



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:11 AM EDT

PDB ID : 1Y2J  
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With 3,5-dimethyl-1-(3-nitro-phenyl)-1H-pyrazole-4-carboxylic acid ethyl ester  
Authors : Card, G.L.; Blasdel, L.; England, B.P.; Zhang, C.; Suzuki, Y.; Gillette, S.; Fong, D.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.  
Deposited on : 2004-11-22  
Resolution : 2.55 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

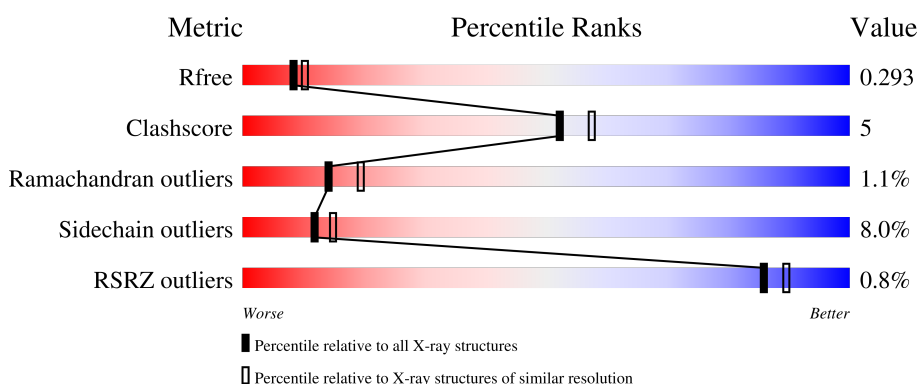
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	398	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>17%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	398	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5336 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2617	1653	441	503	20			
1	B	323	Total	C	N	O	S	0	0	0
			2617	1653	441	503	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	INITIATING METHIONINE	UNP Q07343
A	132	GLY	-	CLONING ARTIFACT	UNP Q07343
A	133	SER	-	CLONING ARTIFACT	UNP Q07343
A	134	SER	-	CLONING ARTIFACT	UNP Q07343
A	135	HIS	-	EXPRESSION TAG	UNP Q07343
A	136	HIS	-	EXPRESSION TAG	UNP Q07343
A	137	HIS	-	EXPRESSION TAG	UNP Q07343
A	138	HIS	-	EXPRESSION TAG	UNP Q07343
A	139	HIS	-	EXPRESSION TAG	UNP Q07343
A	140	HIS	-	EXPRESSION TAG	UNP Q07343
A	141	SER	-	CLONING ARTIFACT	UNP Q07343
A	142	SER	-	CLONING ARTIFACT	UNP Q07343
A	143	GLY	-	CLONING ARTIFACT	UNP Q07343
A	144	LEU	-	CLONING ARTIFACT	UNP Q07343
A	145	VAL	-	CLONING ARTIFACT	UNP Q07343
A	146	PRO	-	CLONING ARTIFACT	UNP Q07343
A	147	ARG	-	CLONING ARTIFACT	UNP Q07343
A	148	GLY	-	CLONING ARTIFACT	UNP Q07343
A	149	SER	-	CLONING ARTIFACT	UNP Q07343
A	150	HIS	-	CLONING ARTIFACT	UNP Q07343
A	151	MET	-	CLONING ARTIFACT	UNP Q07343
A	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343
B	131	MET	-	INITIATING METHIONINE	UNP Q07343
B	132	GLY	-	CLONING ARTIFACT	UNP Q07343
B	133	SER	-	CLONING ARTIFACT	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
B	134	SER	-	CLONING ARTIFACT	UNP Q07343
B	135	HIS	-	EXPRESSION TAG	UNP Q07343
B	136	HIS	-	EXPRESSION TAG	UNP Q07343
B	137	HIS	-	EXPRESSION TAG	UNP Q07343
B	138	HIS	-	EXPRESSION TAG	UNP Q07343
B	139	HIS	-	EXPRESSION TAG	UNP Q07343
B	140	HIS	-	EXPRESSION TAG	UNP Q07343
B	141	SER	-	CLONING ARTIFACT	UNP Q07343
B	142	SER	-	CLONING ARTIFACT	UNP Q07343
B	143	GLY	-	CLONING ARTIFACT	UNP Q07343
B	144	LEU	-	CLONING ARTIFACT	UNP Q07343
B	145	VAL	-	CLONING ARTIFACT	UNP Q07343
B	146	PRO	-	CLONING ARTIFACT	UNP Q07343
B	147	ARG	-	CLONING ARTIFACT	UNP Q07343
B	148	GLY	-	CLONING ARTIFACT	UNP Q07343
B	149	SER	-	CLONING ARTIFACT	UNP Q07343
B	150	HIS	-	CLONING ARTIFACT	UNP Q07343
B	151	MET	-	CLONING ARTIFACT	UNP Q07343
B	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343

