



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:59 pm BST

PDB ID : 2W98  
Title : CRYSTAL STRUCTURE OF HUMAN ZINC-BINDING ALCOHOL DEHYDROGENASE 1 (ZADH1) IN TERNARY COMPLEX WITH NADP AND PHENYLBUTAZONE  
Authors : Shafqat, N.; Yue, W.W.; Muniz, J.; Picaud, S.; Niesen, F.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Oppermann, U.  
Deposited on : 2009-01-22  
Resolution : 1.85 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.

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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 : 2.11  
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) : 2.11

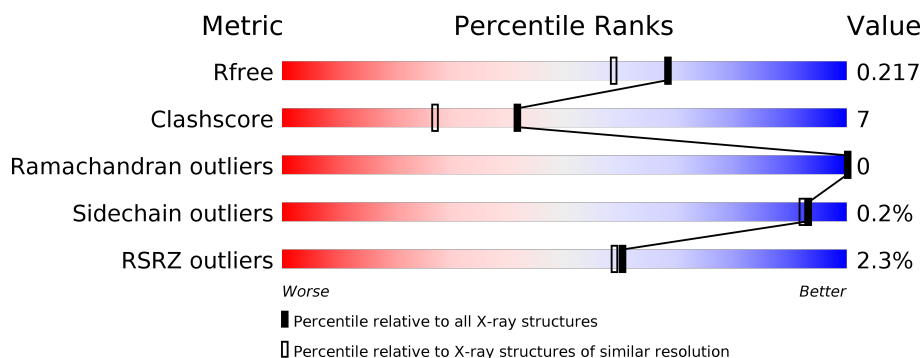
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	357	
1	B	357	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P1Z	A	1351	-	-	X	-
3	P1Z	A	1352	-	-	X	-
3	P1Z	A	1353	-	-	X	-
4	PO4	B	1360	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6268 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 PROSTAGLANDIN REDUCTASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	10	0
			2723	1727	462	514	20			
1	B	355	Total	C	N	O	S	0	8	0
			2759	1749	469	521	20			

There are 16 discrepancies between the modelled and reference sequences:

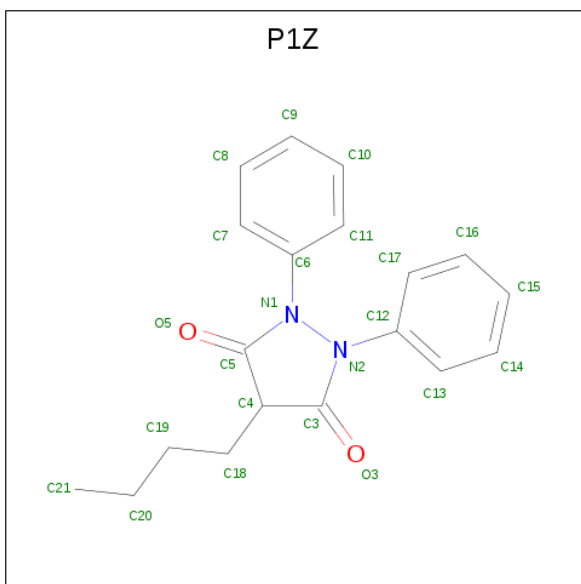
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q8N8N7
A	350	ALA	-	expression tag	UNP Q8N8N7
A	351	GLU	-	expression tag	UNP Q8N8N7
A	352	ASN	-	expression tag	UNP Q8N8N7
A	353	LEU	-	expression tag	UNP Q8N8N7
A	354	TYR	-	expression tag	UNP Q8N8N7
A	355	PHE	-	expression tag	UNP Q8N8N7
A	356	GLN	-	expression tag	UNP Q8N8N7
B	0	MET	-	expression tag	UNP Q8N8N7
B	350	ALA	-	expression tag	UNP Q8N8N7
B	351	GLU	-	expression tag	UNP Q8N8N7
B	352	ASN	-	expression tag	UNP Q8N8N7
B	353	LEU	-	expression tag	UNP Q8N8N7
B	354	TYR	-	expression tag	UNP Q8N8N7
B	355	PHE	-	expression tag	UNP Q8N8N7
B	356	GLN	-	expression tag	UNP Q8N8N7

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is 4-BUTYL-1,2-DIPHENYL-PYRAZOLIDINE-3,5-DIONE (three-letter code: P1Z) (formula:  $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2$ ).



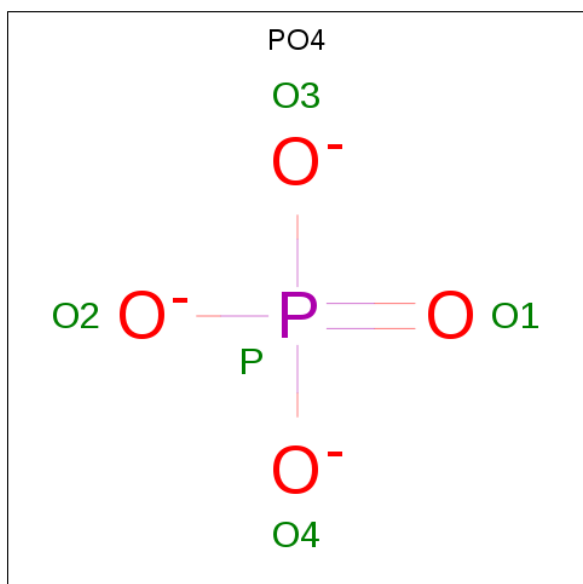
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	19	2	2		

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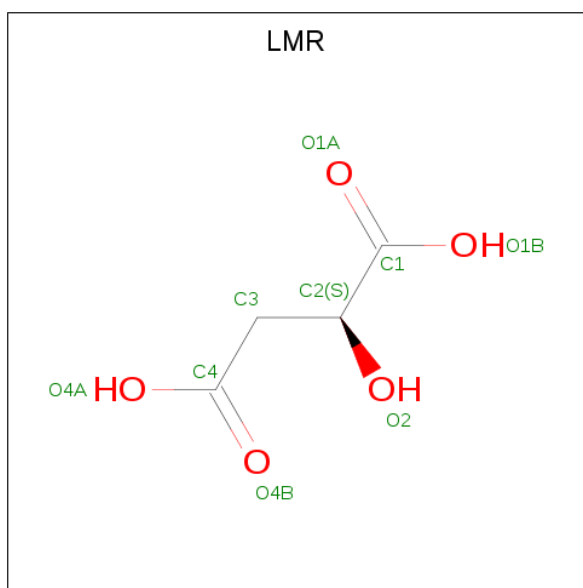
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	19	2	2		
3	A	1	Total	C	N	O	0	0
			23	19	2	2		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

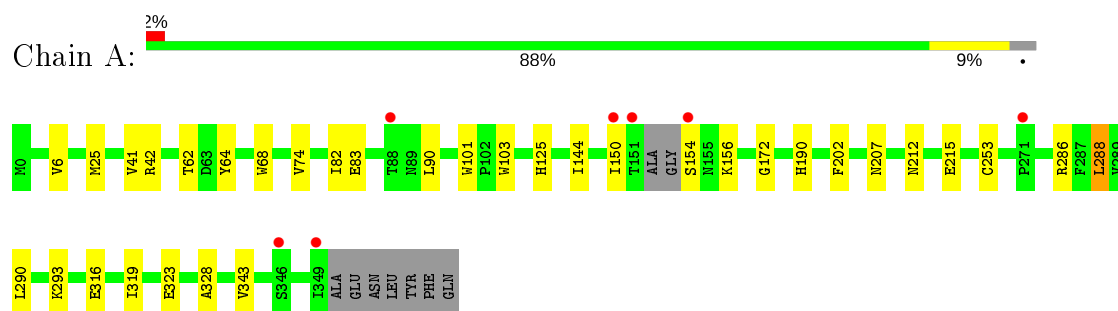
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	239	Total	O	0	0
			239	239		
8	B	254	Total	O	0	0
			254	254		

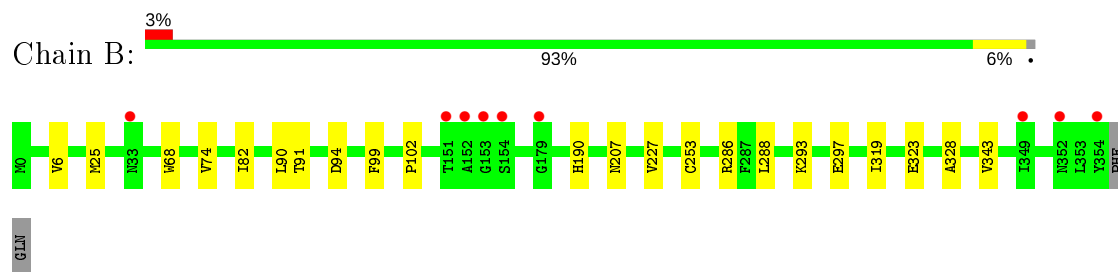
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: PROSTAGLANDIN REDUCTASE 2



#### • Molecule 1: PROSTAGLANDIN REDUCTASE 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.01 Å   82.79 Å   69.10 Å 90.00°   99.77°   90.00°	Depositor
Resolution (Å)	53.40 – 1.85 53.37 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.40-1.85) 99.2 (53.37-1.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 1.86 Å)	Xtrriage
Refinement program	REFMAC 5.5.0055	Depositor
R, $R_{free}$	0.158   ,   0.188 0.185   ,   0.217	Depositor DCC
$R_{free}$ test set	1319 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtrriage
Anisotropy	0.355	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	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 62.96 % 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 1.0407e-05. 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: CL, NA, PO4, NAP, P1Z, LMR

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	0.55	0/2802	0.62	0/3791
1	B	0.52	0/2833	0.61	0/3834
All	All	0.53	0/5635	0.61	0/7625

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

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	2723	0	2736	38	0
1	B	2759	0	2760	22	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
3	A	69	0	59	27	0
3	B	92	0	77	9	0
4	A	15	0	0	0	0
4	B	10	0	0	3	0
5	B	9	0	4	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	239	0	0	2	0
8	B	254	0	0	4	0
All	All	6268	0	5686	80	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 7.

