



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:16 AM EDT

PDB ID : 3H2O  
Title : Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase  
Authors : Yun, M.-K.; White, S.W.  
Deposited on : 2009-04-14  
Resolution : 2.70 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 : 2.35  
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) : 2.35

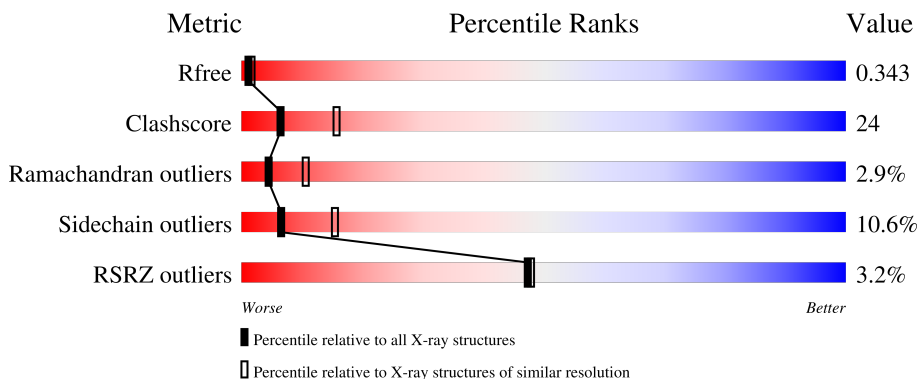
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	297	 3% 52% 30% 6% 11%
1	B	297	 3% 43% 39% 6% 12%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4069 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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2000	1257	345	382	16	0	0	0
1	B	262	1996	1256	344	380	16	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

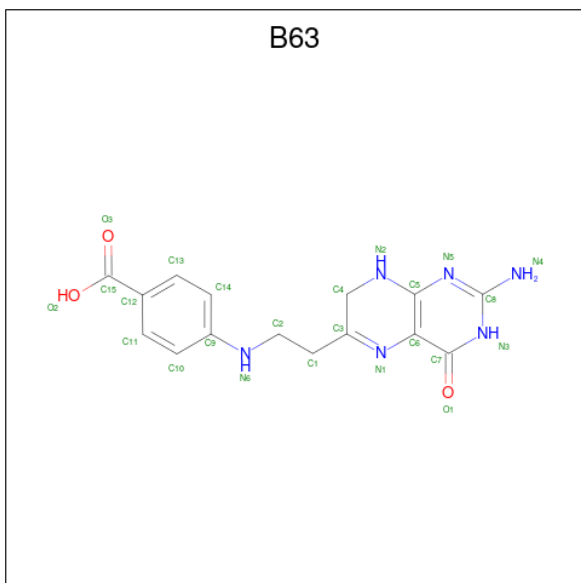
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B1UXN2
A	-18	GLY	-	expression tag	UNP B1UXN2
A	-17	SER	-	expression tag	UNP B1UXN2
A	-16	SER	-	expression tag	UNP B1UXN2
A	-15	HIS	-	expression tag	UNP B1UXN2
A	-14	HIS	-	expression tag	UNP B1UXN2
A	-13	HIS	-	expression tag	UNP B1UXN2
A	-12	HIS	-	expression tag	UNP B1UXN2
A	-11	HIS	-	expression tag	UNP B1UXN2
A	-10	HIS	-	expression tag	UNP B1UXN2
A	-9	SER	-	expression tag	UNP B1UXN2
A	-8	SER	-	expression tag	UNP B1UXN2
A	-7	GLY	-	expression tag	UNP B1UXN2
A	-6	LEU	-	expression tag	UNP B1UXN2
A	-5	VAL	-	expression tag	UNP B1UXN2
A	-4	PRO	-	expression tag	UNP B1UXN2
A	-3	ARG	-	expression tag	UNP B1UXN2
A	-2	GLY	-	expression tag	UNP B1UXN2
A	-1	SER	-	expression tag	UNP B1UXN2
A	0	HIS	-	expression tag	UNP B1UXN2
B	-19	MET	-	expression tag	UNP B1UXN2
B	-18	GLY	-	expression tag	UNP B1UXN2
B	-17	SER	-	expression tag	UNP B1UXN2
B	-16	SER	-	expression tag	UNP B1UXN2
B	-15	HIS	-	expression tag	UNP B1UXN2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B1UXN2
B	-13	HIS	-	expression tag	UNP B1UXN2
B	-12	HIS	-	expression tag	UNP B1UXN2
B	-11	HIS	-	expression tag	UNP B1UXN2
B	-10	HIS	-	expression tag	UNP B1UXN2
B	-9	SER	-	expression tag	UNP B1UXN2
B	-8	SER	-	expression tag	UNP B1UXN2
B	-7	GLY	-	expression tag	UNP B1UXN2
B	-6	LEU	-	expression tag	UNP B1UXN2
B	-5	VAL	-	expression tag	UNP B1UXN2
B	-4	PRO	-	expression tag	UNP B1UXN2
B	-3	ARG	-	expression tag	UNP B1UXN2
B	-2	GLY	-	expression tag	UNP B1UXN2
B	-1	SER	-	expression tag	UNP B1UXN2
B	0	HIS	-	expression tag	UNP B1UXN2