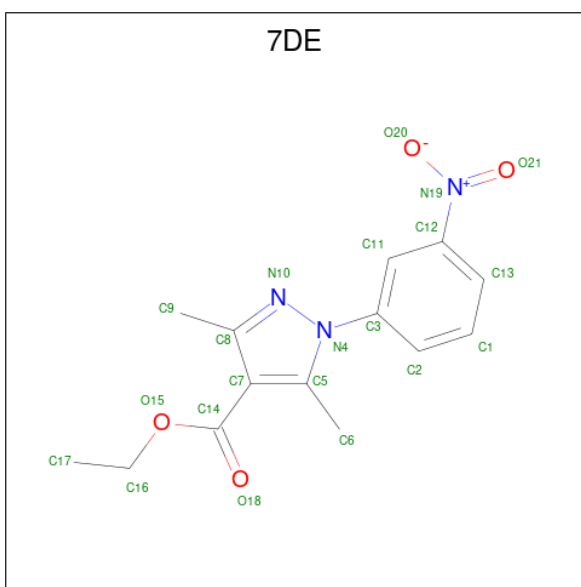
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is 3,5-DIMETHYL-1-(3-NITROPHENYL)-1H-PYRAZOLE-4-CARBOXYLIC ACID ETHYL ESTER (three-letter code: 7DE) (formula: C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	14	3	4		
4	B	1	Total	C	N	O	0	0
			21	14	3	4		

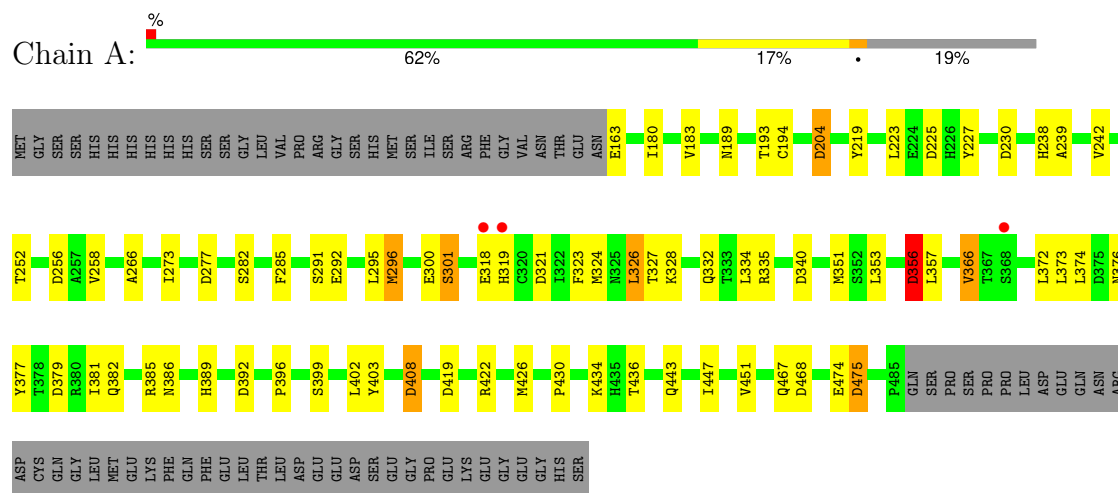
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	28	Total	O	0	0
			28	28		