All (80) 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:288:LEU:CD1	3:A:1351:P1Z:H17	1.55	1.35
1:A:288:LEU:HD11	3:A:1351:P1Z:C17	1.64	1.26
3:A:1352:P1Z:H211	3:A:1353:P1Z:C21	1.72	1.19
1:A:288:LEU:HD12	3:A:1351:P1Z:H17	1.35	1.08
3:A:1352:P1Z:H211	3:A:1353:P1Z:H212	1.37	1.05
3:A:1352:P1Z:H211	3:A:1353:P1Z:H213	1.44	0.99
1:A:288:LEU:CD1	3:A:1351:P1Z:C17	2.32	0.96
1:B:99:PHE:HA	4:B:1360:PO4:O3	1.65	0.96
1:A:190:HIS:CD2	1:A:207:ASN:HD22	1.81	0.95
1:A:25[B]:MET:HG2	8:A:2023:HOH:O	1.66	0.94
1:A:288:LEU:HD11	3:A:1351:P1Z:H17	1.25	0.94
1:B:190:HIS:CD2	1:B:207:ASN:HD22	1.85	0.93
3:A:1352:P1Z:C21	3:A:1353:P1Z:H212	2.02	0.88
1:B:99:PHE:CA	4:B:1360:PO4:O3	2.27	0.82
3:A:1352:P1Z:H202	3:A:1353:P1Z:H192	1.62	0.80
1:B:25[B]:MET:HG2	8:B:2026:HOH:O	1.79	0.80
3:A:1352:P1Z:H202	3:A:1353:P1Z:C19	2.14	0.78
1:A:190:HIS:CD2	1:A:207:ASN:ND2	2.53	0.75
1:A:288:LEU:HD11	3:A:1351:P1Z:C16	2.19	0.73
1:B:190:HIS:CD2	1:B:207:ASN:ND2	2.57	0.72
3:A:1352:P1Z:C20	3:A:1353:P1Z:H212	2.22	0.70
3:A:1352:P1Z:C21	3:A:1353:P1Z:C21	2.59	0.69
1:A:290:LEU:HD12	3:A:1351:P1Z:C16	2.23	0.68
1:B:68:TRP:CE2	1:B:74:VAL:HG13	2.31	0.65
1:A:68:TRP:CE2	1:A:74[A]:VAL:HG13	2.34	0.63
1:A:64:TYR:HB3	3:B:1358:P1Z:H212	1.81	0.62
1:A:290:LEU:HD12	3:A:1351:P1Z:H16	1.82	0.61
3:A:1353:P1Z:C3	3:A:1353:P1Z:H202	2.28	0.60
1:A:293[B]:LYS:HD3	3:A:1352:P1Z:H213	1.84	0.60
1:A:82[A]:ILE:CD1	1:A:90:LEU:HB3	2.33	0.58
1:A:64:TYR:OH	1:A:286:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HG21	1:A:328:ALA:HB2	1.88	0.56
3:A:1351:P1Z:C11	3:A:1351:P1Z:C12	2.81	0.56
3:A:1351:P1Z:H11	3:A:1351:P1Z:C12	2.36	0.55
1:A:290:LEU:HD12	3:A:1351:P1Z:C15	2.37	0.55
1:B:293:LYS:HD2	3:B:1359:P1Z:H213	1.87	0.54
1:A:125:HIS:HE1	1:A:316:GLU:OE2	1.90	0.54
1:A:319:ILE:CG2	1:A:343:VAL:HG22	2.38	0.54
1:A:6:VAL:HG22	1:A:25[A]:MET:SD	2.48	0.54
1:B:319:ILE:CG2	1:B:343:VAL:HG22	2.39	0.53
1:A:42[A]:ARG:NH2	1:A:83:GLU:OE2	2.37	0.53
1:B:82:ILE:HD12	1:B:94:ASP:HB2	1.90	0.53
1:B:319:ILE:HG21	1:B:328:ALA:HB2	1.91	0.51
1:A:74[B]:VAL:HG23	1:A:103:TRP:CD2	2.46	0.51
3:B:1356:P1Z:C6	3:B:1356:P1Z:H13	2.39	0.51
1:B:91:THR:HG22	8:B:2067:HOH:O	2.11	0.50
1:B:25[A]:MET:SD	1:B:323:GLU:HA	2.51	0.50
1:A:190:HIS:HD2	1:A:207:ASN:ND2	2.07	0.48
3:B:1356:P1Z:C13	3:B:1356:P1Z:C6	2.87	0.48
1:A:253:CYS:O	2:A:1350:NAP:H2N	2.14	0.48
3:B:1356:P1Z:C11	3:B:1356:P1Z:C12	2.90	0.47
1:A:74[B]:VAL:HG23	1:A:103:TRP:CE3	2.50	0.47
1:B:253:CYS:O	2:B:1355:NAP:H2N	2.15	0.47
1:B:6:VAL:HG22	1:B:25[A]:MET:SD	2.55	0.47
1:B:297:GLU:HA	3:B:1359:P1Z:H8	1.97	0.46
3:B:1356:P1Z:H11	3:B:1356:P1Z:C12	2.45	0.46
1:B:227:VAL:HG22	8:B:2105:HOH:O	2.16	0.45
1:A:212:ASN:HB3	1:A:215:GLU:HG2	1.99	0.45
1:A:62:THR:CG2	1:A:64:TYR:CE2	3.01	0.44
3:A:1352:P1Z:H212	3:A:1352:P1Z:H181	1.57	0.44
1:A:25[A]:MET:SD	1:A:323:GLU:HA	2.58	0.44
3:A:1352:P1Z:C7	3:B:1357:P1Z:H11	2.49	0.43
1:A:74[B]:VAL:CG2	1:A:103:TRP:CE3	3.01	0.43
1:B:190:HIS:HD2	1:B:207:ASN:ND2	2.15	0.43
1:B:286:ARG:HG3	8:B:2157:HOH:O	2.17	0.43
3:A:1352:P1Z:C12	3:A:1352:P1Z:H11	2.48	0.43
3:A:1352:P1Z:H201	3:A:1353:P1Z:H212	1.99	0.42
1:A:154:SER:HB2	1:A:156:LYS:HG3	2.02	0.42
1:A:172:GLY:HA3	1:A:202:PHE:CZ	2.54	0.42
1:B:102:PRO:HG2	4:B:1361:PO4:O1	2.19	0.42
1:B:288[A]:LEU:HD11	3:B:1356:P1Z:C17	2.50	0.42
3:A:1353:P1Z:O3	3:A:1353:P1Z:H202	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TRP:CZ2	1:B:74:VAL:HG13	2.55	0.41
1:A:144:ILE:HG23	1:A:150:ILE:HD12	2.01	0.41
1:A:68:TRP:CZ2	1:A:74[A]:VAL:HG13	2.55	0.41
1:A:82[A]:ILE:HD13	1:A:90:LEU:HB3	2.00	0.41
1:B:82:ILE:CD1	1:B:90:LEU:HB3	2.50	0.41
1:A:25[B]:MET:CE	8:A:2023:HOH:O	2.69	0.40
1:A:290:LEU:CD1	3:A:1351:P1Z:C16	2.97	0.40
1:A:41:VAL:HG11	1:A:101:TRP:CH2	2.57	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	354/357 (99%)	345 (98%)	9 (2%)	0	100	100
1	B	361/357 (101%)	354 (98%)	7 (2%)	0	100	100
All	All	715/714 (100%)	699 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	303/304 (100%)	302 (100%)	1 (0%)	92	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	303/304 (100%)	303 (100%)	0	100	100
All	All	606/608 (100%)	605 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LEU

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	89	ASN
1	A	125	HIS
1	A	190	HIS
1	B	89	ASN
1	B	149	HIS
1	B	190	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	PO4	A	1356	-	4,4,4	0.84	0	6,6,6	0.56	0
3	P1Z	B	1358	-	23,25,25	2.70	5 (21%)	23,34,34	3.14	12 (52%)
3	P1Z	B	1357	-	23,25,25	2.61	4 (17%)	23,34,34	3.05	12 (52%)
3	P1Z	B	1359	-	23,25,25	2.64	3 (13%)	23,34,34	2.56	11 (47%)
4	PO4	B	1360	-	4,4,4	1.26	1 (25%)	6,6,6	1.12	0
5	LMR	B	1362	7	2,8,8	0.39	0	3,10,10	1.64	1 (33%)
2	NAP	A	1350	-	45,52,52	1.52	3 (6%)	56,80,80	1.59	9 (16%)
4	PO4	A	1355	-	4,4,4	0.94	0	6,6,6	0.82	0
3	P1Z	A	1353	-	23,25,25	2.74	4 (17%)	23,34,34	2.79	9 (39%)
2	NAP	B	1355	-	45,52,52	1.39	4 (8%)	56,80,80	1.53	11 (19%)
3	P1Z	A	1352	-	23,25,25	2.72	4 (17%)	23,34,34	2.71	11 (47%)
4	PO4	B	1361	-	4,4,4	0.92	0	6,6,6	0.72	0
3	P1Z	B	1356	-	23,25,25	2.73	4 (17%)	23,34,34	2.62	10 (43%)
4	PO4	A	1354	-	4,4,4	1.11	0	6,6,6	0.69	0
3	P1Z	A	1351	-	23,25,25	2.68	4 (17%)	23,34,34	2.37	6 (26%)