- Molecule 2 is 4-{[2-(2-amino-4-oxo-3,4,7,8-tetrahydropteridin-6-yl)ethyl]amino}benzoic acid (three-letter code: B63) (formula: C<sub>15</sub>H<sub>16</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	24	15	6	3	0	0
2	B	1	24	15	6	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	3	Total O 3 3	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.29Å 99.29Å 263.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.78 – 2.70 48.78 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.78-2.70) 93.7 (48.78-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.64 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.271 , 0.311 0.301 , 0.343	Depositor DCC
$R_{free}$ test set	1158 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtrriage
Anisotropy	0.930	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0926e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: B63, SO4

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	1.10	9/2029 (0.4%)	1.06	7/2744 (0.3%)
1	B	0.93	1/2024 (0.0%)	1.03	3/2733 (0.1%)
All	All	1.02	10/4053 (0.2%)	1.04	10/5477 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	LYS	CE-NZ	8.21	1.69	1.49
1	A	73	LYS	N-CA	8.10	1.62	1.46
1	A	248	LYS	CE-NZ	7.63	1.68	1.49
1	A	73	LYS	CA-CB	7.33	1.70	1.53
1	A	211	TYR	CE1-CZ	6.71	1.47	1.38
1	A	211	TYR	CG-CD2	6.28	1.47	1.39
1	A	34	SER	CB-OG	5.64	1.49	1.42
1	A	247	GLU	CB-CG	-5.26	1.42	1.52
1	A	252	PHE	CE1-CZ	5.03	1.47	1.37
1	B	95	LYS	CE-NZ	5.01	1.61	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	203	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	B	148	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	263	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	214	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	B	21	LEU	CA-CB-CG	-5.45	102.77	115.30
1	A	96	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	248	LYS	CD-CE-NZ	5.27	123.83	111.70
1	A	234	ARG	NE-CZ-NH1	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASP	CB-CG-OD1	-5.07	113.74	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2000	0	1974	87	0
1	B	1996	0	1984	103	0
2	A	24	0	15	4	0
2	B	24	0	15	2	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
All	All	4069	0	3988	192	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 24.