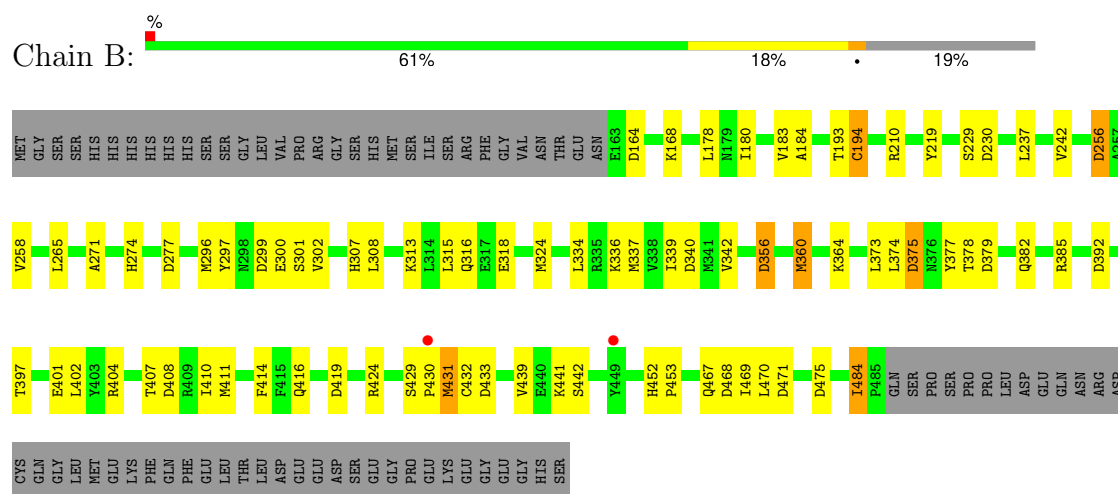
### 3 Residue-property plots

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: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



#### • Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.48Å 94.23Å 106.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.55 64.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	84.5 (70.71-2.55) 85.2 (64.89-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.244 , 0.297 0.243 , 0.293	Depositor DCC
$R_{free}$ test set	1505 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.26 % 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 1.1752e-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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, ZN, 7DE, MG

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	0.60	0/2661	0.89	13/3608 (0.4%)
1	B	0.65	0/2661	0.88	11/3608 (0.3%)
All	All	0.63	0/5322	0.89	24/7216 (0.3%)

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 (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	392	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	230	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	408	ASP	CB-CG-OD2	7.07	124.67	118.30
1	A	419	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	468	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	321	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	299	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	277	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	379	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	408	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	356	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	277	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	433	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	230	ASP	CB-CG-OD2	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	475	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	392	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	471	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	475	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	468	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	256	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	356	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	204	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	419	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	194	CME	Mainchain

## 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	2617	0	2546	27	0
1	B	2617	0	2546	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	15	4	0
4	B	21	0	15	0	0
5	A	28	0	0	3	0
5	B	28	0	0	0	0
All	All	5336	0	5122	57	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 5.