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	P1Z	B	1358	-	-	4/12/32/32	0/3/3/3
3	P1Z	B	1357	-	-	2/12/32/32	0/3/3/3
3	P1Z	B	1359	-	-	3/12/32/32	0/3/3/3
2	NAP	B	1355	-	-	5/31/67/67	0/5/5/5
2	NAP	A	1350	-	-	4/31/67/67	0/5/5/5
3	P1Z	A	1353	-	-	6/12/32/32	0/3/3/3
3	P1Z	A	1352	-	-	4/12/32/32	0/3/3/3
3	P1Z	B	1356	-	-	4/12/32/32	0/3/3/3
5	LMR	B	1362	7	-	2/2/8/8	-
3	P1Z	A	1351	-	-	4/12/32/32	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1353	P1Z	N1-N2	-9.73	1.26	1.42
3	B	1359	P1Z	N1-N2	-9.62	1.26	1.42
3	A	1351	P1Z	N1-N2	-9.38	1.27	1.42
3	A	1352	P1Z	N1-N2	-9.19	1.27	1.42
3	B	1357	P1Z	N1-N2	-8.90	1.27	1.42
3	B	1356	P1Z	N1-N2	-8.78	1.28	1.42
3	B	1358	P1Z	N1-N2	-8.56	1.28	1.42
3	B	1358	P1Z	C12-N2	-6.63	1.32	1.43
3	A	1352	P1Z	C12-N2	-6.52	1.32	1.43
3	B	1356	P1Z	C12-N2	-6.51	1.32	1.43
3	A	1351	P1Z	C12-N2	-6.45	1.32	1.43
3	A	1353	P1Z	C12-N2	-6.04	1.33	1.43
3	B	1358	P1Z	C6-N1	-5.71	1.33	1.43
3	B	1359	P1Z	C12-N2	-5.59	1.33	1.43
2	A	1350	NAP	P2B-O2B	5.57	1.69	1.59
3	B	1357	P1Z	C6-N1	-5.45	1.34	1.43
3	B	1357	P1Z	C12-N2	-5.41	1.34	1.43
3	B	1359	P1Z	C6-N1	-5.22	1.34	1.43
2	B	1355	NAP	O7N-C7N	4.99	1.33	1.24
3	A	1352	P1Z	C6-N1	-4.96	1.35	1.43
2	A	1350	NAP	O7N-C7N	4.71	1.33	1.24
2	B	1355	NAP	P2B-O2B	4.68	1.68	1.59
3	B	1356	P1Z	C6-N1	-4.66	1.35	1.43
3	A	1353	P1Z	C6-N1	-4.36	1.35	1.43
3	B	1356	P1Z	C4-C3	-4.09	1.44	1.52
3	A	1351	P1Z	C6-N1	-3.42	1.37	1.43
3	A	1351	P1Z	C4-C3	-3.21	1.46	1.52
3	A	1353	P1Z	C4-C5	-3.17	1.46	1.52
2	A	1350	NAP	C6N-N1N	2.72	1.42	1.35
2	B	1355	NAP	C6N-N1N	2.63	1.41	1.35
3	A	1352	P1Z	C4-C3	-2.45	1.47	1.52
2	B	1355	NAP	C2N-N1N	2.27	1.37	1.35
4	B	1360	PO4	P-O3	-2.23	1.47	1.54
3	B	1357	P1Z	C4-C3	-2.12	1.48	1.52
3	B	1358	P1Z	C4-C3	-2.10	1.48	1.52
3	B	1358	P1Z	C17-C12	2.02	1.43	1.39

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1358	P1Z	C13-C12-N2	8.42	134.25	119.57
3	A	1353	P1Z	C17-C12-N2	7.25	132.21	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1359	P1Z	C13-C12-N2	6.87	131.54	119.57
3	B	1357	P1Z	C11-C6-N1	6.65	131.17	119.57
3	A	1351	P1Z	C17-C12-N2	6.34	130.63	119.57
3	B	1358	P1Z	C17-C12-N2	-6.32	108.55	119.57
3	B	1356	P1Z	C17-C12-N2	6.14	130.26	119.57
3	B	1357	P1Z	C17-C12-N2	6.09	130.19	119.57
3	A	1352	P1Z	C13-C12-N2	5.88	129.82	119.57
3	A	1353	P1Z	C13-C12-N2	-5.78	109.49	119.57
3	A	1351	P1Z	C13-C12-N2	-4.97	110.91	119.57
3	B	1356	P1Z	C7-C6-N1	4.92	128.15	119.57
3	A	1352	P1Z	O3-C3-C4	-4.90	121.00	127.30
3	B	1357	P1Z	C13-C12-N2	-4.85	111.11	119.57
3	B	1359	P1Z	C17-C12-N2	-4.73	111.33	119.57
3	A	1352	P1Z	O5-C5-C4	-4.67	121.30	127.30
2	B	1355	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
3	B	1357	P1Z	O3-C3-C4	-4.53	121.48	127.30
2	A	1350	NAP	C6N-N1N-C2N	-4.46	117.91	121.97
3	A	1353	P1Z	C12-N2-N1	4.46	128.17	117.30
3	B	1356	P1Z	C19-C18-C4	-4.38	100.68	114.46
3	B	1358	P1Z	C7-C6-N1	4.29	127.04	119.57
2	A	1350	NAP	C3N-C2N-N1N	4.28	124.61	120.43
3	B	1357	P1Z	C7-C6-N1	-4.27	112.13	119.57
3	A	1352	P1Z	C17-C12-N2	-4.17	112.30	119.57
2	A	1350	NAP	N3A-C2A-N1A	-4.13	122.22	128.68
3	B	1357	P1Z	C8-C7-C6	4.05	124.97	119.68
2	A	1350	NAP	C6N-C5N-C4N	4.02	125.28	119.44
3	A	1353	P1Z	O5-C5-C4	-4.02	122.14	127.30
3	A	1351	P1Z	O5-C5-C4	-3.94	122.23	127.30
3	B	1359	P1Z	C7-C6-N1	3.93	126.42	119.57
3	A	1353	P1Z	C19-C18-C4	-3.74	102.69	114.46
2	B	1355	NAP	C6N-N1N-C2N	-3.64	118.65	121.97
3	B	1357	P1Z	C19-C18-C4	-3.64	103.00	114.46
3	B	1358	P1Z	C10-C11-C6	3.63	124.42	119.68
3	B	1358	P1Z	O5-C5-C4	-3.61	122.65	127.30
3	B	1356	P1Z	C13-C12-N2	-3.54	113.40	119.57
3	A	1352	P1Z	C7-C6-N1	3.52	125.70	119.57
3	B	1359	P1Z	C6-N1-N2	3.52	125.88	117.30
3	A	1352	P1Z	C16-C17-C12	3.46	124.20	119.68
2	B	1355	NAP	C6N-C5N-C4N	3.40	124.37	119.44
3	B	1356	P1Z	C10-C11-C6	3.35	124.06	119.68
3	A	1351	P1Z	C19-C18-C4	-3.34	103.93	114.46
3	B	1358	P1Z	C16-C17-C12	3.31	124.01	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1353	P1Z	C11-C6-N1	3.25	125.23	119.57
3	A	1353	P1Z	C6-N1-N2	3.24	125.20	117.30
3	A	1352	P1Z	C12-N2-N1	3.17	125.03	117.30
3	A	1351	P1Z	C7-C6-N1	3.11	124.98	119.57
3	B	1359	P1Z	O5-C5-C4	-3.07	123.35	127.30
3	B	1358	P1Z	C12-N2-N1	3.00	124.63	117.30
2	B	1355	NAP	C5N-C4N-C3N	-2.98	116.82	120.34
3	B	1358	P1Z	C6-N1-N2	2.97	124.55	117.30
3	B	1358	P1Z	C19-C18-C4	-2.96	105.16	114.46
2	A	1350	NAP	O4D-C1D-C2D	-2.93	102.64	106.93
3	B	1359	P1Z	C19-C18-C4	-2.89	105.36	114.46
3	B	1356	P1Z	C11-C6-N1	-2.87	114.58	119.57
3	B	1356	P1Z	O5-C5-C4	-2.85	123.64	127.30
3	A	1352	P1Z	C6-N1-N2	2.84	124.23	117.30
3	B	1357	P1Z	C6-N1-N2	2.83	124.21	117.30
2	A	1350	NAP	C5N-C4N-C3N	-2.81	117.02	120.34
3	B	1359	P1Z	C12-N2-N1	2.79	124.11	117.30
5	B	1362	LMR	C3-C2-C1	2.79	114.64	111.10
3	B	1356	P1Z	C14-C13-C12	2.75	123.28	119.68
2	A	1350	NAP	C5N-C6N-N1N	-2.74	116.47	120.40
3	B	1356	P1Z	C12-N2-N1	2.73	123.96	117.30
3	B	1359	P1Z	C16-C17-C12	2.70	123.21	119.68
3	A	1353	P1Z	C14-C13-C12	2.70	123.21	119.68
3	B	1357	P1Z	C12-N2-N1	2.56	123.53	117.30
3	B	1358	P1Z	C9-C8-C7	2.54	124.06	120.19
3	B	1358	P1Z	O3-C3-C4	-2.54	124.04	127.30
2	B	1355	NAP	O4B-C4B-C5B	-2.52	101.07	109.37
3	A	1351	P1Z	C14-C13-C12	2.51	122.97	119.68
3	A	1352	P1Z	C10-C11-C6	2.49	122.94	119.68
3	B	1357	P1Z	O5-C5-C4	-2.48	124.12	127.30
2	B	1355	NAP	O4D-C1D-C2D	-2.47	103.31	106.93
2	A	1350	NAP	O3X-P2B-O2X	2.46	117.05	107.64
2	B	1355	NAP	C3N-C2N-N1N	2.38	122.75	120.43
2	B	1355	NAP	C2A-N1A-C6A	2.36	122.79	118.75
3	B	1359	P1Z	O3-C3-C4	-2.35	124.28	127.30
3	B	1357	P1Z	C9-C10-C11	2.33	123.73	120.19
3	B	1357	P1Z	C14-C13-C12	2.27	122.65	119.68
2	A	1350	NAP	O4B-C4B-C5B	-2.27	101.91	109.37
3	B	1359	P1Z	C11-C6-N1	-2.20	115.73	119.57
2	B	1355	NAP	O7N-C7N-C3N	2.19	122.25	119.63
3	B	1356	P1Z	C13-C12-C17	-2.16	114.77	119.16
3	A	1353	P1Z	C8-C7-C6	2.16	122.50	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1358	P1Z	C15-C14-C13	2.15	123.46	120.19
3	A	1352	P1Z	C15-C14-C13	2.10	123.39	120.19
2	B	1355	NAP	C5N-C6N-N1N	-2.08	117.42	120.40
2	B	1355	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
3	A	1352	P1Z	C11-C6-N1	-2.05	115.99	119.57
3	B	1359	P1Z	C10-C11-C6	2.01	122.31	119.68

