



## Full wwPDB X-ray Structure Validation Report

Aug 16, 2023 – 05:06 AM EDT

PDB ID : 1ZG7  
Title : Crystal Structure of 2-(5-{[amino(imino)methyl]amino}-2-chlorophenyl)-3-sulfanylpropanoic acid Bound to Activated Porcine Pancreatic Carboxypeptidase B  
Authors : Adler, M.; Bryant, J.; Buckman, B.; Islam, I.; Larsen, B.; Finster, S.; Kent, L.; May, K.; Mohan, R.; Yuan, S.; Whitlow, M.  
Deposited on : 2005-04-20  
Resolution : 1.75 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

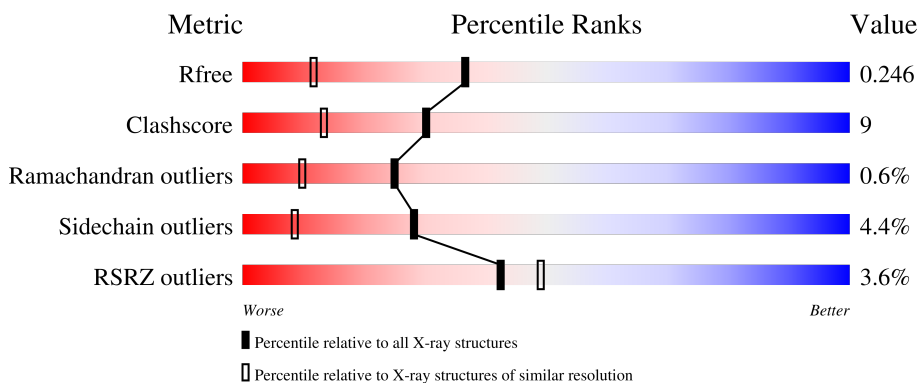
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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	306	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">81%      16%      .</p>
1	B	306	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">81%      18%      .</p>
1	C	306	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8%      70%      27%      ..</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8019 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.

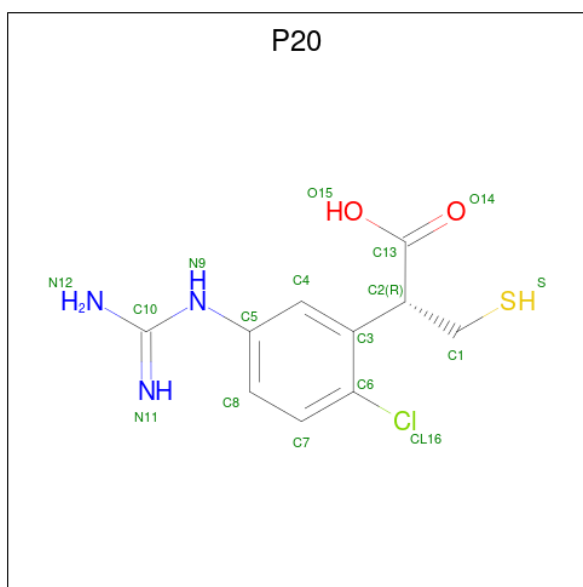
- Molecule 1 is a protein called procarboxypeptidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2443	1564	398	469	12	0	0	0
1	B	305	2443	1564	398	469	12	0	0	0
1	C	304	2434	1558	397	467	12	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 2-(5-{[AMINO(IMINO)METHYL]AMINO}-2-CHLOROPHENYL)-3-SULFANYLPROPANOIC ACID (three-letter code: P20) (formula: C<sub>10</sub>H<sub>12</sub>ClN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	Total	C	Cl	N	O	S	0	0
			17	10	1	3	2	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			17	10	1	3	2	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			17	10	1	3	2	1		

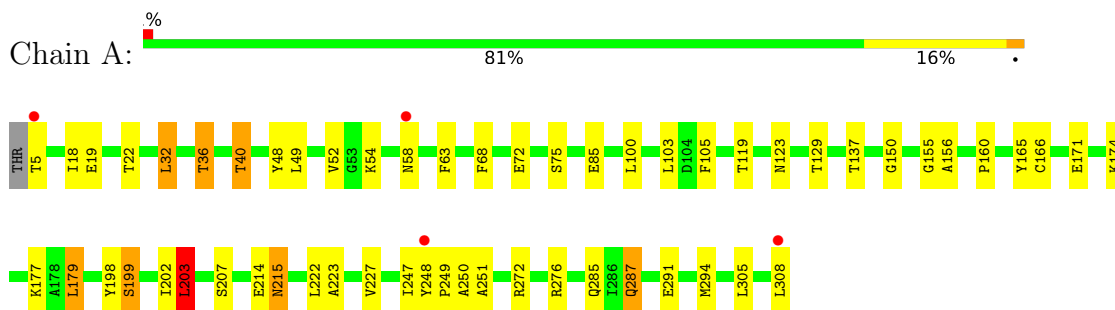
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		
4	B	247	Total	O	0	0
			247	247		
4	C	149	Total	O	0	0
			149	149		