All (57) 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:340:ASP:OD2	1:B:385:ARG:HD3	1.82	0.79
1:B:439:VAL:O	1:B:442:SER:OG	2.14	0.65
1:B:258:VAL:HG11	1:B:374:LEU:HD12	1.80	0.64
1:B:411:MET:HG3	1:B:439:VAL:HG22	1.81	0.62
1:B:274:HIS:O	1:B:307:HIS:CD2	2.53	0.61
1:B:256:ASP:OD1	1:B:256:ASP:C	2.39	0.61
1:A:163:GLU:N	1:A:163:GLU:OE2	2.35	0.59
1:A:300:GLU:O	1:A:301:SER:C	2.41	0.57
1:B:219:TYR:CE1	1:B:315:LEU:HD23	2.39	0.57
1:B:397:THR:HB	1:B:469:ILE:HG23	1.87	0.57
1:A:443:GLN:OE1	4:A:101:7DE:H161	2.06	0.56
1:A:266:ALA:HB2	1:A:334:LEU:HD12	1.89	0.54
1:B:300:GLU:O	1:B:301:SER:C	2.46	0.53
1:A:296:MET:SD	1:B:296:MET:SD	3.07	0.53
1:B:180:ILE:HA	1:B:183:VAL:HG13	1.89	0.53
1:B:308:LEU:HG	1:B:342:VAL:HG11	1.92	0.52
1:B:258:VAL:CG1	1:B:374:LEU:HD12	2.39	0.51
1:A:399:SER:OG	1:A:402:LEU:HG	2.09	0.51
1:B:407:THR:O	1:B:410:ILE:HG22	2.11	0.50
1:B:265:LEU:HD23	1:B:334:LEU:HD12	1.94	0.50
1:A:340:ASP:OD2	1:A:385:ARG:HD3	2.12	0.49
1:A:396:PRO:HG2	1:A:451:VAL:HG21	1.96	0.48
1:B:334:LEU:C	1:B:334:LEU:HD23	2.35	0.47
1:A:223:LEU:HD11	1:A:273:ILE:HG22	1.95	0.47
1:A:408:ASP:HA	5:A:26:HOH:O	2.14	0.47
1:A:227:TYR:CZ	1:A:239:ALA:HB2	2.50	0.47
1:B:360:MET:HB2	1:B:382:GLN:NE2	2.30	0.47
1:A:219:TYR:CZ	1:A:223:LEU:HD13	2.50	0.46
1:A:180:ILE:HA	1:A:183:VAL:HG13	1.98	0.46
1:B:364:LYS:O	1:B:364:LYS:HG3	2.15	0.45
1:A:443:GLN:HE22	4:A:101:7DE:H162	1.79	0.45
1:A:403:TYR:OH	1:A:447:ILE:HD11	2.16	0.45
1:A:366:VAL:HG12	1:A:372:LEU:HA	1.98	0.45
1:B:297:TYR:HB2	1:B:302:VAL:HG22	1.99	0.45
1:B:414:PHE:O	1:B:432:CYS:HB3	2.17	0.44
1:A:292:GLU:CD	1:B:313:LYS:HZ3	2.21	0.44
1:A:353:LEU:HD23	1:A:389:HIS:CD2	2.52	0.44
4:A:101:7DE:H13	5:A:1006:HOH:O	2.17	0.44
1:A:238:HIS:O	1:A:242:VAL:HG23	2.18	0.43
1:B:452:HIS:HB3	1:B:453:PRO:HD3	2.00	0.43
1:A:356:ASP:HB3	1:A:382:GLN:NE2	2.34	0.42
1:A:357:LEU:HD22	1:A:386:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:CG1	1:A:374:LEU:HD12	2.49	0.42
1:A:381:ILE:O	1:A:385:ARG:HG3	2.19	0.42
1:A:285:PHE:CE2	1:A:426:MET:HE3	2.55	0.42
4:A:101:7DE:O15	4:A:101:7DE:H61	2.20	0.42
1:B:308:LEU:CD2	1:B:339:ILE:HA	2.50	0.42
1:A:376:ASN:CG	1:A:377:TYR:H	2.23	0.42
1:B:337:MET:HG2	1:B:377:TYR:OH	2.19	0.42
1:B:184:ALA:HB2	1:B:237:LEU:CD1	2.50	0.41
1:B:441:LYS:HG2	1:B:484:ILE:HD13	2.01	0.41
1:B:429:SER:O	1:B:431:MET:N	2.53	0.41
1:B:242:VAL:HG12	1:B:271:ALA:HB1	2.02	0.41
1:B:375:ASP:HB2	1:B:379:ASP:OD2	2.20	0.41
1:A:323:PHE:O	1:A:326:LEU:HB2	2.20	0.41
1:A:340:ASP:HB2	5:A:12:HOH:O	2.20	0.41
1:B:237:LEU:O	1:B:237:LEU:HG	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/398 (80%)	297 (93%)	19 (6%)	4 (1%)	12	16
1	B	320/398 (80%)	299 (93%)	18 (6%)	3 (1%)	17	24
All	All	640/796 (80%)	596 (93%)	37 (6%)	7 (1%)	14	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	ASP
1	A	301	SER
1	A	430	PRO

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Mol	Chain	Res	Type
1	A	193	THR
1	B	193	THR
1	B	430	PRO
1	A	366	VAL

### 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	292/359 (81%)	268 (92%)	24 (8%)	11	14
1	B	292/359 (81%)	269 (92%)	23 (8%)	12	15
All	All	584/718 (81%)	537 (92%)	47 (8%)	12	15