All (192) 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:81:LYS:CE	1:A:81:LYS:NZ	1.69	1.52
1:A:248:LYS:CE	1:A:248:LYS:NZ	1.68	1.51
1:B:9:CYS:HB2	1:B:12:TYR:O	1.65	0.96
1:A:2:LYS:HD3	1:A:2:LYS:C	1.95	0.85
1:A:242:VAL:HG13	1:A:253:VAL:HG11	1.59	0.84
1:B:214:LEU:HD23	1:B:215:LEU:N	1.91	0.84
1:B:79:GLU:O	1:B:83:VAL:HG12	1.78	0.83
1:A:121:ASP:OD2	1:A:123:TRP:N	2.11	0.82
1:A:2:LYS:HD3	1:A:2:LYS:O	1.80	0.81
1:B:51:GLU:O	1:B:55:GLU:HG2	1.84	0.78
1:B:227:LEU:HB3	1:B:229:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HB3	1:A:229:LEU:CD1	2.13	0.78
1:A:2:LYS:C	1:A:2:LYS:CD	2.51	0.77
1:B:216:GLY:O	1:B:220:LYS:NZ	2.19	0.76
1:A:227:LEU:O	1:A:229:LEU:CD1	2.36	0.73
1:A:133:GLU:O	1:A:136:ALA:HB3	1.90	0.71
1:A:227:LEU:C	1:A:229:LEU:HD12	2.11	0.71
1:A:227:LEU:O	1:A:229:LEU:HD11	1.92	0.70
1:A:172:LYS:HD2	1:A:178:ASP:OD1	1.95	0.66
1:A:216:GLY:O	1:A:220:LYS:NZ	2.28	0.66
1:A:112:ILE:HD11	1:A:119:ILE:HD11	1.77	0.66
1:B:8:ARG:HH11	1:B:8:ARG:HA	1.61	0.66
1:A:218:SER:HB2	1:A:255:VAL:HA	1.78	0.65
1:B:59:ILE:HG23	1:B:97:PRO:HG2	1.79	0.64
1:B:221:SER:H	2:B:502:B63:C15	2.10	0.64
1:B:26:LEU:HD21	1:B:45:ALA:HB1	1.78	0.64
1:B:117:HIS:O	1:B:140:VAL:HB	1.98	0.64
1:B:149:ASP:N	1:B:149:ASP:OD1	2.30	0.64
1:B:156:LEU:HD23	1:B:198:GLU:HG3	1.79	0.64
1:B:201:ARG:O	1:B:248:LYS:HE3	1.97	0.63
1:B:123:TRP:HB2	1:B:127:ALA:HB2	1.81	0.62
1:B:178:ASP:HA	1:B:181:ILE:HD12	1.81	0.62
1:A:104:LYS:HB3	1:A:107:VAL:HG23	1.81	0.62
1:A:121:ASP:OD2	1:A:121:ASP:C	2.39	0.61
1:A:235:LEU:HD11	1:A:260:GLU:HG3	1.81	0.61
1:A:123:TRP:CB	1:A:127:ALA:HB2	2.32	0.60
1:B:27:ASN:HB2	1:B:48:HIS:ND1	2.17	0.59
1:B:145:MET:HA	1:B:184:ASP:O	2.02	0.59
1:B:87:ILE:O	1:B:91:SER:HB3	2.03	0.59
1:B:215:LEU:HD23	1:B:253:VAL:HG12	1.84	0.59
1:B:83:VAL:O	1:B:86:MET:HB2	2.03	0.58
1:A:123:TRP:HB2	1:A:127:ALA:HB2	1.85	0.58
1:A:227:LEU:O	1:A:229:LEU:HD12	2.03	0.58
1:A:104:LYS:HE3	1:A:104:LYS:HA	1.86	0.58
1:A:51:GLU:O	1:A:55:GLU:HG2	2.04	0.57
1:B:182:ILE:HG22	1:B:183:LEU:N	2.18	0.57
1:B:146:HIS:HB3	1:B:185:PRO:O	2.04	0.57
1:B:218:SER:HB2	1:B:255:VAL:HA	1.86	0.57
1:A:204:GLU:OE2	1:A:248:LYS:HD3	2.05	0.57
1:B:87:ILE:HD12	1:B:114:ALA:HB3	1.86	0.56
1:B:214:LEU:HG	1:B:252:PHE:HB2	1.88	0.56
1:A:245:GLY:C	1:A:250:CYS:HG	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASP:O	1:B:170:ILE:HG13	2.06	0.56
1:B:123:TRP:CB	1:B:127:ALA:HB2	2.34	0.56
1:B:192:THR:HB	1:B:193:PRO:CD	2.36	0.56
1:B:259:LYS:HB3	1:B:260:GLU:OE1	2.06	0.56
1:A:55:GLU:HB2	1:A:258:VAL:CG1	2.37	0.55
1:A:96:LEU:HB3	1:A:97:PRO:HD2	1.87	0.55
1:B:208:VAL:HG23	1:B:209:LEU:HD23	1.87	0.55
1:A:259:LYS:HB3	1:A:260:GLU:OE2	2.07	0.55
1:A:214:LEU:HG	1:A:252:PHE:HB2	1.88	0.55
1:B:214:LEU:HD23	1:B:214:LEU:C	2.27	0.55
1:A:43:ASP:O	1:A:47:ARG:HG3	2.07	0.54
1:B:5:TYR:CE1	1:B:179:GLU:HA	2.43	0.54
1:B:182:ILE:CG2	1:B:183:LEU:N	2.71	0.54
1:B:104:LYS:HB3	1:B:128:GLU:OE2	2.08	0.53
1:B:257:ASP:O	1:B:258:VAL:C	2.44	0.53
1:A:57:ALA:HB2	1:A:258:VAL:HG11	1.89	0.53
1:A:20:THR:OG1	1:A:269:ASP:OD2	2.26	0.53
1:A:193:PRO:HA	1:A:196:ASN:HD22	1.72	0.53
1:B:8:ARG:HD2	1:B:13:THR:HG23	1.89	0.53
1:A:121:ASP:OD2	1:A:124:GLY:N	2.41	0.53
1:A:227:LEU:HB3	1:A:229:LEU:HD13	1.90	0.52
1:A:155:ASN:HB3	1:A:158:ALA:HB3	1.90	0.52
1:B:232:GLU:CD	1:B:232:GLU:H	2.13	0.52
1:B:130:LYS:HD2	1:B:130:LYS:H	1.73	0.52
1:B:165:TYR:HE1	1:B:209:LEU:HD22	1.75	0.52
1:A:221:SER:N	2:A:501:B63:O2	2.34	0.52
1:B:156:LEU:HD23	1:B:198:GLU:CG	2.40	0.52
1:A:149:ASP:N	1:A:149:ASP:OD1	2.43	0.51
1:A:252:PHE:CD1	1:A:252:PHE:N	2.77	0.51
1:B:151:MET:HG2	1:B:190:ALA:O	2.10	0.51
1:B:252:PHE:CD1	1:B:252:PHE:N	2.79	0.51
1:B:86:MET:O	1:B:90:VAL:HG23	2.10	0.51
1:A:200:MET:SD	1:A:215:LEU:HD11	2.51	0.51
1:B:140:VAL:HG23	1:B:141:PRO:O	2.09	0.51
1:A:53:ARG:NH1	1:A:54:ASP:OD1	2.44	0.51
1:B:18:GLU:HG3	1:B:19:LYS:HG2	1.92	0.51
1:B:128:GLU:O	1:B:129:PRO:C	2.48	0.51
1:B:142:ILE:CG1	1:B:143:ILE:N	2.74	0.51
1:B:25:ILE:HD12	1:B:256:HIS:N	2.25	0.50
1:B:25:ILE:HD12	1:B:255:VAL:C	2.31	0.50
1:B:122:ILE:HB	1:B:145:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:O	1:B:250:CYS:SG	2.69	0.50
1:B:254:ARG:O	1:B:254:ARG:HG2	2.10	0.50
1:B:214:LEU:HD23	1:B:215:LEU:H	1.73	0.50
1:A:104:LYS:HB3	1:A:107:VAL:CG2	2.41	0.49
1:A:258:VAL:O	1:A:262:SER:HB2	2.13	0.49