### 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.

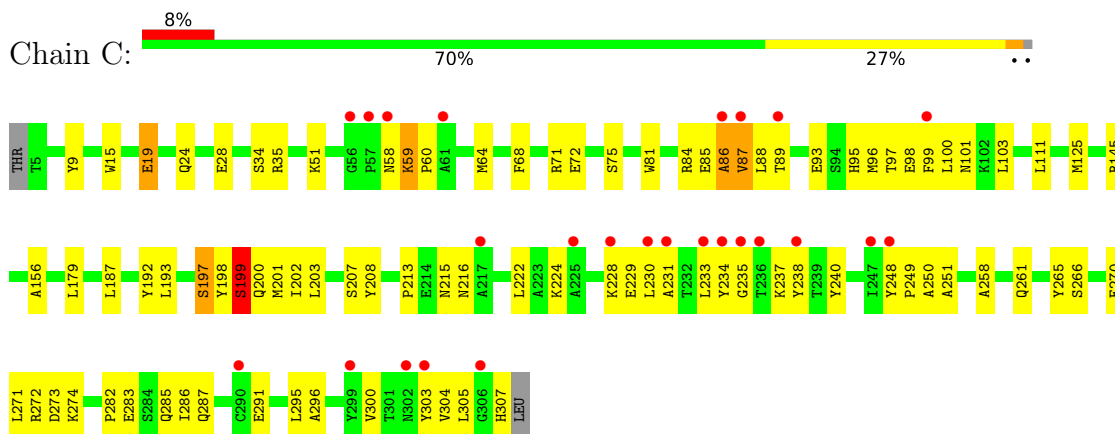
- Molecule 1: procarboxypeptidase B



- Molecule 1: procarboxypeptidase B



- Molecule 1: procarboxypeptidase B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.50Å 100.37Å 136.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.75 8.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (8.00-1.75) 100.0 (8.00-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 1.75Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.208 , 0.262 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	3543 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: ZN, P20

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	0.58	0/2512	0.73	1/3418 (0.0%)
1	B	0.57	0/2512	0.74	0/3418
1	C	0.56	0/2503	0.74	1/3407 (0.0%)
All	All	0.57	0/7527	0.74	2/10243 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ALA	N-CA-C	-6.27	94.07	111.00
1	A	203	LEU	CA-CB-CG	-5.15	103.46	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	TYR	Sidechain