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	204	ASP
1	A	252	THR
1	A	282	SER
1	A	291	SER
1	A	295	LEU
1	A	296	MET
1	A	318	GLU
1	A	319	HIS
1	A	324	MET
1	A	326	LEU
1	A	327	THR
1	A	328	LYS
1	A	332	GLN
1	A	335	ARG
1	A	351	MET
1	A	356	ASP
1	A	373	LEU
1	A	422	ARG

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Mol	Chain	Res	Type
1	A	434	LYS
1	A	436	THR
1	A	467	GLN
1	A	474	GLU
1	A	475	ASP
1	B	164	ASP
1	B	168	LYS
1	B	178	LEU
1	B	210	ARG
1	B	229	SER
1	B	256	ASP
1	B	316	GLN
1	B	318	GLU
1	B	324	MET
1	B	336	LYS
1	B	356	ASP
1	B	360	MET
1	B	373	LEU
1	B	378	THR
1	B	401	GLU
1	B	402	LEU
1	B	404	ARG
1	B	416	GLN
1	B	424	ARG
1	B	431	MET
1	B	467	GLN
1	B	470	LEU
1	B	484	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	382	GLN
1	B	201	GLN
1	B	382	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	B	194	1	8,9,10	1.39	1 (12%)	6,9,11	2.12	4 (66%)
1	CME	A	194	1	8,9,10	1.55	1 (12%)	6,9,11	2.76	4 (66%)

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
1	CME	B	194	1	-	2/5/8/10	-
1	CME	A	194	1	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	CME	OH-CZ	-3.59	1.23	1.42
1	A	194	CME	OH-CZ	-3.57	1.23	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	CME	CB-SG-SD	4.93	116.61	103.86
1	B	194	CME	CB-SG-SD	2.67	110.78	103.86
1	A	194	CME	CB-CA-C	2.64	117.98	110.80
1	B	194	CME	CA-CB-SG	-2.54	104.05	114.45
1	B	194	CME	OH-CZ-CE	2.53	120.71	110.82
1	A	194	CME	OH-CZ-CE	2.48	120.49	110.82
1	A	194	CME	CE-SD-SG	2.36	113.84	103.46
1	B	194	CME	CE-SD-SG	2.20	113.11	103.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	194	CME	SD-CE-CZ-OH
1	A	194	CME	CA-CB-SG-SD
1	A	194	CME	N-CA-CB-SG
1	B	194	CME	CZ-CE-SD-SG
1	A	194	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
4	7DE	A	101	-	18,22,22	1.62	4 (22%)	19,31,31	1.55	4 (21%)
4	7DE	B	102	-	18,22,22	1.76	3 (16%)	19,31,31	1.44	3 (15%)

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
4	7DE	A	101	-	-	3/9/15/15	0/2/2/2
4	7DE	B	102	-	-	3/9/15/15	0/2/2/2



All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	102	7DE	C11-C3	-3.99	1.37	1.40
4	B	102	7DE	C12-N19	-3.74	1.36	1.45
4	A	101	7DE	C12-N19	-3.07	1.37	1.45
4	A	101	7DE	C11-C3	-3.04	1.38	1.40
4	A	101	7DE	C8-N10	-2.55	1.27	1.33
4	B	102	7DE	C8-N10	-2.51	1.27	1.33
4	A	101	7DE	C11-C12	2.20	1.41	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	7DE	O21-N19-C12	-4.29	112.91	118.82
4	A	101	7DE	C11-C12-N19	2.60	120.98	118.74
4	B	102	7DE	C9-C8-N10	2.54	125.16	119.75
4	B	102	7DE	C13-C12-N19	2.29	121.33	119.34
4	B	102	7DE	C2-C1-C13	-2.22	117.58	121.00
4	A	101	7DE	C1-C2-C3	2.06	122.56	121.19
4	A	101	7DE	O15-C14-C7	2.06	116.94	112.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	7DE	C13-C12-N19-O21
4	A	101	7DE	C11-C12-N19-O21
4	B	102	7DE	O18-C14-O15-C16
4	B	102	7DE	C13-C12-N19-O21
4	B	102	7DE	C11-C12-N19-O21
4	A	101	7DE	O18-C14-O15-C16