1:A:236:GLU:H	1:A:236:GLU:CD	2.16	0.49
1:B:63:GLY:HA2	1:B:101:ASP:HB3	1.94	0.49
1:B:221:SER:N	2:B:502:B63:O2	2.40	0.49
1:B:3:TRP:CH2	1:B:212:PRO:HD3	2.48	0.49
1:A:221:SER:H	2:A:501:B63:C15	2.26	0.48
1:B:131:ILE:O	1:B:134:VAL:HB	2.13	0.48
1:A:26:LEU:HD21	1:A:45:ALA:HB1	1.96	0.48
1:A:81:LYS:NZ	1:A:81:LYS:CD	2.69	0.48
1:B:242:VAL:HG22	1:B:253:VAL:HG11	1.95	0.48
1:A:189:PHE:O	1:A:191:LYS:HG3	2.14	0.47
1:A:203:LEU:HD21	1:A:215:LEU:HD13	1.96	0.47
1:B:121:ASP:OD2	1:B:123:TRP:N	2.36	0.47
1:A:91:SER:HA	1:A:98:ILE:CD1	2.44	0.47
1:B:55:GLU:HB3	1:B:258:VAL:CG1	2.44	0.47
1:A:42:VAL:O	1:A:45:ALA:N	2.45	0.47
1:A:157:MET:O	1:A:158:ALA:C	2.52	0.47
1:B:7:LEU:HA	1:B:7:LEU:HD23	1.39	0.47
1:B:236:GLU:H	1:B:236:GLU:CD	2.17	0.47
1:B:156:LEU:O	1:B:159:ASP:N	2.46	0.47
1:A:123:TRP:O	1:A:126:LYS:HB2	2.15	0.47
1:B:58:HIS:O	1:B:97:PRO:HD2	2.15	0.47
1:B:104:LYS:CB	1:B:128:GLU:OE2	2.63	0.46
1:B:156:LEU:O	1:B:159:ASP:HB2	2.15	0.46
1:B:214:LEU:HA	1:B:252:PHE:O	2.15	0.46
1:B:23:MET:HB3	1:B:254:ARG:HB2	1.97	0.46
1:A:42:VAL:O	1:A:43:ASP:C	2.52	0.46
1:A:227:LEU:HB3	1:A:229:LEU:HD12	1.96	0.46
1:B:123:TRP:O	1:B:126:LYS:HB2	2.15	0.46
1:B:255:VAL:HG11	1:B:261:MET:HG3	1.98	0.46
1:A:232:GLU:H	1:A:232:GLU:CD	2.19	0.45
1:A:257:ASP:HB3	1:A:260:GLU:HG2	1.98	0.45
1:B:141:PRO:HA	1:B:180:ASN:HB3	1.99	0.45
1:A:92:LYS:O	1:A:92:LYS:HG3	2.16	0.45
1:B:268:MET:O	1:B:271:MET:N	2.48	0.45
1:A:28:VAL:HG21	1:A:63:GLY:C	2.37	0.45
1:B:81:LYS:HE3	1:B:81:LYS:HB2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:MET:O	1:A:203:LEU:HD12	2.16	0.45
1:B:231:VAL:HA	1:B:234:ARG:HD2	1.97	0.45
1:A:52:MET:HA	1:A:55:GLU:CG	2.47	0.45
1:B:27:ASN:HB2	1:B:48:HIS:CE1	2.51	0.45
1:B:5:TYR:CZ	1:B:179:GLU:HA	2.52	0.45
1:B:42:VAL:O	1:B:43:ASP:C	2.55	0.45
1:A:112:ILE:CD1	1:A:119:ILE:HD11	2.46	0.44
1:A:29:THR:HA	1:A:30:PRO:HD3	1.88	0.44
1:B:214:LEU:C	1:B:214:LEU:CD2	2.85	0.44
1:A:227:LEU:C	1:A:229:LEU:CD1	2.82	0.44
1:B:55:GLU:HB3	1:B:258:VAL:HG12	1.98	0.44
1:B:192:THR:HB	1:B:193:PRO:HD2	1.99	0.44
1:A:2:LYS:HD2	1:A:3:TRP:CD1	2.53	0.44
1:B:3:TRP:CZ3	1:B:212:PRO:HD3	2.53	0.44
1:A:25:ILE:HD12	1:A:256:HIS:CD2	2.53	0.44
1:A:203:LEU:HB2	1:A:248:LYS:HD2	1.99	0.44
1:B:26:LEU:HB2	1:B:61:ASP:O	2.17	0.44
1:B:157:MET:HA	1:B:160:MET:HG3	1.99	0.44
1:B:231:VAL:C	1:B:233:GLU:H	2.20	0.43
1:A:268:MET:HE2	1:A:268:MET:HB3	1.58	0.43
1:A:7:LEU:HD21	1:A:182:ILE:HD11	2.01	0.43
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.68	0.43
1:A:16:LEU:HA	1:A:16:LEU:HD23	1.71	0.43
1:A:63:GLY:HA2	1:A:101:ASP:HB3	2.00	0.43
1:A:187:ILE:HG21	1:A:217:THR:HG22	2.01	0.43
1:A:12:TYR:CE1	1:A:96:LEU:C	2.93	0.43
1:B:203:LEU:HA	1:B:203:LEU:HD22	1.70	0.43
1:A:218:SER:HA	1:A:238:THR:CG2	2.50	0.42
2:A:501:B63:H1A	3:A:279:SO4:O4	2.19	0.42
1:B:112:ILE:HG23	1:B:116:ALA:O	2.19	0.42
1:A:58:HIS:C	1:A:59:ILE:HG13	2.40	0.42
1:B:245:GLY:C	1:B:250:CYS:HG	2.22	0.42
1:A:49:ALA:O	1:A:52:MET:N	2.53	0.42
1:B:59:ILE:HG21	1:B:118:ILE:HD12	2.02	0.42
1:A:218:SER:HA	1:A:238:THR:HG23	2.01	0.42
1:A:121:ASP:OD2	1:A:122:ILE:N	2.53	0.42
1:A:2:LYS:CD	1:A:3:TRP:N	2.83	0.42
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.80	0.42
1:B:122:ILE:HA	1:B:145:MET:HB3	2.01	0.41
1:B:146:HIS:HD2	1:B:163:ASP:HB2	1.84	0.41
1:B:192:THR:O	1:B:196:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLU:OE2	1:B:204:GLU:N	2.45	0.41
1:A:8:ARG:HA	1:A:13:THR:HG23	2.01	0.41
2:A:501:B63:H16	2:A:501:B63:H2A	1.79	0.41
1:B:267:MET:HG3	1:B:271:MET:CE	2.51	0.41
1:B:142:ILE:HG13	1:B:143:ILE:N	2.36	0.41
1:B:154:ARG:HE	1:B:154:ARG:HB3	1.62	0.41
1:B:25:ILE:O	1:B:52:MET:HE2	2.21	0.40
1:B:197:LEU:O	1:B:200:MET:HB2	2.21	0.40
1:A:35:ASP:O	1:A:82:ARG:NH1	2.54	0.40
1:A:155:ASN:O	1:A:156:LEU:C	2.59	0.40
1:B:26:LEU:HD22	1:B:62:ILE:HG12	2.02	0.40
1:B:112:ILE:HD11	1:B:119:ILE:HD11	2.04	0.40
1:A:155:ASN:HD22	1:A:158:ALA:HB2	1.85	0.40
1:B:192:THR:C	1:B:194:GLU:H	2.24	0.40
1:A:30:PRO:HB3	1:A:82:ARG:HH21	1.86	0.40
1:A:52:MET:O	1:A:53:ARG:C	2.59	0.40
1:B:184:ASP:C	1:B:184:ASP:OD2	2.60	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	260/297 (88%)	221 (85%)	33 (13%)	6 (2%)	6	16
1	B	256/297 (86%)	222 (87%)	25 (10%)	9 (4%)	3	8
All	All	516/594 (87%)	443 (86%)	58 (11%)	15 (3%)	4	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	LEU