## 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	2443	0	2324	36	0
1	B	2443	0	2324	33	0
1	C	2434	0	2313	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	17	0	9	1	0
3	B	17	0	9	1	0
3	C	17	0	9	0	0
4	A	249	0	0	2	0
4	B	247	0	0	1	0
4	C	149	0	0	2	0
All	All	8019	0	6988	134	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 9.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:HD13	1:C:295:LEU:HD11	1.43	0.98
1:A:203:LEU:HD13	3:A:401:P20:H7	1.49	0.92
1:B:203:LEU:HD13	3:B:501:P20:H7	1.54	0.87
1:C:85:GLU:O	1:C:89:THR:HB	1.81	0.80
1:C:60:PRO:HG2	1:C:103:LEU:HB3	1.65	0.78
1:B:272:ARG:HH11	1:B:285:GLN:HE21	1.34	0.74
1:A:215:ASN:H	1:A:215:ASN:HD22	1.36	0.74
1:B:198:TYR:O	1:B:199:SER:HB2	1.88	0.74
1:B:303:TYR:O	1:B:307:HIS:HD2	1.71	0.73
1:C:224:LYS:O	1:C:228:LYS:HG2	1.89	0.71
1:C:233:LEU:HD23	1:C:234:TYR:CE2	2.27	0.70
1:C:224:LYS:HG3	1:C:240:TYR:OH	1.93	0.69
1:B:287:GLN:HG3	4:B:1021:HOH:O	1.94	0.68
1:C:287:GLN:O	1:C:291:GLU:HG3	1.92	0.68
1:A:137:THR:HG21	1:B:39:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:PRO:HG2	1:C:285:GLN:HG3	1.76	0.67
1:A:40:THR:HG22	1:A:174:LYS:NZ	2.11	0.66
1:C:97:THR:HG22	1:C:101:ASN:ND2	2.12	0.65
1:C:303:TYR:O	1:C:307:HIS:HD2	1.80	0.65
1:C:9:TYR:CE1	1:C:84:ARG:HB2	2.34	0.63
1:C:71:ARG:HD3	1:C:125:MET:O	2.01	0.60
1:A:305:LEU:HD23	1:A:308:LEU:HD11	1.84	0.58
1:C:72:GLU:O	1:C:75:SER:HB3	2.03	0.58
1:A:85:GLU:HG2	1:A:294:MET:CE	2.34	0.58
1:C:231:ALA:O	1:C:235:GLY:HA2	2.03	0.58
1:C:303:TYR:O	1:C:307:HIS:CD2	2.57	0.57
1:C:202:ILE:O	1:C:240:TYR:HA	2.05	0.56
1:B:272:ARG:HH11	1:B:285:GLN:NE2	2.03	0.56
1:B:233:LEU:HD13	1:B:295:LEU:HD11	1.87	0.56
1:A:32:LEU:CD1	1:A:54:LYS:HD2	2.36	0.55
1:C:238:TYR:OH	1:C:271:LEU:HA	2.06	0.55
1:B:287:GLN:O	1:B:291:GLU:HG3	2.08	0.54
1:C:86:ALA:O	1:C:87:VAL:HG13	2.07	0.54
1:C:198:TYR:O	1:C:199:SER:HB2	2.07	0.54
1:C:96:MET:SD	1:C:100:LEU:CD1	2.96	0.54
1:C:89:THR:HG23	1:C:93:GLU:HB3	1.90	0.54
1:C:200:GLN:HB3	1:C:238:TYR:CD1	2.43	0.53
1:C:15:TRP:O	1:C:19:GLU:HB2	2.08	0.53
1:C:248:TYR:CE1	1:C:250:ALA:HB2	2.43	0.53
1:A:40:THR:HG22	1:A:174:LYS:HZ1	1.74	0.52
1:C:248:TYR:HE1	1:C:250:ALA:HB2	1.75	0.52
1:C:224:LYS:HG2	1:C:228:LYS:HE3	1.92	0.51
1:A:160:PRO:HA	1:A:165:TYR:CG	2.45	0.51
1:A:287:GLN:O	1:A:291:GLU:HG3	2.10	0.51
1:B:198:TYR:O	1:B:199:SER:CB	2.59	0.51
1:C:201:MET:HE1	1:C:203:LEU:HD11	1.93	0.51
1:B:215:ASN:H	1:B:215:ASN:HD22	1.59	0.51
1:C:97:THR:HG22	1:C:101:ASN:HD21	1.76	0.51
1:B:85:GLU:HG2	1:B:294:MET:CE	2.40	0.51
1:B:72:GLU:O	1:B:75:SER:HB3	2.11	0.50
1:A:215:ASN:H	1:A:215:ASN:ND2	2.05	0.50
1:C:233:LEU:HD23	1:C:234:TYR:HE2	1.75	0.50
1:C:207:SER:O	1:C:249:PRO:HA	2.11	0.50
1:C:300:VAL:O	1:C:304:VAL:HG23	2.11	0.50
1:A:156:ALA:HB1	1:A:166:CYS:HB3	1.93	0.49
1:B:40:THR:O	1:B:174:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.78	0.49
1:A:85:GLU:HG2	1:A:294:MET:HE2	1.95	0.49
1:A:215:ASN:HD22	1:A:215:ASN:N	2.03	0.49
1:B:156:ALA:HB1	1:B:166:CYS:HB3	1.95	0.49
1:B:209:ASP:HB3	1:B:211:LYS:HG2	1.94	0.48
1:A:155:GLY:HA3	1:A:250:ALA:HA	1.95	0.48
1:A:272:ARG:HH11	1:A:285:GLN:HE21	1.62	0.48
1:C:99:PHE:HD2	1:C:305:LEU:HD11	1.78	0.48
1:C:270:GLU:HA	1:C:270:GLU:OE1	2.13	0.48
1:A:19:GLU:HG3	1:A:48:TYR:CE2	2.49	0.48
1:C:265:TYR:CE1	1:C:303:TYR:HE2	2.31	0.48
1:C:95:HIS:HA	1:C:98:GLU:HG2	1.96	0.47
1:C:213:PRO:HD2	1:C:216:ASN:HB3	1.95	0.47
1:C:64:MET:HA	1:C:193:LEU:O	2.14	0.47
1:C:283:GLU:O	1:C:286:ILE:HG13	2.14	0.47
1:A:198:TYR:O	1:A:199:SER:CB	2.62	0.47
1:C:230:LEU:HB2	1:C:296:ALA:HB2	1.96	0.47
1:C:231:ALA:HB2	4:C:1451:HOH:O	2.14	0.47