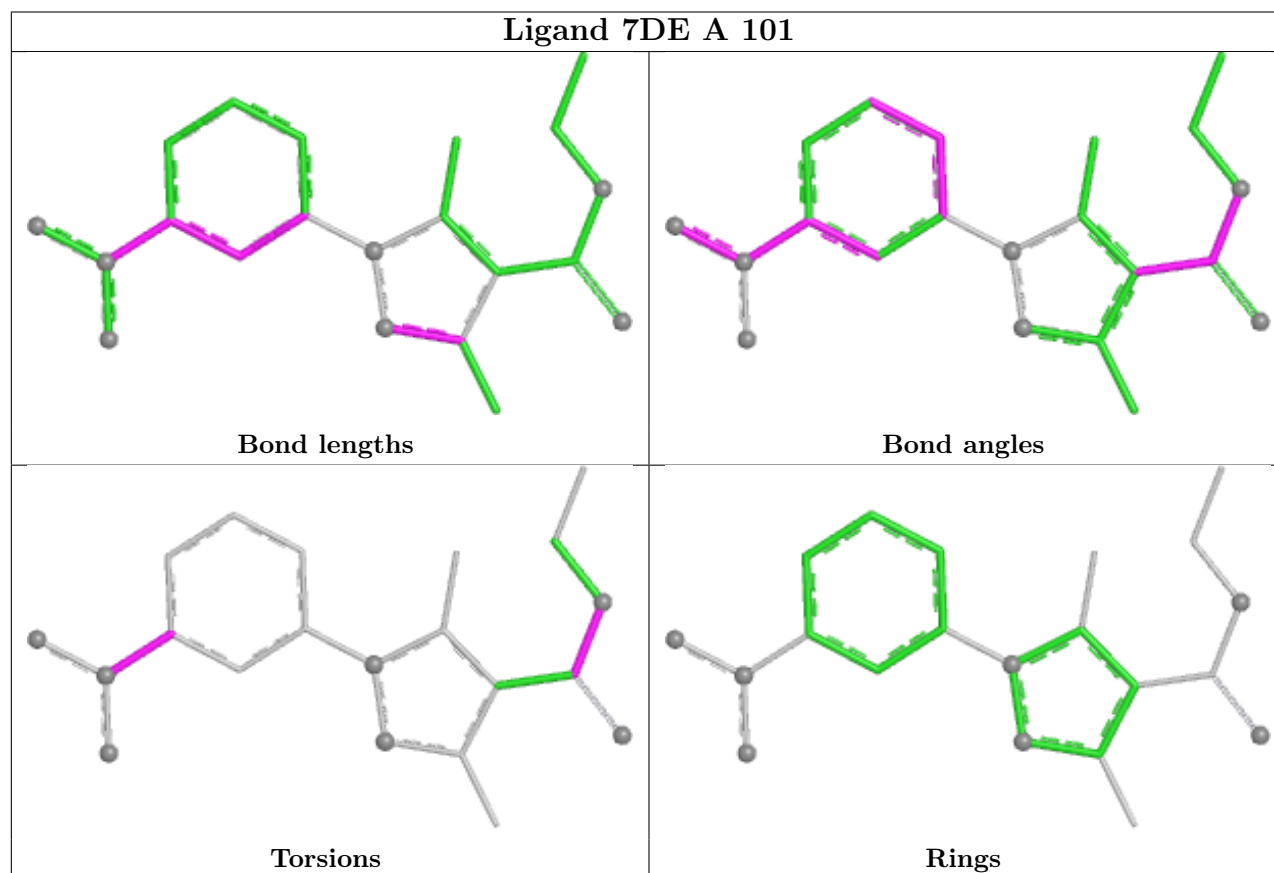
There are no ring outliers.

