2	A	0	HBM	O33-C18-N19-C20

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	0	HBM	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.



## 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	350/372 (94%)	0.34	29 (8%) <b>11</b> <b>6</b>	12, 37, 82, 102	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	GLY	7.5
1	A	264	ASP	5.4
1	A	290	GLU	4.2
1	A	286	PRO	4.1
1	A	120	GLY	3.8
1	A	355	ASP	3.6
1	A	123	LYS	3.4
1	A	289	THR	3.3
1	A	151	GLN	3.2
1	A	212	PRO	3.2
1	A	260	ASP	3.1
1	A	261	SER	3.0
1	A	218	CYS	2.9
1	A	121	GLU	2.7
1	A	300	PRO	2.6
1	A	285	ASN	2.5
1	A	259	GLY	2.5
1	A	211	GLU	2.4
1	A	283	GLU	2.3
1	A	125	GLU	2.3
1	A	146	TYR	2.3
1	A	47	GLY	2.3
1	A	150	LYS	2.2
1	A	302	THR	2.1
1	A	149	ALA	2.1
1	A	346	PRO	2.1
1	A	279	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	2.0
1	A	303	LYS	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](#)

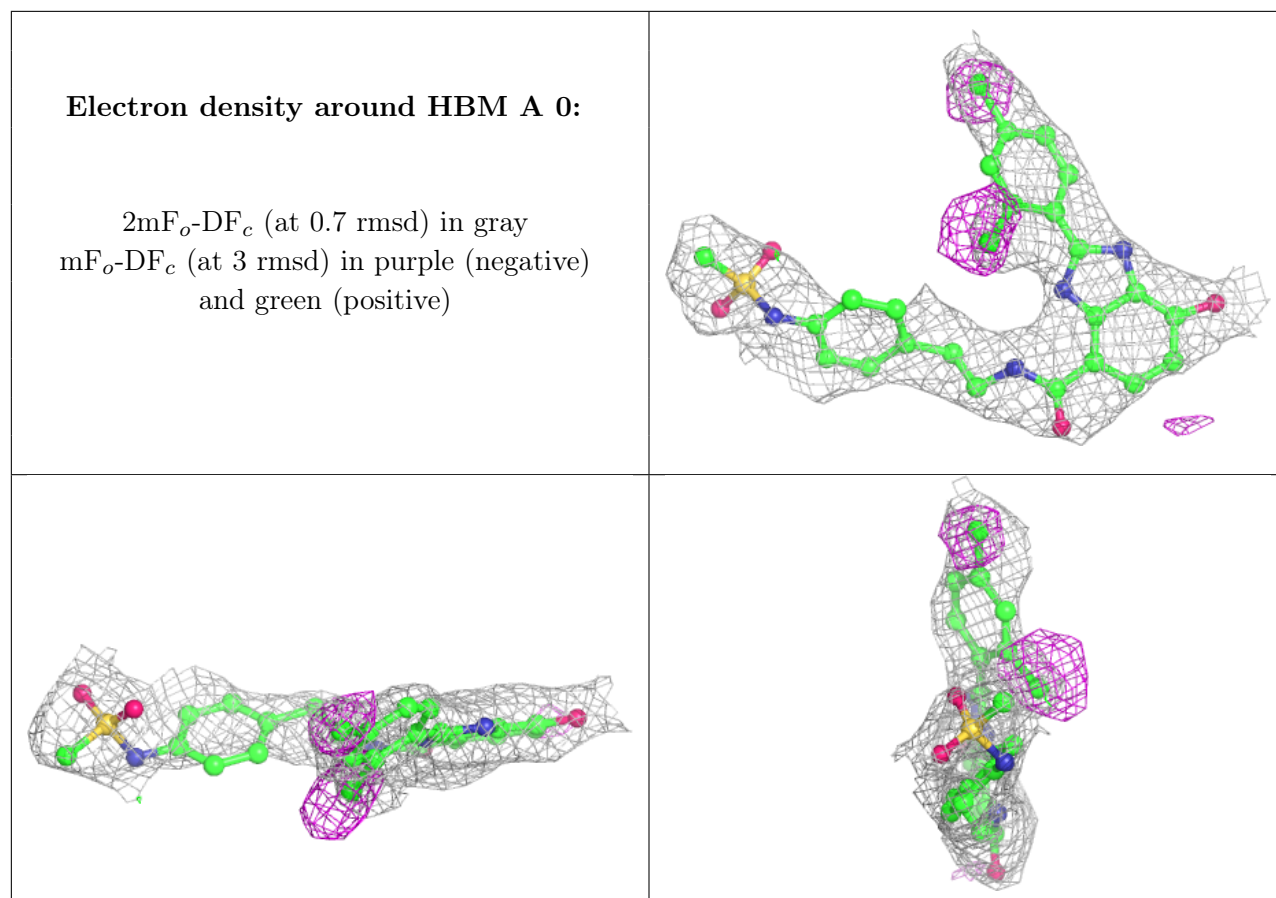
There are no monosaccharides in this entry.

## 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	HBM	A	0	34/34	0.76	0.32	36,44,83,85	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.