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1358	P1Z	C19-C18-C4-C3
3	B	1358	P1Z	C19-C18-C4-C5
3	B	1357	P1Z	C19-C18-C4-C3
3	B	1357	P1Z	C19-C18-C4-C5
3	B	1359	P1Z	C19-C18-C4-C3
3	B	1359	P1Z	C19-C18-C4-C5
2	B	1355	NAP	O4D-C1D-N1N-C6N
5	B	1362	LMR	O2-C2-C3-C4
3	A	1353	P1Z	C19-C18-C4-C3
3	A	1353	P1Z	C19-C18-C4-C5
3	A	1352	P1Z	C19-C18-C4-C3
3	A	1352	P1Z	C19-C18-C4-C5
3	B	1356	P1Z	C19-C18-C4-C5
3	A	1351	P1Z	C19-C18-C4-C3
3	A	1351	P1Z	C19-C18-C4-C5
3	A	1351	P1Z	C4-C18-C19-C20
3	B	1358	P1Z	C4-C18-C19-C20
3	A	1353	P1Z	C4-C18-C19-C20
3	B	1356	P1Z	C17-C12-N2-C3
3	B	1356	P1Z	C17-C12-N2-N1
3	A	1353	P1Z	C11-C6-N1-C5
5	B	1362	LMR	C1-C2-C3-C4
3	B	1359	P1Z	C18-C19-C20-C21
2	A	1350	NAP	C4B-C5B-O5B-PA
3	B	1356	P1Z	C4-C18-C19-C20
2	B	1355	NAP	C4B-C5B-O5B-PA
3	A	1351	P1Z	C18-C19-C20-C21
3	A	1353	P1Z	C7-C6-N1-C5
3	A	1352	P1Z	C7-C6-N1-N2
3	B	1358	P1Z	C7-C6-N1-N2
2	B	1355	NAP	C3B-C4B-C5B-O5B

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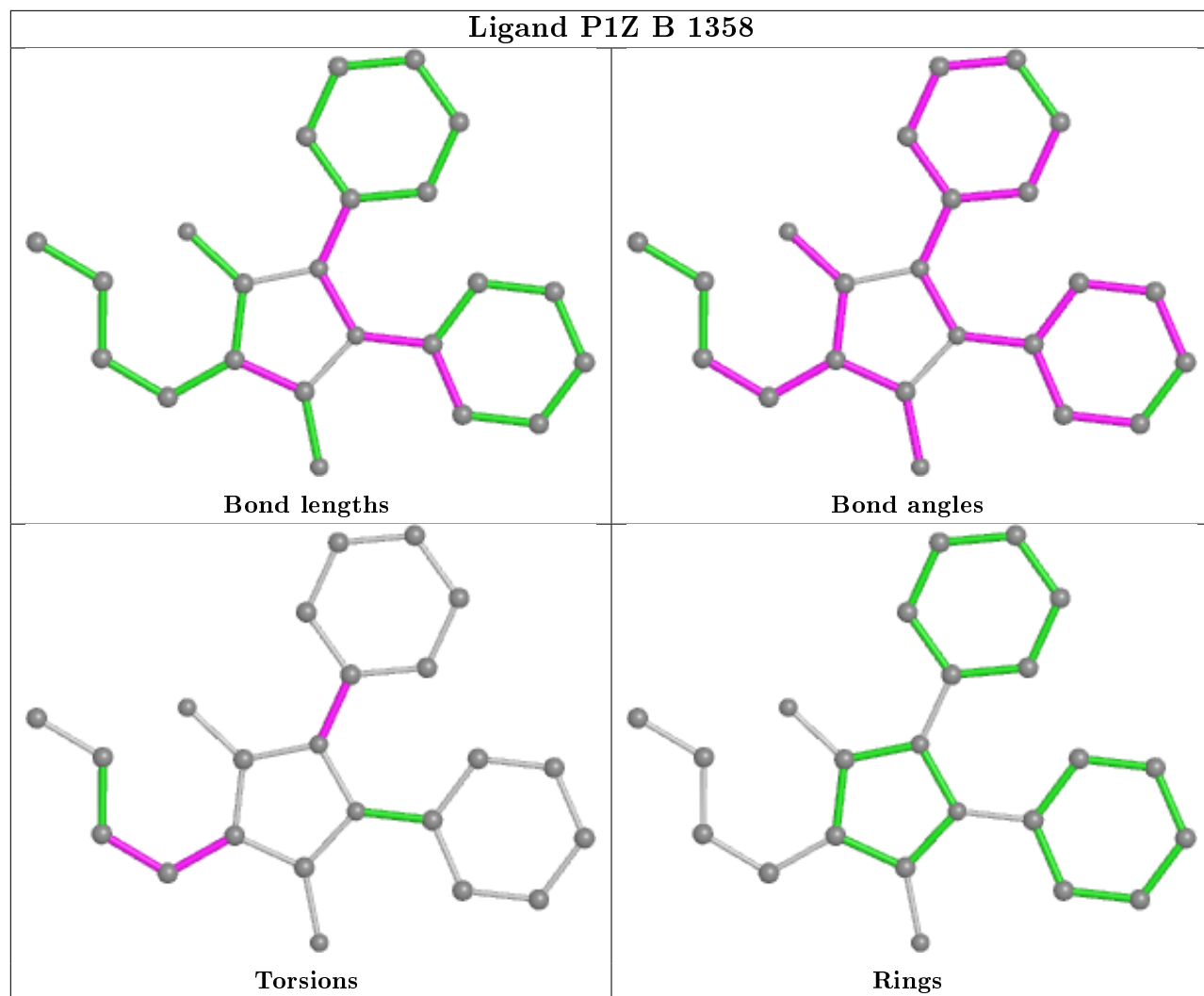
Mol	Chain	Res	Type	Atoms
2	A	1350	NAP	C3B-C4B-C5B-O5B
2	A	1350	NAP	O4B-C4B-C5B-O5B
2	B	1355	NAP	PA-O3-PN-O1N
2	B	1355	NAP	O4B-C4B-C5B-O5B
3	A	1353	P1Z	C18-C19-C20-C21
3	A	1352	P1Z	C18-C19-C20-C21
2	A	1350	NAP	C1B-C2B-O2B-P2B

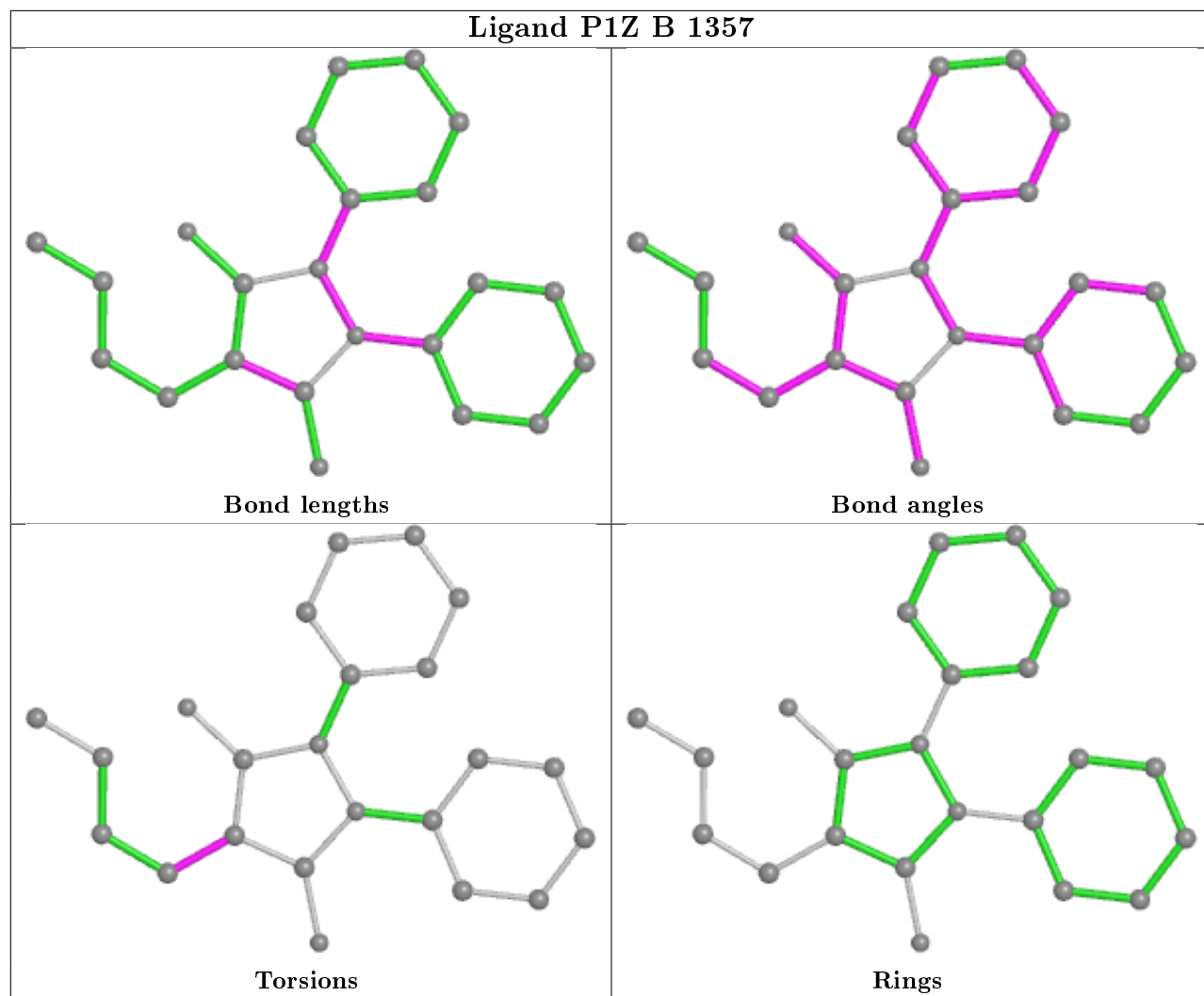
There are no ring outliers.