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Mol	Chain	Res	Type
1	B	179	GLU
1	B	239	GLY
1	B	258	VAL
1	A	37	GLY
1	A	115	GLY
1	A	156	LEU
1	B	91	SER
1	A	38	SER
1	B	127	ALA
1	A	31	ASP
1	B	115	GLY
1	A	28	VAL
1	B	29	THR
1	B	129	PRO

### 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	208/247 (84%)	185 (89%)	23 (11%)	6	14
1	B	208/247 (84%)	187 (90%)	21 (10%)	7	17
All	All	416/494 (84%)	372 (89%)	44 (11%)	6	15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	7	LEU
1	A	11	GLU
1	A	13	THR
1	A	20	THR
1	A	26	LEU
1	A	28	VAL
1	A	35	ASP
1	A	38	SER

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	76	VAL
1	A	83	VAL
1	A	104	LYS
1	A	130	LYS
1	A	149	ASP
1	A	151	MET
1	A	170	ILE
1	A	203	LEU
1	A	213	VAL
1	A	218	SER
1	A	247	GLU
1	A	252	PHE
1	A	253	VAL
1	B	7	LEU
1	B	11	GLU
1	B	13	THR
1	B	19	LYS
1	B	23	MET
1	B	47	ARG
1	B	59	ILE
1	B	76	VAL
1	B	77	GLU
1	B	87	ILE
1	B	91	SER
1	B	95	LYS
1	B	100	ILE
1	B	106	GLU
1	B	152	ASN
1	B	154	ARG
1	B	203	LEU
1	B	213	VAL
1	B	215	LEU
1	B	252	PHE
1	B	272	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	155	ASN
1	A	180	ASN