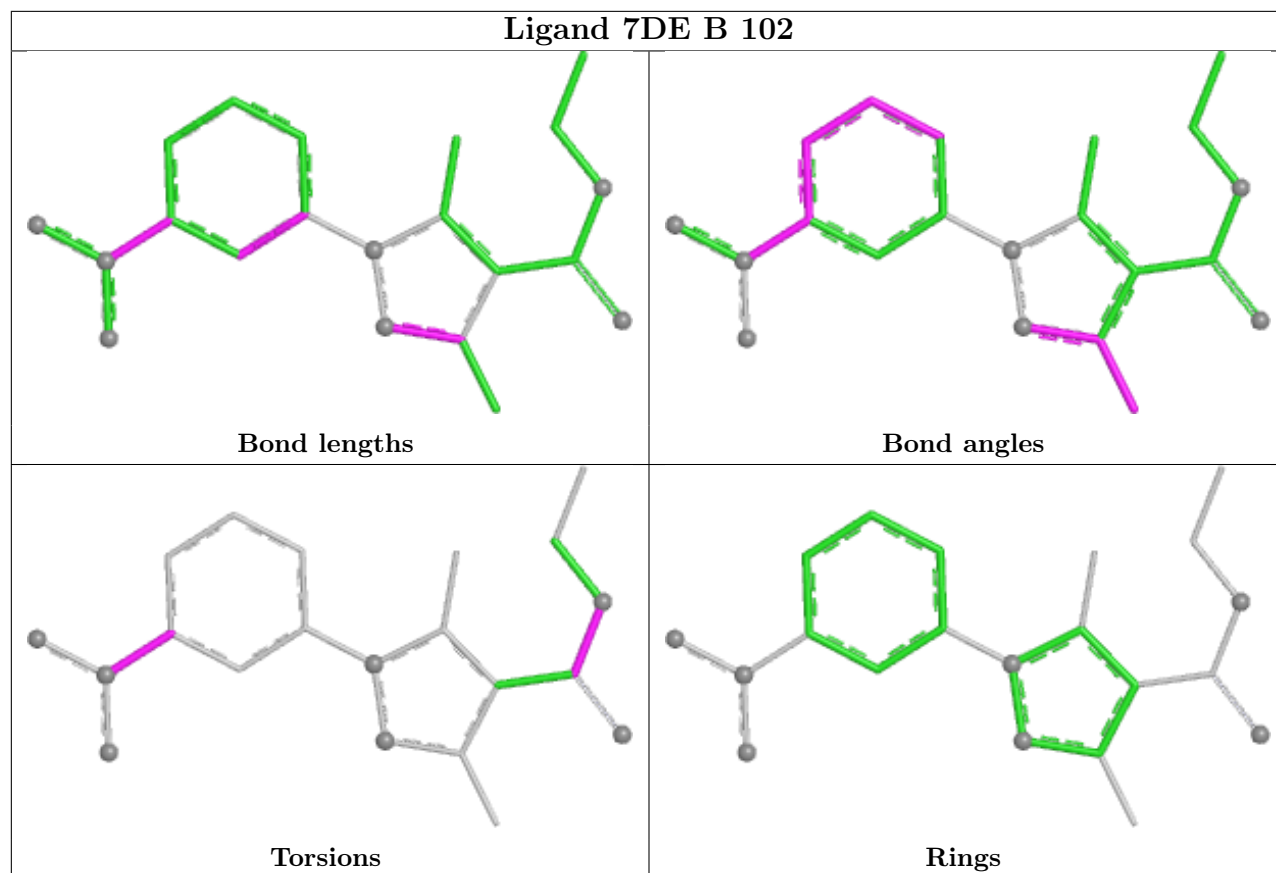
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	7DE	4	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	322/398 (80%)	0.23	3 (0%) 84 88	8, 17, 22, 26	0
1	B	322/398 (80%)	0.22	2 (0%) 89 92	5, 16, 21, 26	0
All	All	644/796 (80%)	0.22	5 (0%) 86 89	5, 17, 21, 26	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	SER	3.1
1	A	319	HIS	3.1
1	B	449	TYR	2.5
1	A	318	GLU	2.3
1	B	430	PRO	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	A	194	10/11	0.91	0.11	31,34,58,58	0
1	CME	B	194	10/11	0.93	0.15	31,35,57,57	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