1:A:119:THR:HA	1:A:123:ASN:O	2.15	0.47
1:C:96:MET:SD	1:C:100:LEU:HD11	2.55	0.47
1:A:202:ILE:HD12	1:A:227:VAL:HG12	1.97	0.47
1:B:85:GLU:HG2	1:B:294:MET:HE2	1.95	0.46
1:C:283:GLU:HA	1:C:286:ILE:HG13	1.97	0.46
1:B:160:PRO:HA	1:B:165:TYR:CG	2.50	0.46
1:C:72:GLU:HG2	1:C:197:SER:O	2.15	0.46
1:A:129:THR:HB	4:A:1088:HOH:O	2.15	0.46
1:A:36:THR:HG22	1:A:49:LEU:HB3	1.98	0.46
1:C:248:TYR:C	1:C:248:TYR:CD1	2.89	0.46
1:C:208:TYR:HB3	1:C:251:ALA:HA	1.98	0.45
1:A:72:GLU:O	1:A:75:SER:HB3	2.17	0.45
1:A:207:SER:O	1:A:249:PRO:HA	2.16	0.45
1:B:24:GLN:O	1:B:28:GLU:HG3	2.17	0.45
1:A:63:PHE:CZ	1:A:179:LEU:HD21	2.50	0.45
1:C:58:ASN:O	1:C:59:LYS:HB2	2.17	0.45
1:C:198:TYR:O	1:C:199:SER:CB	2.64	0.45
1:C:100:LEU:HD12	1:C:100:LEU:N	2.32	0.45
1:B:42:PHE:CD2	1:B:131:SER:HA	2.52	0.44
1:C:87:VAL:CG2	1:C:88:LEU:N	2.80	0.44
1:A:5:THR:HG21	4:A:1521:HOH:O	2.15	0.44
1:A:150:GLY:O	1:A:251:ALA:HB1	2.17	0.44
1:B:33:ILE:HD11	1:B:87:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:MET:SD	1:C:100:LEU:HD13	2.57	0.44
1:B:303:TYR:O	1:B:307:HIS:CD2	2.61	0.44
1:C:258:ALA:O	1:C:261:GLN:HB2	2.18	0.44
1:B:238:TYR:OH	1:B:271:LEU:HA	2.18	0.43
1:C:34:SER:OG	1:C:51:LYS:HB3	2.18	0.43
1:A:103:LEU:HD23	1:A:305:LEU:HG	2.00	0.43
1:B:107:VAL:O	1:B:109:PRO:HD3	2.18	0.43
1:C:215:ASN:HB3	4:C:1271:HOH:O	2.17	0.43
1:C:145:ARG:HD2	1:C:156:ALA:HB2	2.01	0.43
1:A:247:ILE:HG22	1:A:248:TYR:CD2	2.54	0.43
1:B:155:GLY:HA3	1:B:250:ALA:HA	2.01	0.43
1:C:111:LEU:HD22	1:C:179:LEU:HD22	2.01	0.43
1:B:207:SER:O	1:B:249:PRO:HA	2.19	0.42
1:C:86:ALA:O	1:C:87:VAL:HG22	2.20	0.42
1:A:52:VAL:HB	1:A:105:PHE:HB2	2.01	0.42
1:C:201:MET:HE2	1:C:201:MET:HB3	1.91	0.42
1:B:215:ASN:ND2	1:B:259:TYR:OH	2.53	0.42
1:B:294:MET:O	1:B:298:LYS:HG3	2.20	0.42
1:C:87:VAL:HG23	1:C:88:LEU:N	2.35	0.42
1:B:201:MET:HG2	1:B:239:THR:OG1	2.20	0.41
1:A:32:LEU:HD13	1:A:54:LYS:HD2	2.02	0.41
1:C:192:TYR:O	1:C:266:SER:HA	2.21	0.41
1:B:272:ARG:HA	1:B:273:ASP:HA	1.86	0.41
1:C:24:GLN:O	1:C:28:GLU:HG3	2.21	0.41
1:A:202:ILE:HD12	1:A:227:VAL:CG1	2.51	0.41
1:B:54:LYS:HA	1:B:54:LYS:HD2	1.92	0.41
1:C:81:TRP:CH2	1:C:287:GLN:HG3	2.54	0.41
1:C:199:SER:HB3	1:C:201:MET:HG3	2.02	0.41
1:B:150:GLY:O	1:B:251:ALA:HB1	2.20	0.41
1:C:9:TYR:CD1	1:C:84:ARG:HB2	2.55	0.41
1:A:18:ILE:O	1:A:22:THR:HG23	2.21	0.41
1:A:171:GLU:OE2	1:A:177:LYS:HD3	2.21	0.40
1:A:223:ALA:O	1:A:227:VAL:HG13	2.21	0.40
1:C:89:THR:HG23	1:C:93:GLU:CB	2.50	0.40
1:C:272:ARG:HB3	1:C:273:ASP:HA	2.04	0.40
1:B:264:LYS:HD3	1:B:264:LYS:HA	1.89	0.40
1:C:229:GLU:HG3	1:C:295:LEU:HB3	2.03	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	303/306 (99%)	293 (97%)	9 (3%)	1 (0%)	41	22
1	B	303/306 (99%)	292 (96%)	10 (3%)	1 (0%)	41	22
1	C	302/306 (99%)	283 (94%)	16 (5%)	3 (1%)	15	4
All	All	908/918 (99%)	868 (96%)	35 (4%)	5 (1%)	25	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	VAL
1	A	199	SER
1	B	199	SER
1	C	199	SER
1	C	59	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/259 (100%)	246 (95%)	12 (5%)	26	7
1	B	258/259 (100%)	245 (95%)	13 (5%)	24	6
1	C	257/259 (99%)	248 (96%)	9 (4%)	36	13
All	All	773/777 (100%)	739 (96%)	34 (4%)	28	8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	36	THR
1	A	40	THR
1	A	58	ASN
1	A	68	PHE
1	A	100	LEU
1	A	179	LEU
1	A	203	LEU
1	A	214	GLU
1	A	215	ASN
1	A	222	LEU
1	A	287	GLN
1	B	32	LEU
1	B	35	ARG
1	B	58	ASN
1	B	68	PHE
1	B	148	ASP
1	B	199	SER
1	B	203	LEU
1	B	214	GLU
1	B	215	ASN
1	B	229	GLU
1	B	248	TYR
1	B	287	GLN
1	B	308	LEU
1	C	19	GLU
1	C	35	ARG
1	C	68	PHE
1	C	187	LEU
1	C	197	SER
1	C	199	SER
1	C	222	LEU
1	C	237	LYS
1	C	274	LYS