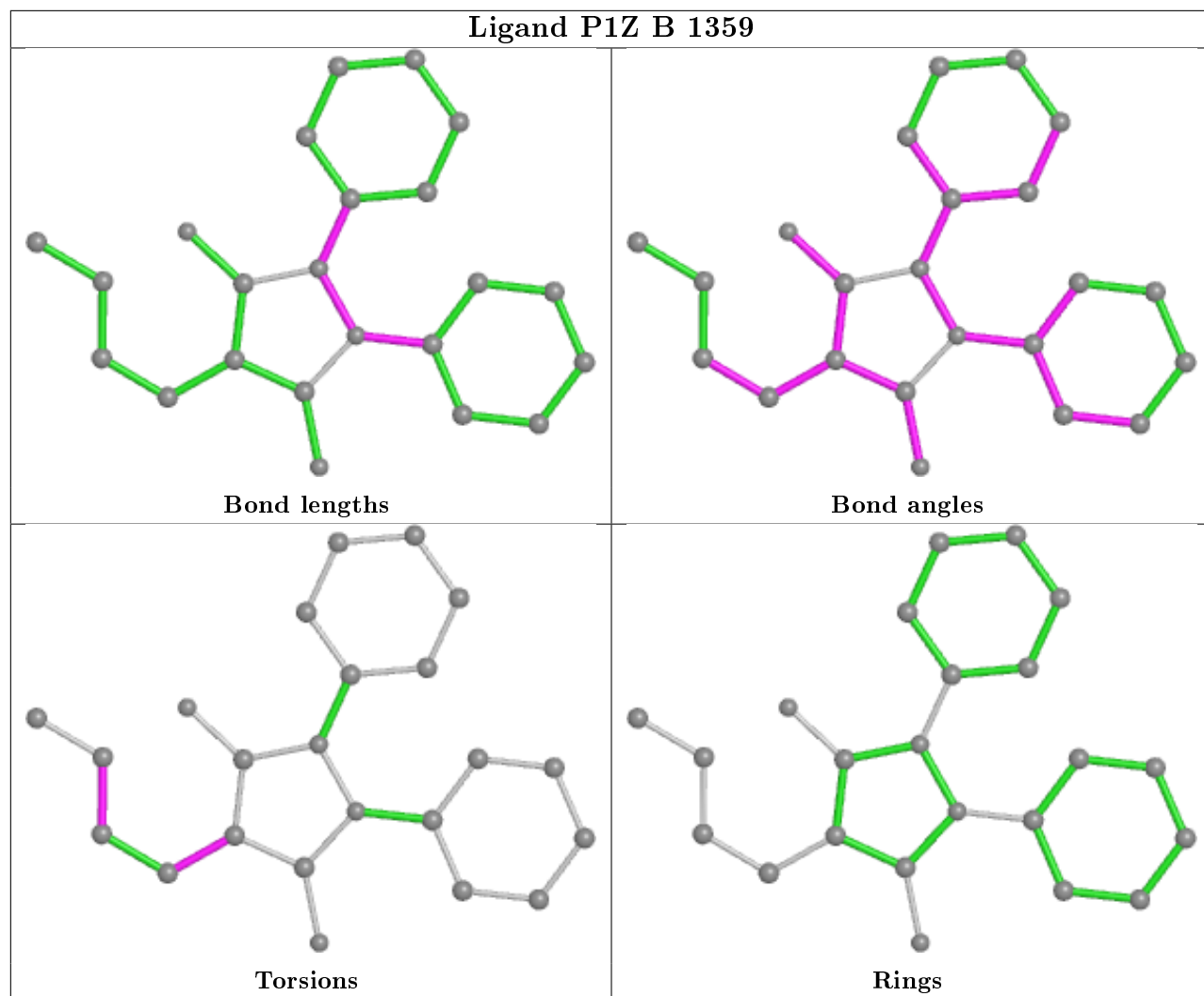
11 monomers are involved in 40 short contacts:

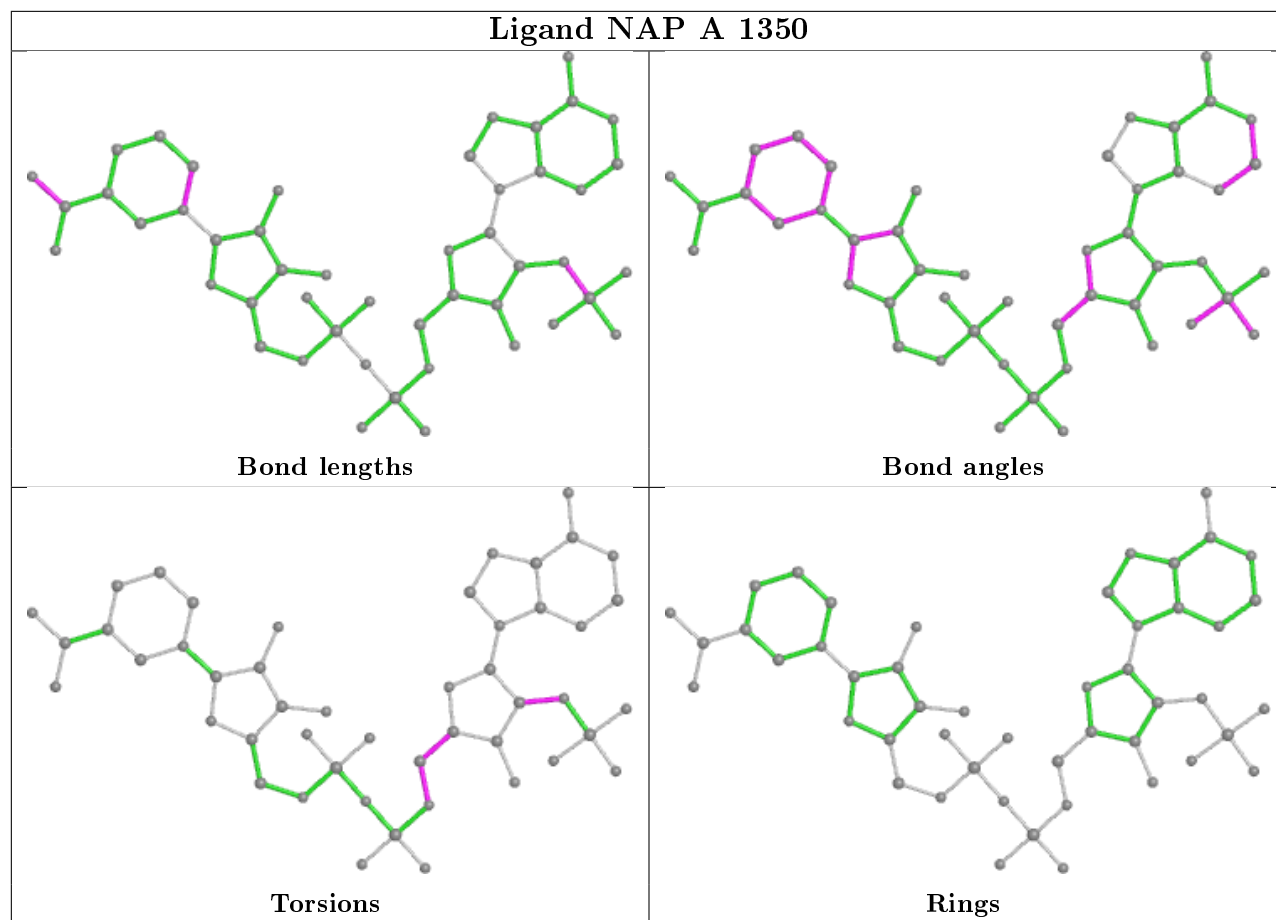
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1358	P1Z	1	0
3	B	1357	P1Z	1	0
3	B	1359	P1Z	2	0
4	B	1360	PO4	2	0
2	A	1350	NAP	1	0
3	A	1353	P1Z	11	0
2	B	1355	NAP	1	0
3	A	1352	P1Z	13	0
4	B	1361	PO4	1	0
3	B	1356	P1Z	5	0
3	A	1351	P1Z	12	0

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.