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Mol	Chain	Res	Type
1	B	88	GLN
1	B	146	HIS
1	B	152	ASN
1	B	180	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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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
3	SO4	A	278	-	4,4,4	0.53	0	6,6,6	0.82	0
2	B63	B	502	-	23,26,26	1.15	2 (8%)	26,36,36	1.81	6 (23%)
2	B63	A	501	-	23,26,26	1.43	3 (13%)	26,36,36	1.38	3 (11%)
3	SO4	A	279	-	4,4,4	0.57	0	6,6,6	0.31	0
3	SO4	B	279	-	4,4,4	0.37	0	6,6,6	0.64	0
3	SO4	B	278	-	4,4,4	0.43	0	6,6,6	1.19	1 (16%)

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	B63	A	501	-	-	5/10/19/19	0/3/3/3
2	B63	B	502	-	-	5/10/19/19	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B63	C6-C5	4.58	1.51	1.40
2	B	502	B63	C6-C5	2.94	1.47	1.40
2	A	501	B63	C7-N3	-2.40	1.34	1.38
2	A	501	B63	C8-N5	2.19	1.38	1.33
2	B	502	B63	O2-C15	-2.03	1.24	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	B63	C8-N5-C5	6.19	124.60	113.43
2	A	501	B63	C8-N5-C5	3.26	119.31	113.43
2	B	502	B63	N4-C8-N3	2.85	122.79	116.71
2	A	501	B63	C2-C1-C3	-2.80	107.20	112.31
2	B	502	B63	C6-N1-C3	2.71	121.61	116.24
2	B	502	B63	O1-C7-C6	-2.56	119.80	126.60
2	A	501	B63	C6-N1-C3	2.50	121.20	116.24
2	B	502	B63	N3-C8-N5	-2.31	119.01	123.32
2	B	502	B63	C6-C7-N3	2.25	118.90	113.19
3	B	278	SO4	O4-S-O3	2.23	118.59	109.06

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	B63	C3-C1-C2-N6
2	A	501	B63	C2-C1-C3-N1
2	B	502	B63	C3-C1-C2-N6
2	B	502	B63	C1-C2-N6-C9
2	A	501	B63	C1-C2-N6-C9
2	B	502	B63	C10-C9-N6-C2
2	A	501	B63	C14-C9-N6-C2
2	B	502	B63	C14-C9-N6-C2
2	A	501	B63	C10-C9-N6-C2

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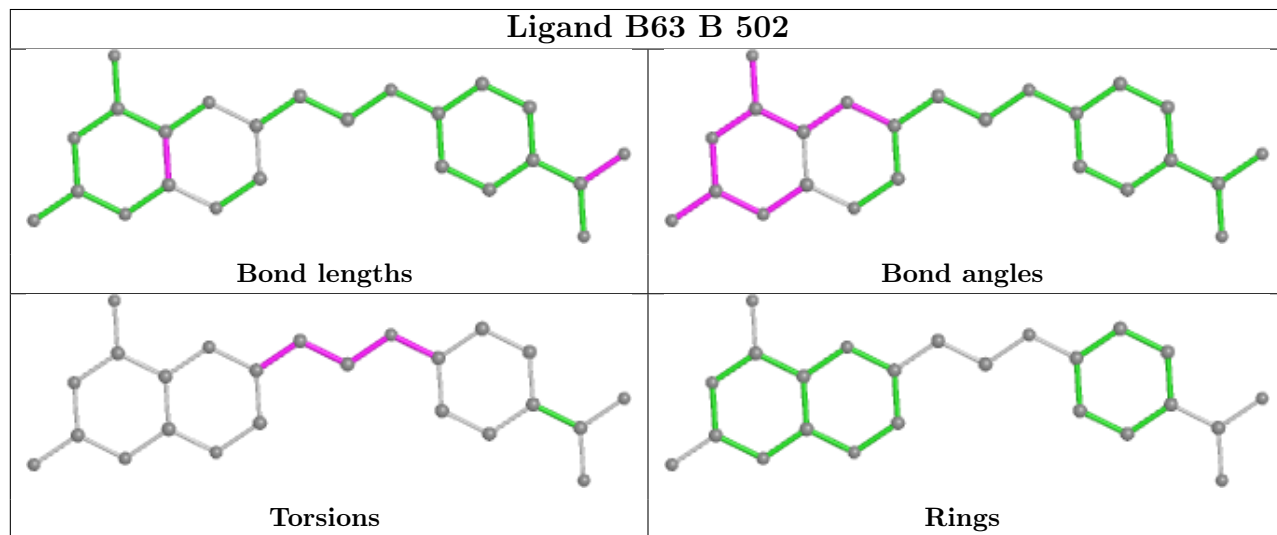
Mol	Chain	Res	Type	Atoms
2	B	502	B63	C2-C1-C3-N1