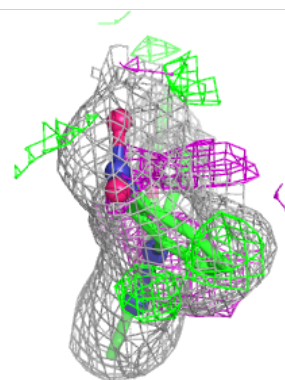
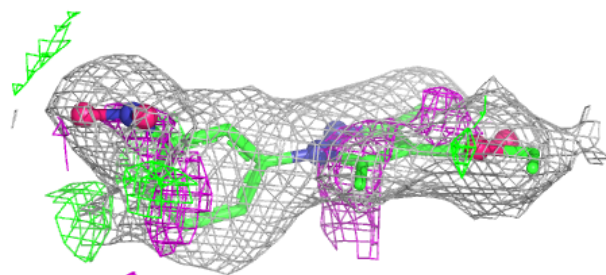
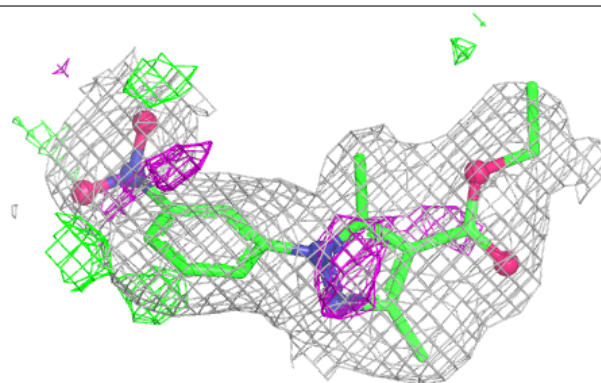
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	7DE	A	101	21/21	0.90	0.18	49,52,54,58	0
3	MG	A	1002	1/1	0.94	0.15	25,25,25,25	0
4	7DE	B	102	21/21	0.94	0.19	47,51,56,57	0
3	MG	B	1002	1/1	0.95	0.17	37,37,37,37	0
2	ZN	A	1001	1/1	0.98	0.14	36,36,36,36	0
2	ZN	B	1001	1/1	0.99	0.13	37,37,37,37	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.

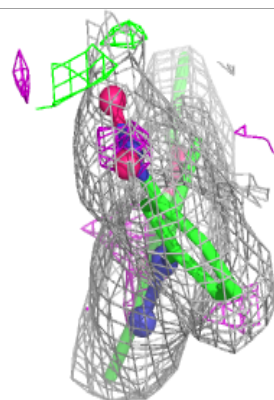
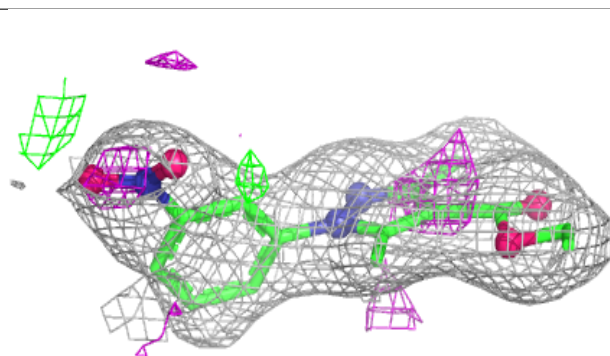
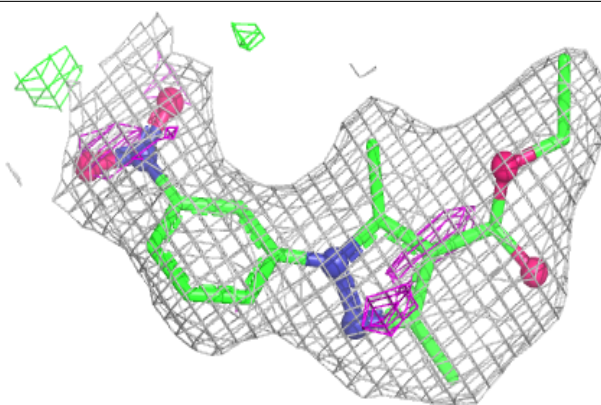
### Electron density around 7DE A 101:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)



**Electron density around 7DE B 102:**

$2mF_o - DF_c$  (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.