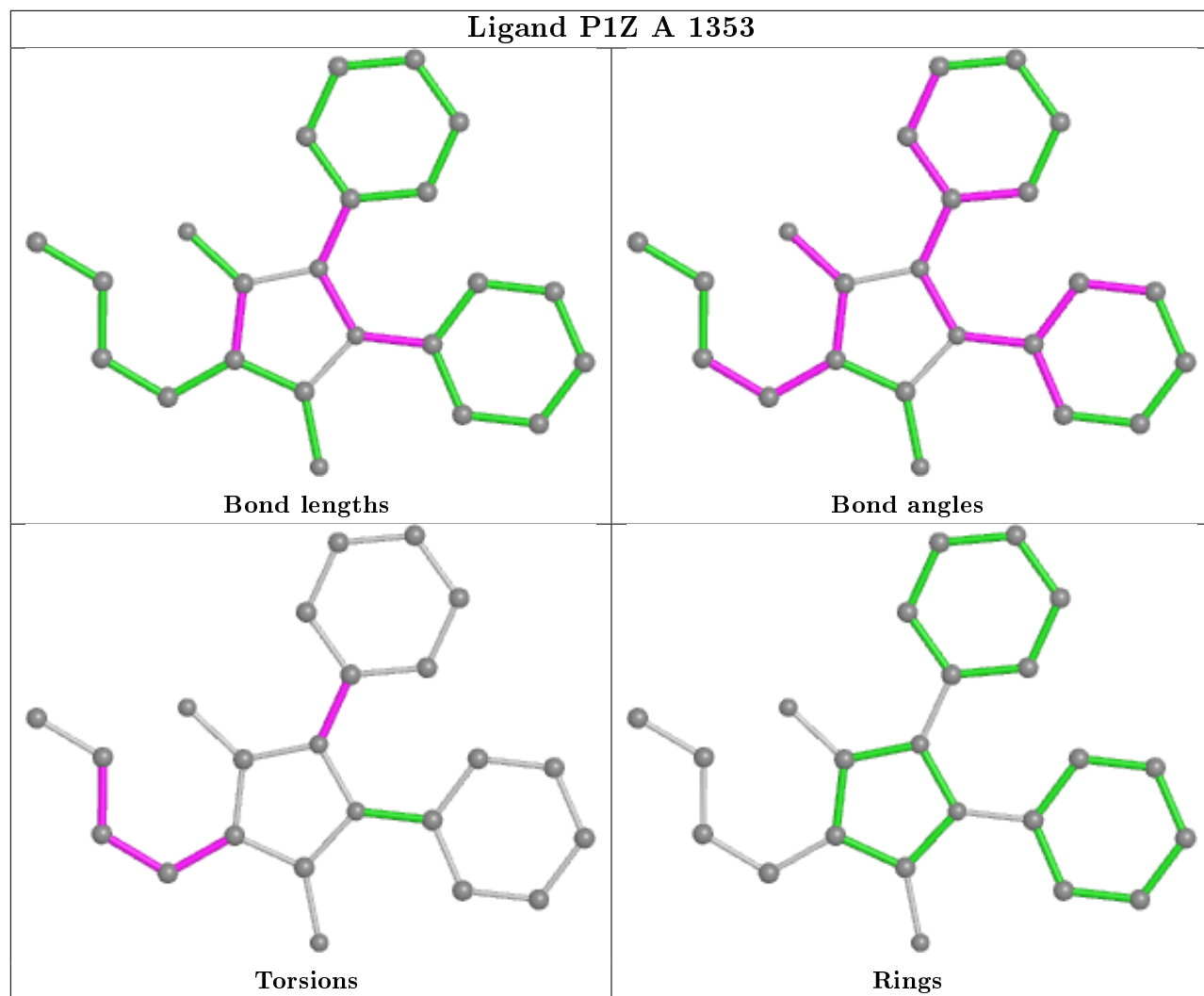


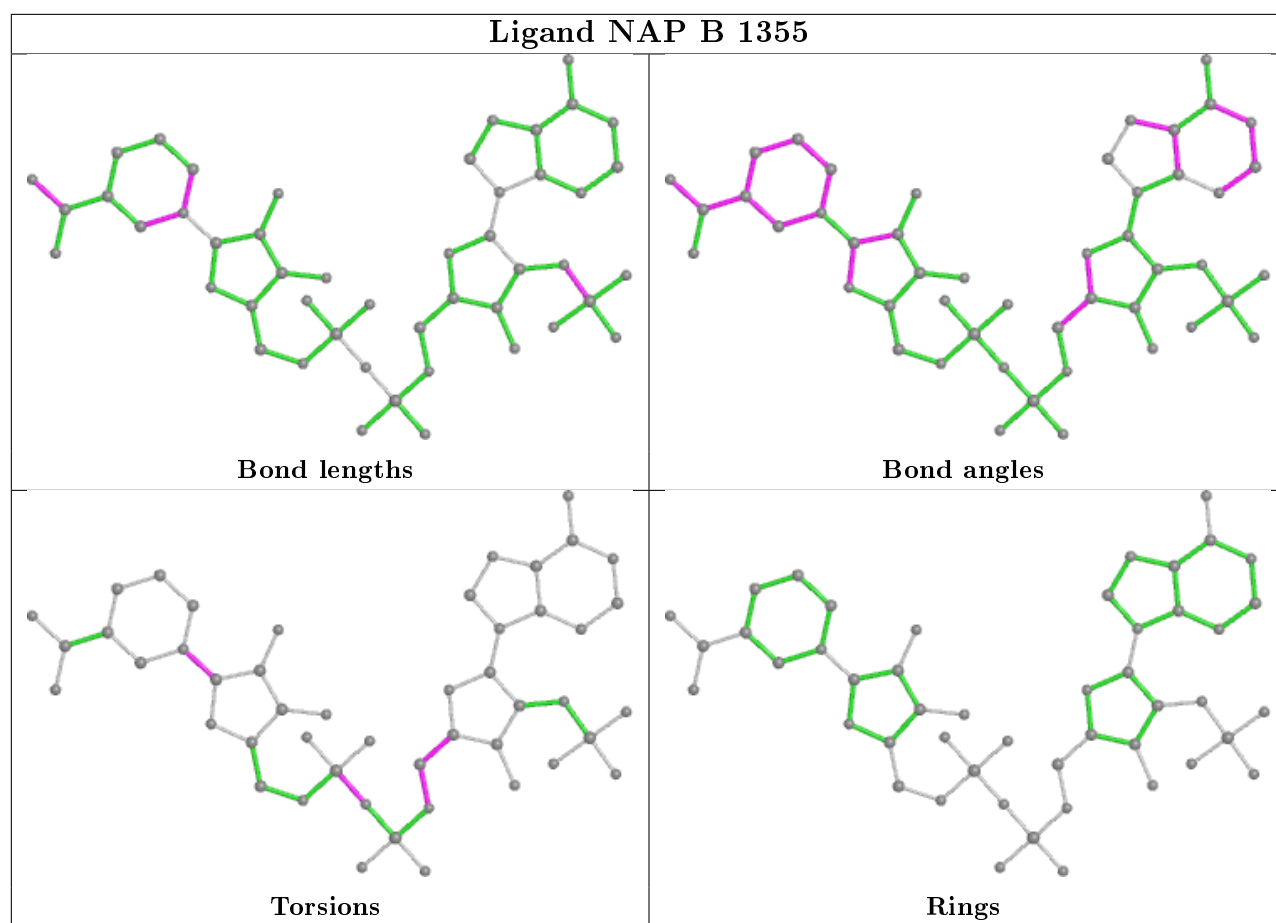


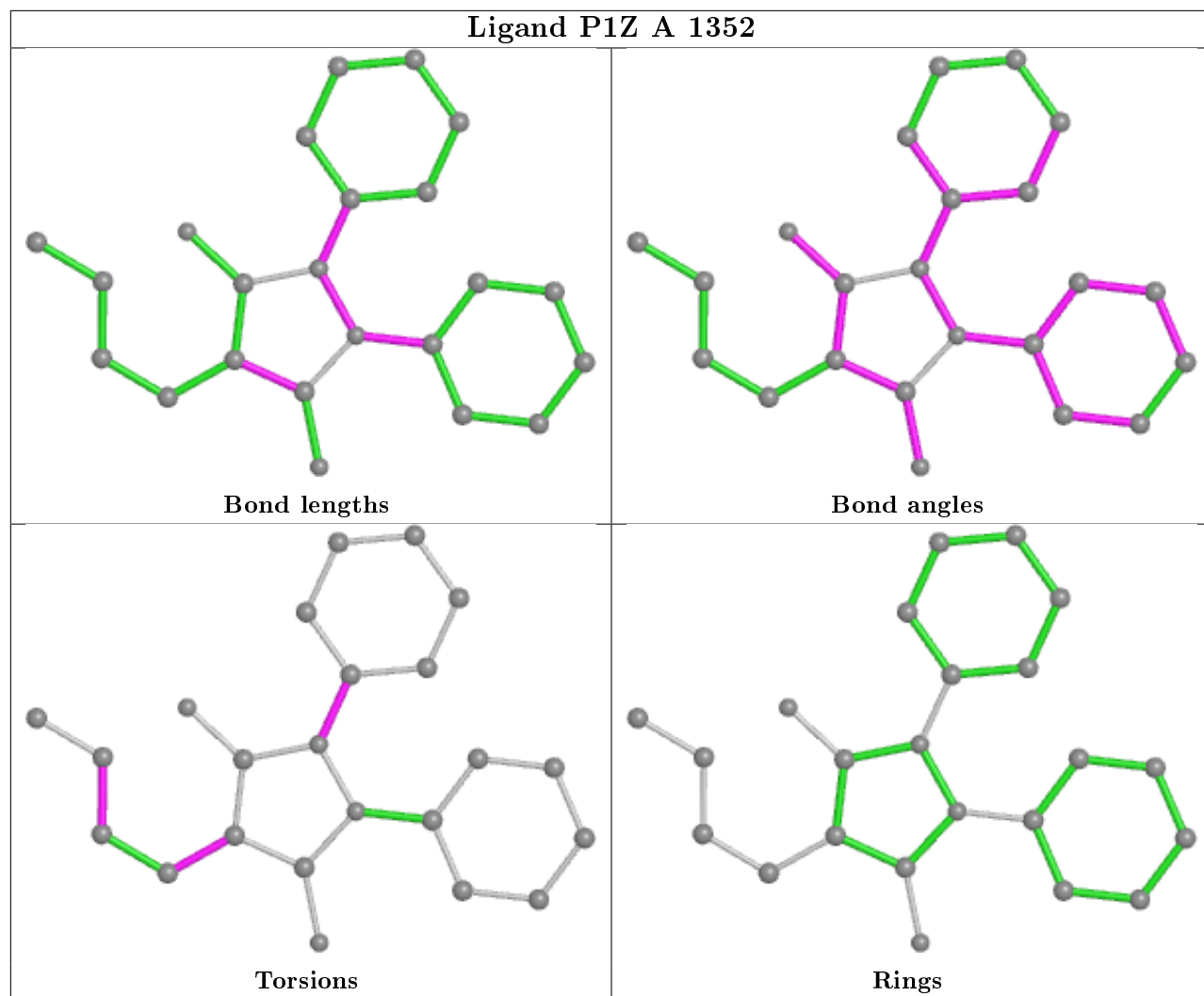


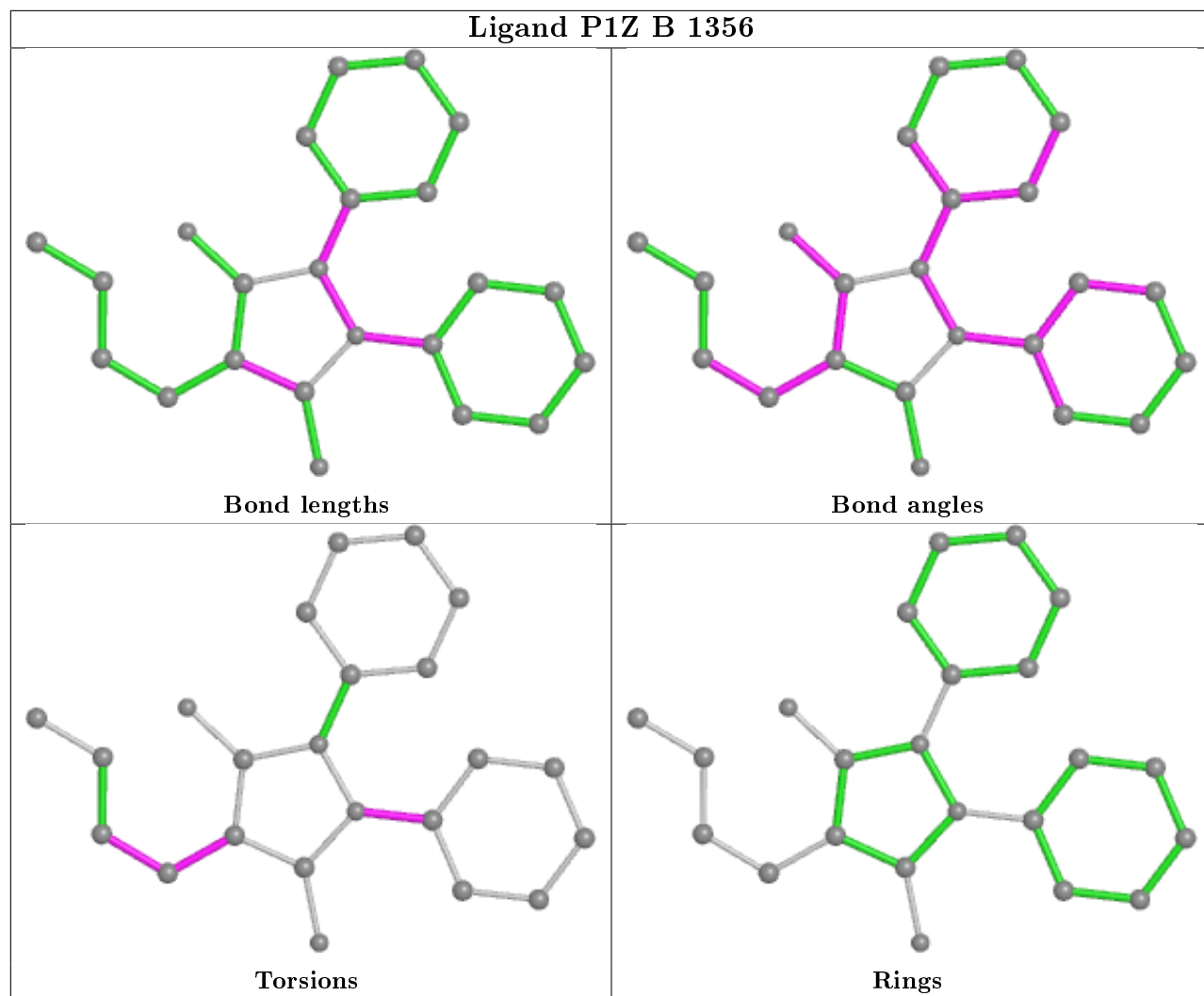


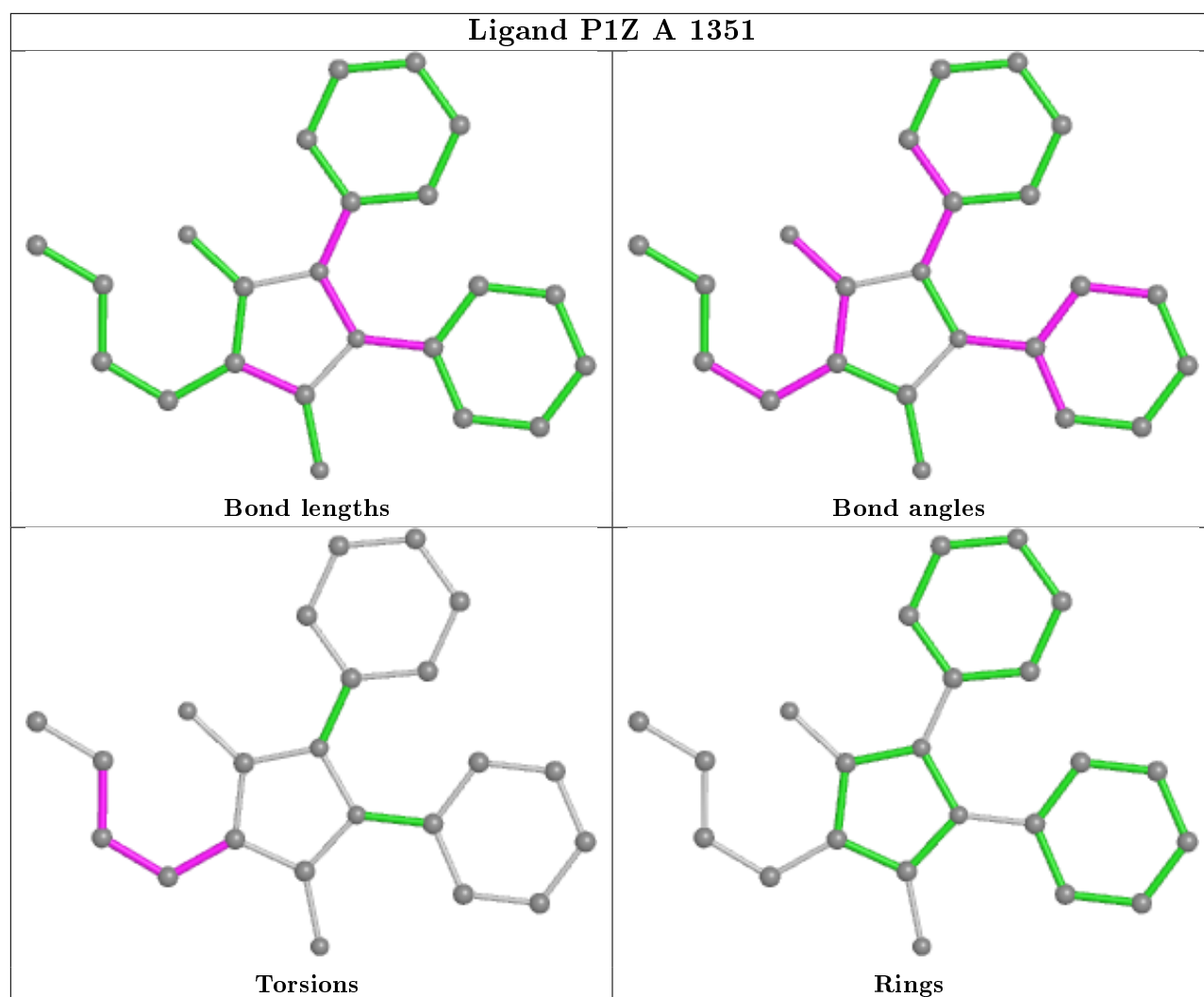












## 5.7 Other polymers [i](#)

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	348/357 (97%)	-0.17	7 (2%) 65 64	2, 7, 22, 47	0
1	B	355/357 (99%)	-0.06	9 (2%) 57 56	2, 7, 26, 47	0
All	All	703/714 (98%)	-0.11	16 (2%) 60 59	2, 7, 23, 47	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ALA	9.5
1	A	349	ILE	5.3
1	B	151	THR	4.8
1	B	153	GLY	4.8
1	B	154	SER	4.6
1	A	151	THR	3.9
1	A	271	PRO	2.8
1	A	154	SER	2.6
1	B	354	TYR	2.6
1	A	88	THR	2.5
1	B	349	ILE	2.5
1	B	33	ASN	2.4
1	A	346	SER	2.2
1	A	150	ILE	2.2
1	B	352	ASN	2.1
1	B	179	GLY	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