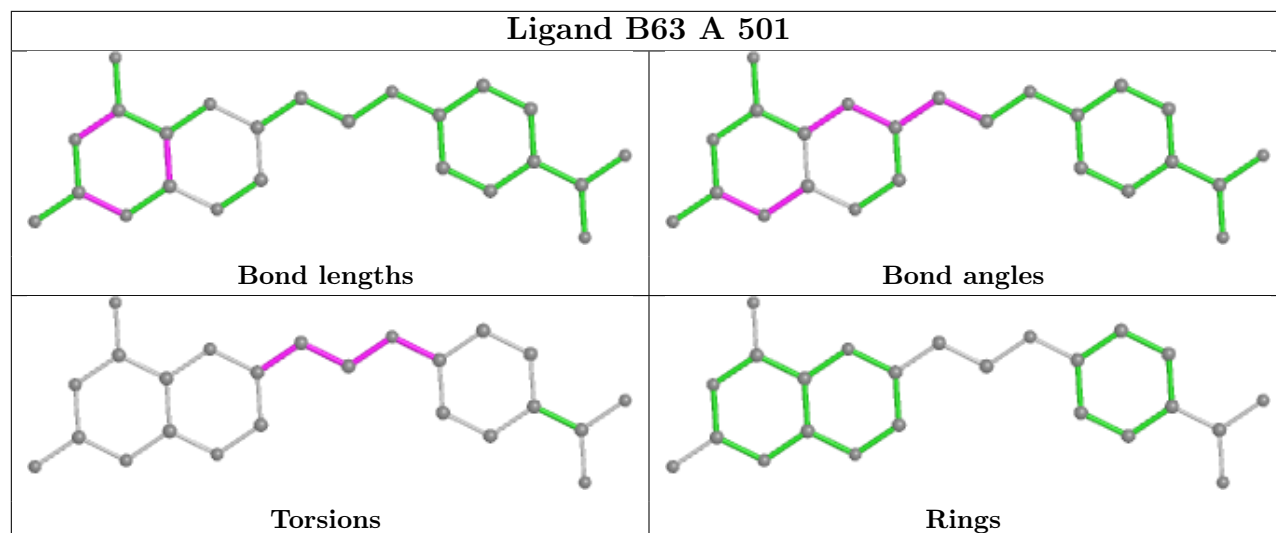
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	B63	2	0
2	A	501	B63	4	0
3	A	279	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 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 [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, 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	264/297 (88%)	0.50	9 (3%) 45 45	31, 48, 68, 76	0
1	B	262/297 (88%)	0.32	8 (3%) 49 49	34, 49, 60, 69	0
All	All	526/594 (88%)	0.41	17 (3%) 47 48	31, 48, 63, 76	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	3.8
1	B	36	GLY	3.7
1	B	76	VAL	3.0
1	B	35	ASP	2.9
1	A	73	LYS	2.8
1	A	7	LEU	2.5
1	B	112	ILE	2.4
1	A	84	VAL	2.4
1	A	61	ASP	2.3
1	A	151	MET	2.3
1	B	115	GLY	2.2
1	B	109	LYS	2.2
1	A	88	GLN	2.2
1	B	7	LEU	2.1
1	B	84	VAL	2.1
1	A	262	SER	2.1
1	A	158	ALA	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](#)

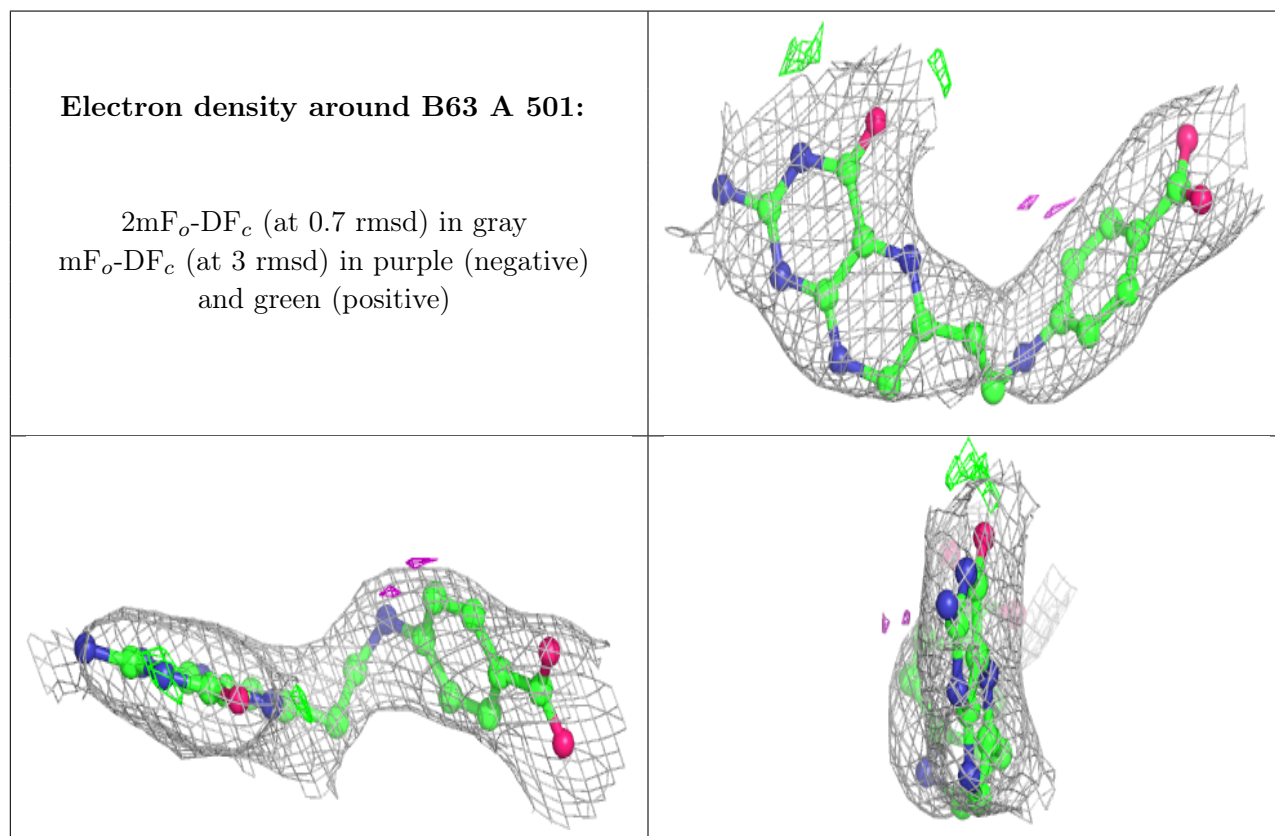
There are no monosaccharides in this entry.