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	215	ASN
1	A	285	GLN
1	A	307	HIS
1	B	46	ASN
1	B	215	ASN

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Mol	Chain	Res	Type
1	B	285	GLN
1	B	287	GLN
1	B	307	HIS
1	C	24	GLN
1	C	302	ASN
1	C	307	HIS

### 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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	P20	A	401	2	16,17,17	1.70	3 (18%)	23,23,23	1.19	2 (8%)
3	P20	C	601	2	16,17,17	1.81	4 (25%)	23,23,23	1.30	2 (8%)
3	P20	B	501	2	16,17,17	1.67	3 (18%)	23,23,23	1.23	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P20	A	401	2	-	1/14/14/14	0/1/1/1
3	P20	C	601	2	-	1/14/14/14	0/1/1/1
3	P20	B	501	2	-	1/14/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	P20	C5-N9	-3.80	1.34	1.41
3	C	601	P20	C5-N9	-3.36	1.34	1.41
3	A	401	P20	C5-N9	-3.19	1.35	1.41
3	C	601	P20	C3-C2	-2.93	1.49	1.52
3	A	401	P20	C6-C3	2.81	1.42	1.39
3	C	601	P20	C6-C3	2.80	1.42	1.39
3	C	601	P20	C10-N9	-2.60	1.34	1.37
3	B	501	P20	C7-C6	2.53	1.44	1.38
3	B	501	P20	C6-C3	2.40	1.42	1.39
3	A	401	P20	C6-CL16	-2.07	1.68	1.73

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	P20	O15-C13-O14	-3.45	116.25	124.09
3	C	601	P20	O15-C13-O14	-3.06	117.13	124.09
3	A	401	P20	C2-C1-S	-3.04	110.86	114.19
3	A	401	P20	O15-C13-O14	-2.82	117.69	124.09
3	C	601	P20	C2-C1-S	-2.75	111.17	114.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	P20	C13-C2-C3-C4
3	C	601	P20	C13-C2-C3-C4
3	A	401	P20	C13-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	P20	1	0

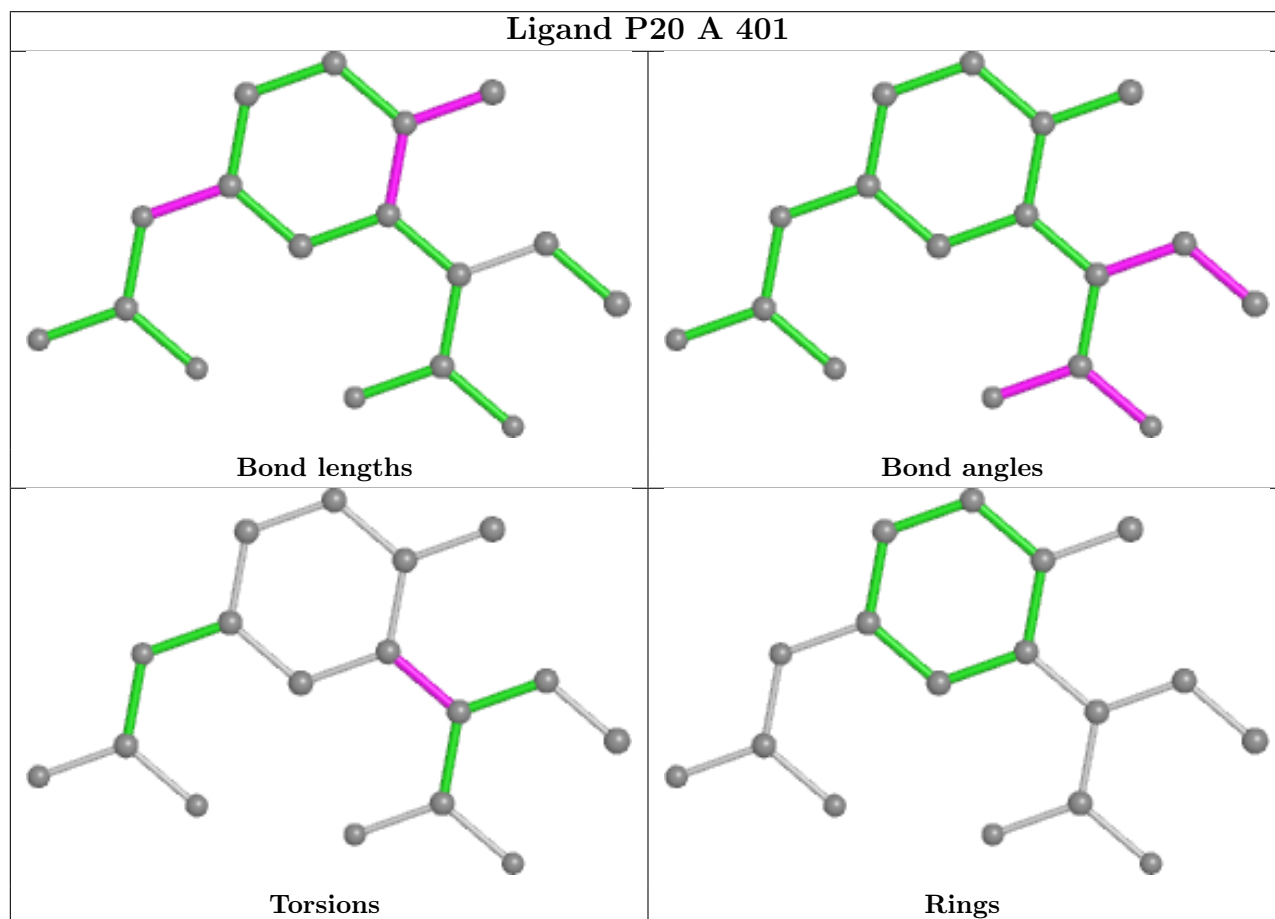
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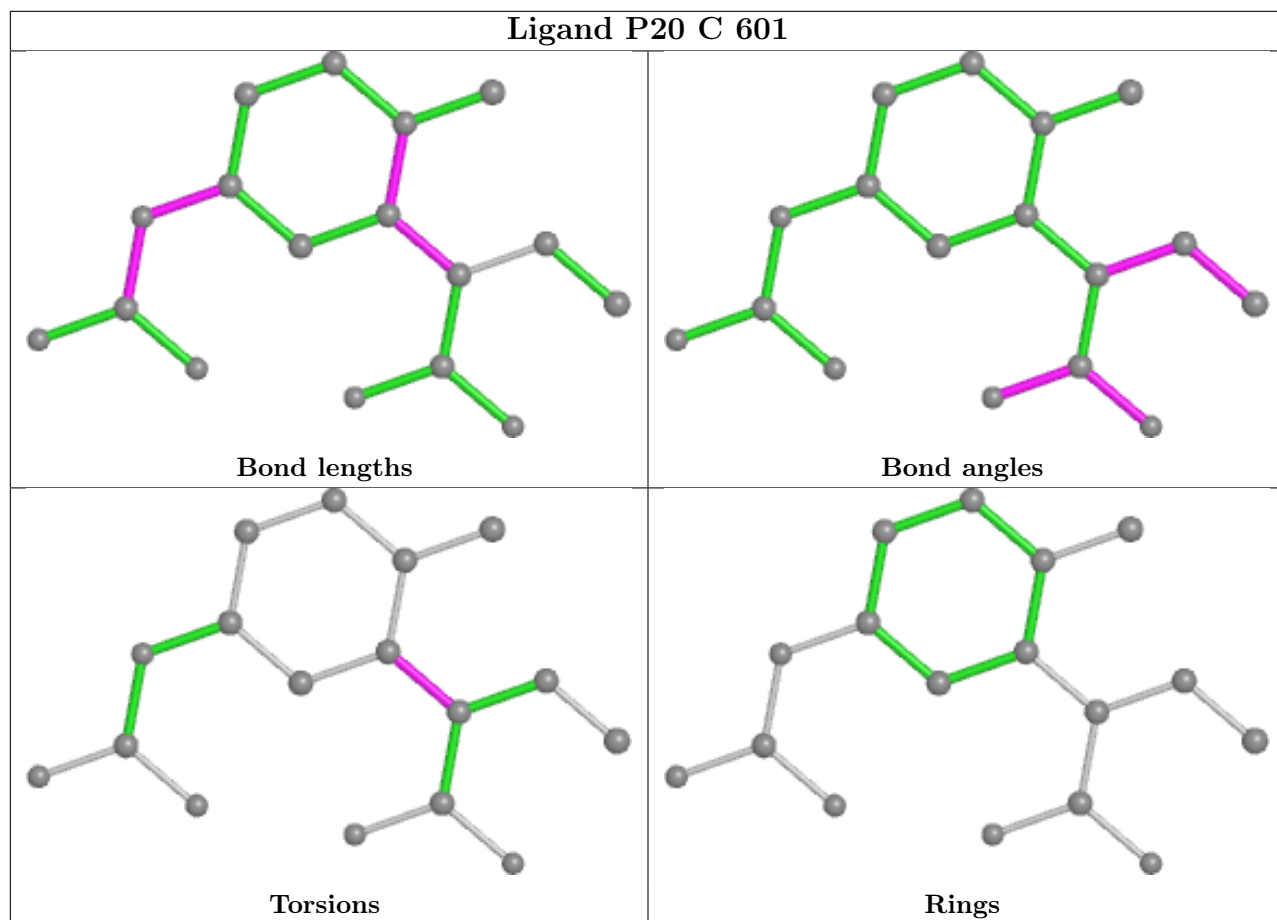