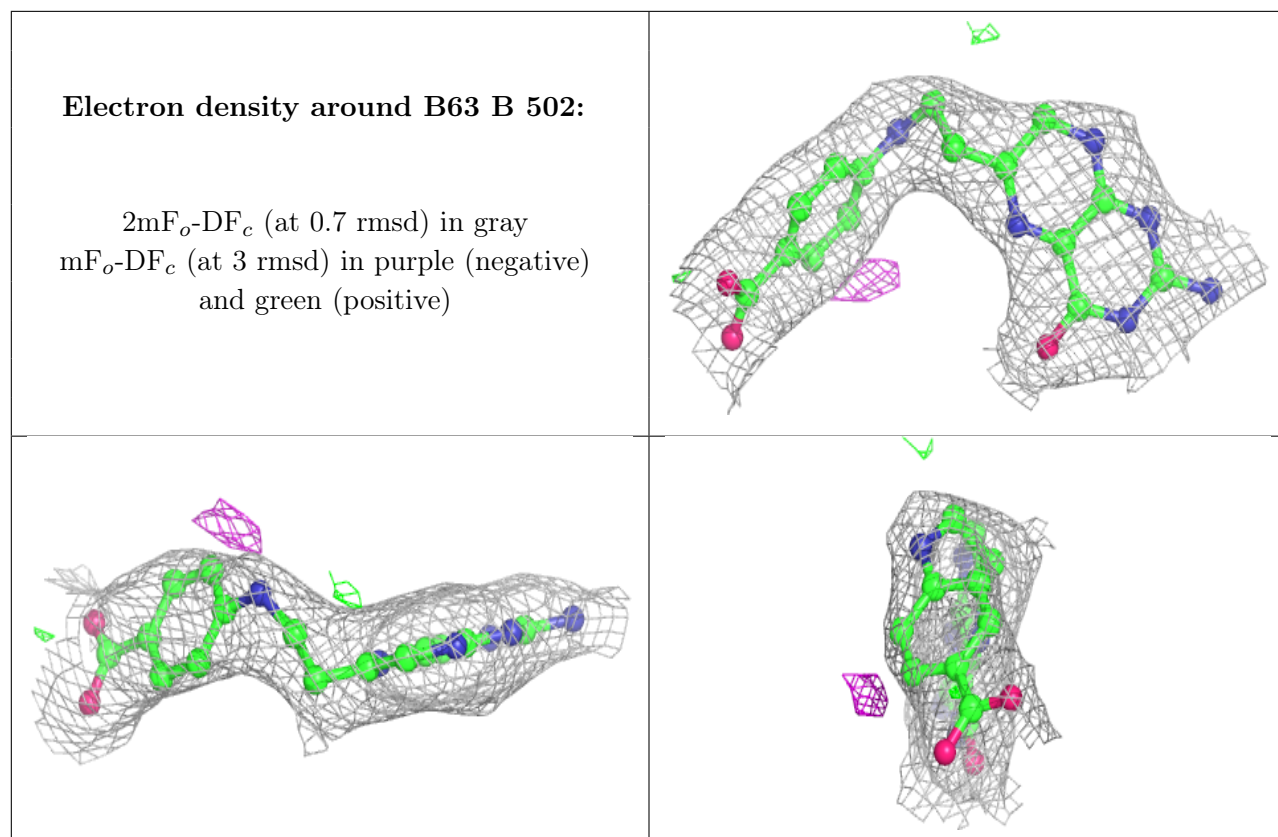
### 6.4 Ligands [i](#)

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
3	SO4	B	278	5/5	0.56	0.30	92,95,96,97	0
3	SO4	A	279	5/5	0.67	0.30	92,93,95,96	0
3	SO4	B	279	5/5	0.71	0.23	89,89,90,90	0
3	SO4	A	278	5/5	0.86	0.17	90,90,90,90	0
2	B63	A	501	24/24	0.91	0.19	39,41,42,43	0
2	B63	B	502	24/24	0.93	0.18	36,42,44,44	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.