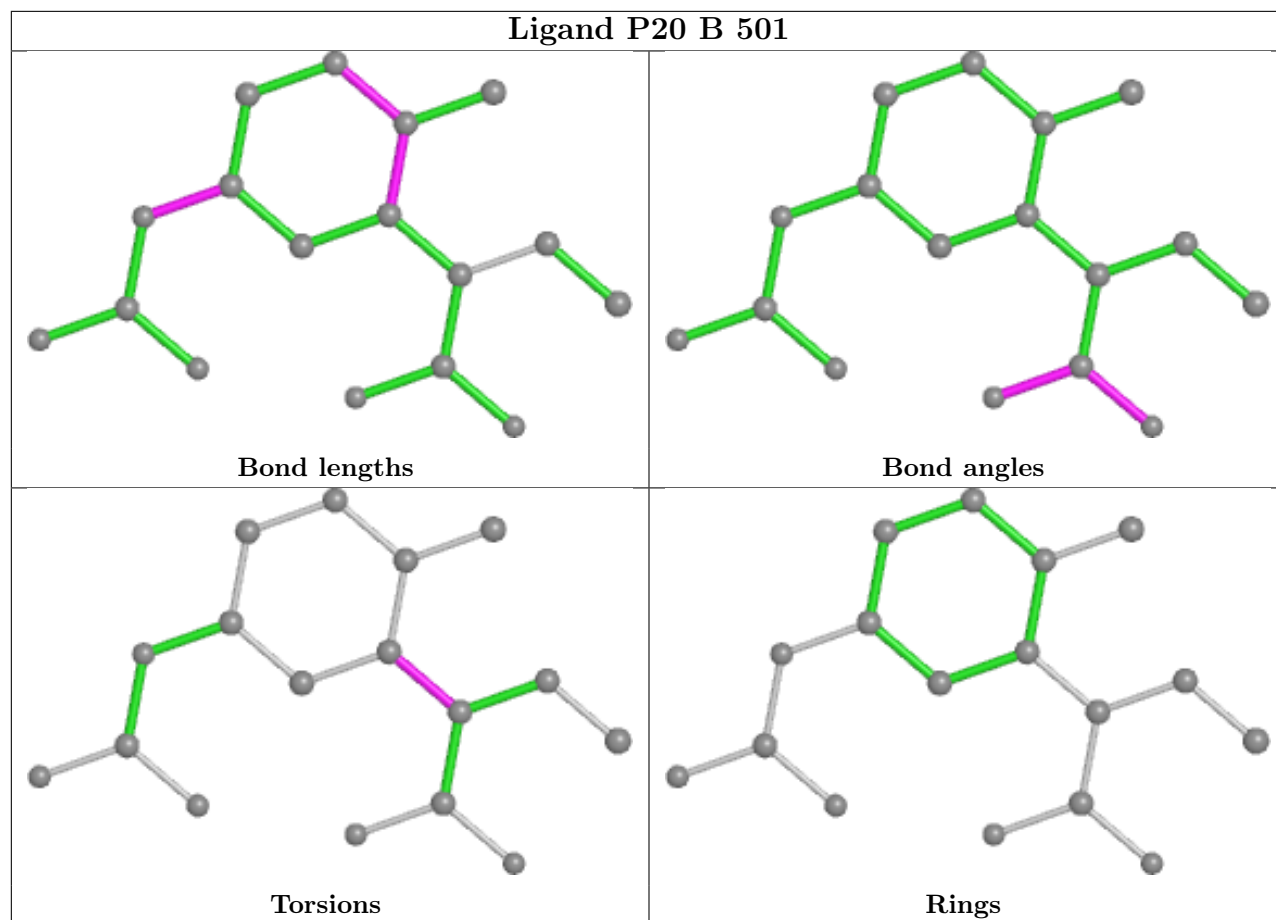
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	P20	1	0

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	305/306 (99%)	-0.26	4 (1%) 77 83	17, 23, 35, 52	0
1	B	305/306 (99%)	-0.23	4 (1%) 77 83	17, 23, 38, 51	0
1	C	304/306 (99%)	0.59	25 (8%) 11 15	19, 35, 52, 69	0
All	All	914/918 (99%)	0.03	33 (3%) 42 49	17, 26, 47, 69	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	VAL	5.7
1	C	58	ASN	5.4
1	C	248	TYR	4.2
1	C	231	ALA	4.0
1	C	303	TYR	3.9
1	C	86	ALA	3.5
1	C	228	LYS	3.5
1	C	306	GLY	3.3
1	C	299	TYR	2.9
1	C	234	TYR	2.9
1	C	57	PRO	2.7
1	C	302	ASN	2.7
1	A	248	TYR	2.7
1	B	248	TYR	2.7
1	C	235	GLY	2.6
1	B	308	LEU	2.6
1	A	58	ASN	2.6
1	C	290	CYS	2.6
1	B	5	THR	2.5
1	B	58	ASN	2.4
1	A	308	LEU	2.3
1	C	56	GLY	2.3
1	C	230	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	217	ALA	2.2
1	C	233	LEU	2.2
1	C	238	TYR	2.2
1	C	61	ALA	2.2
1	C	89	THR	2.2
1	C	236	THR	2.2
1	C	247	ILE	2.1
1	C	225	ALA	2.1
1	C	99	PHE	2.1
1	A	5	THR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

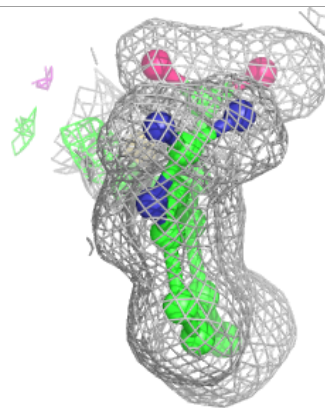
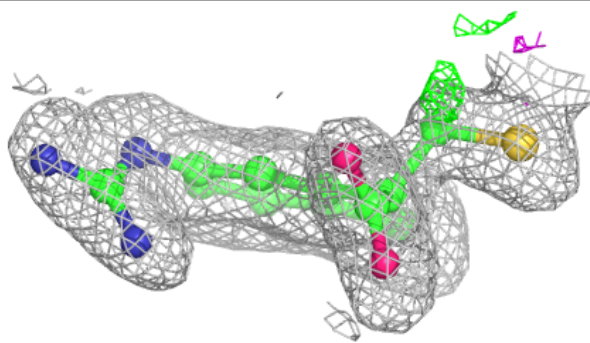
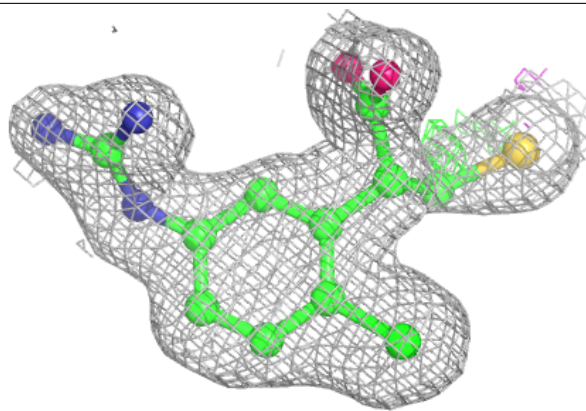
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	P20	C	601	17/17	0.94	0.10	24,31,36,38	0
2	ZN	C	600	1/1	0.95	0.04	28,28,28,28	0
3	P20	B	501	17/17	0.96	0.06	18,21,29,31	0
2	ZN	B	500	1/1	0.96	0.06	25,25,25,25	0
3	P20	A	401	17/17	0.97	0.07	17,22,25,27	0
2	ZN	A	400	1/1	0.99	0.05	25,25,25,25	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.

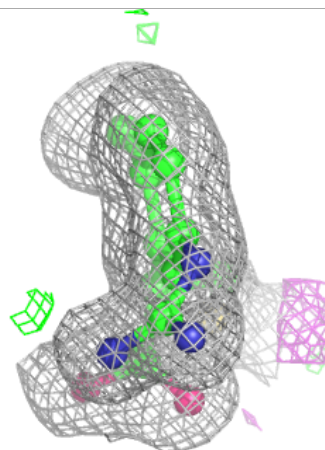
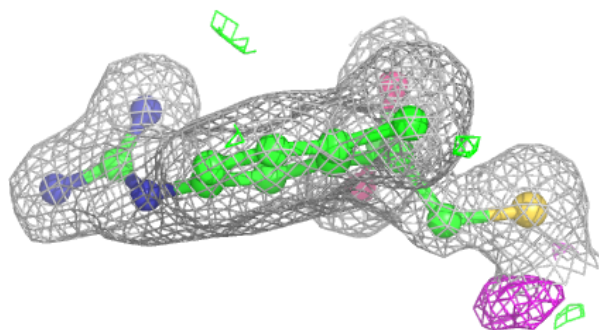
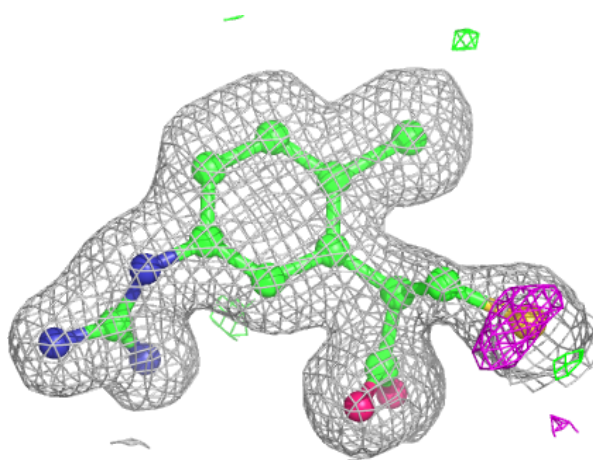
**Electron density around P20 C 601:**

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

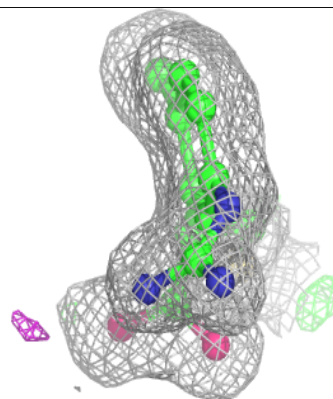
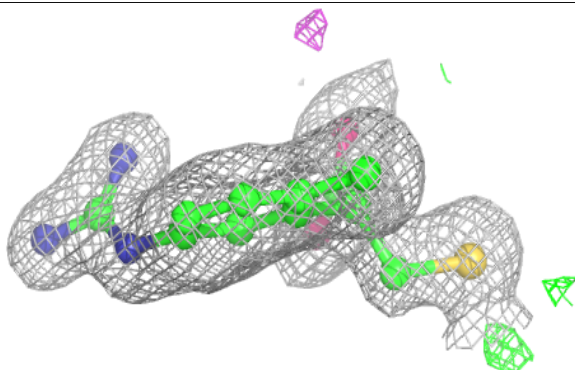
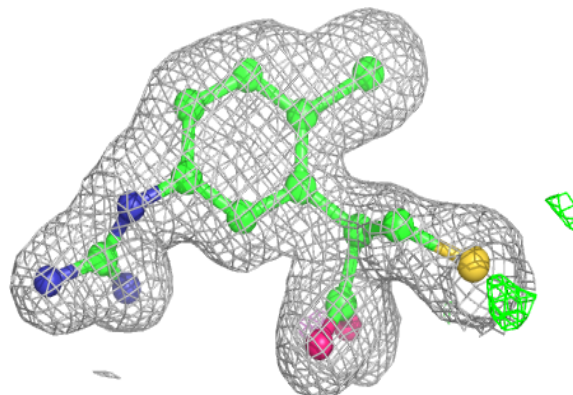


**Electron density around P20 B 501:**

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

**Electron density around P20 A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.