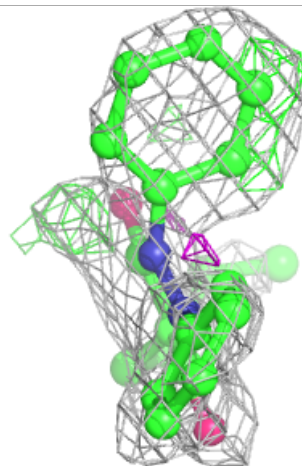
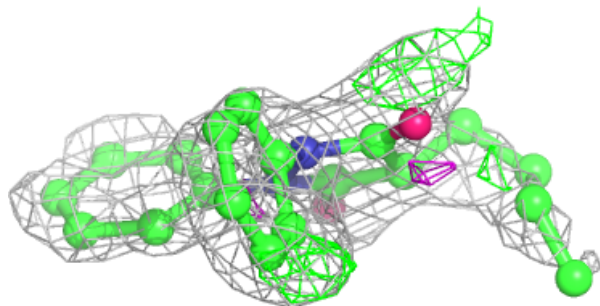
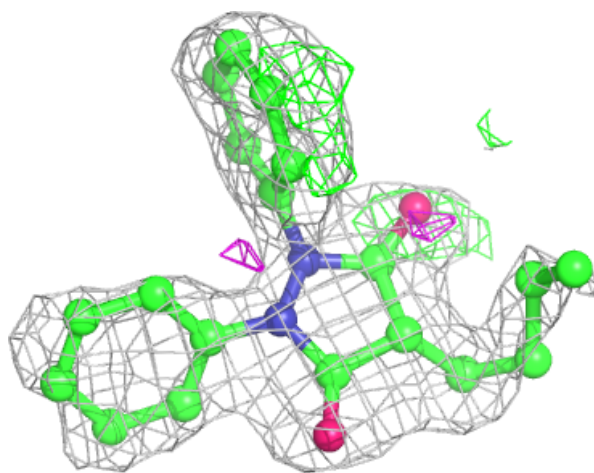
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	LMR	B	1362	9/9	0.77	0.20	45,48,52,54	0
7	NA	B	1364	1/1	0.79	0.24	50,50,50,50	0
3	P1Z	A	1353	23/23	0.80	0.23	22,28,37,39	22
3	P1Z	B	1357	23/23	0.85	0.22	13,16,22,26	23
3	P1Z	B	1358	23/23	0.85	0.25	12,18,24,28	23
3	P1Z	B	1359	23/23	0.87	0.23	15,27,38,44	23
3	P1Z	A	1352	23/23	0.89	0.24	12,17,37,48	23
3	P1Z	B	1356	23/23	0.89	0.17	9,17,21,24	0
4	PO4	A	1355	5/5	0.90	0.31	20,24,36,46	5
3	P1Z	A	1351	23/23	0.91	0.15	9,17,32,34	0
4	PO4	A	1354	5/5	0.93	0.27	16,18,30,50	5
4	PO4	B	1360	5/5	0.94	0.26	15,16,27,43	5
4	PO4	B	1361	5/5	0.95	0.27	16,17,27,45	5
4	PO4	A	1356	5/5	0.95	0.16	34,35,42,46	5
2	NAP	A	1350	48/48	0.96	0.16	9,14,19,24	0
2	NAP	B	1355	48/48	0.96	0.16	9,14,19,21	0
6	CL	B	1363	1/1	0.97	0.16	43,43,43,43	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 P1Z A 1353:**

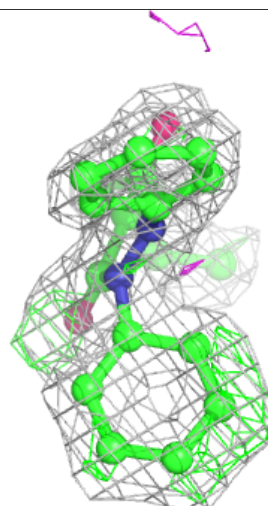
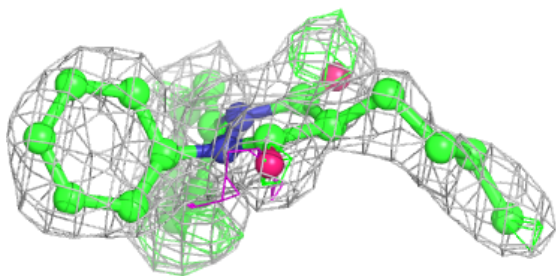
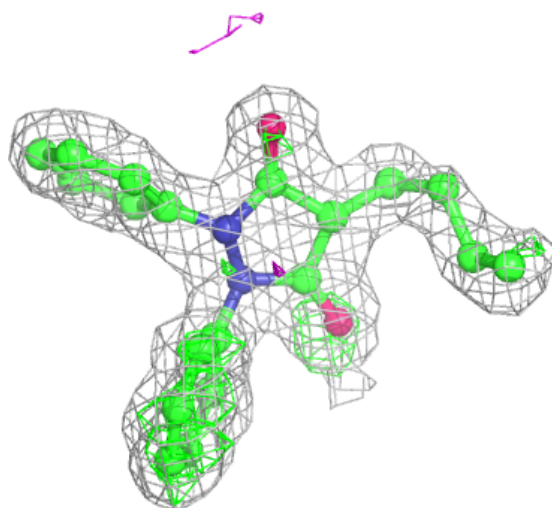
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





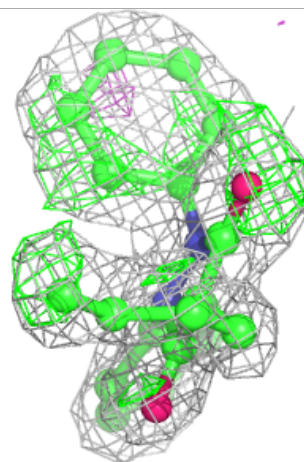
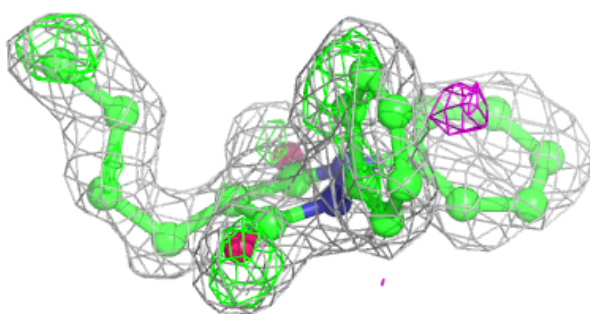
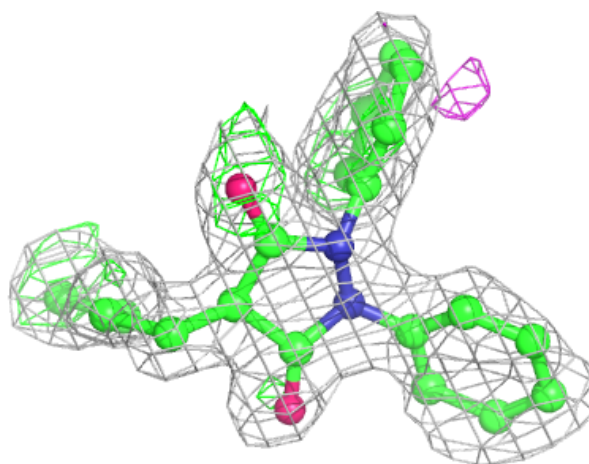
**Electron density around P1Z B 1357:**

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and green (positive)



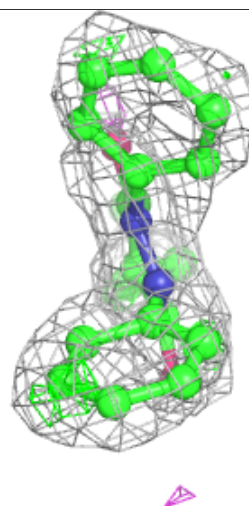
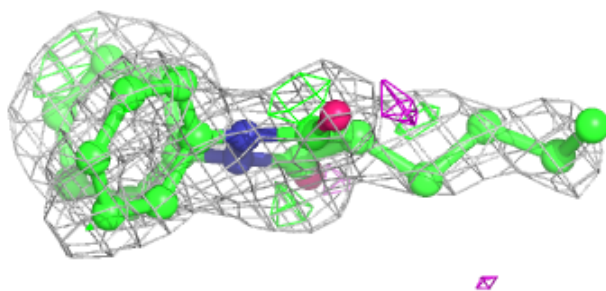
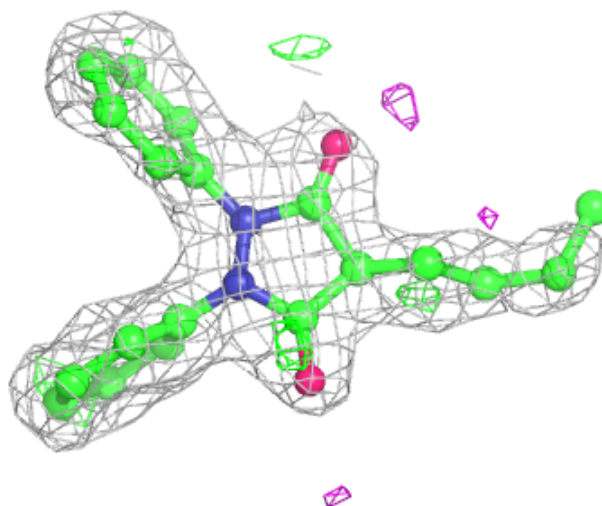
**Electron density around P1Z B 1358:**

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



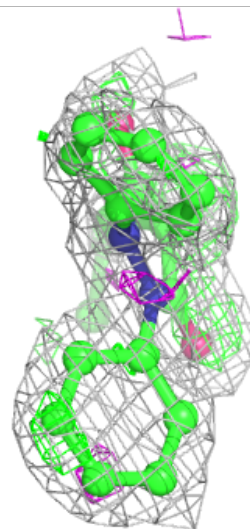
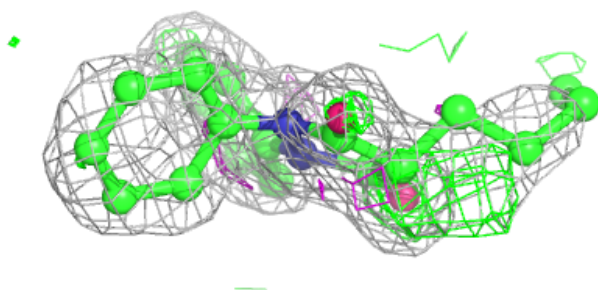
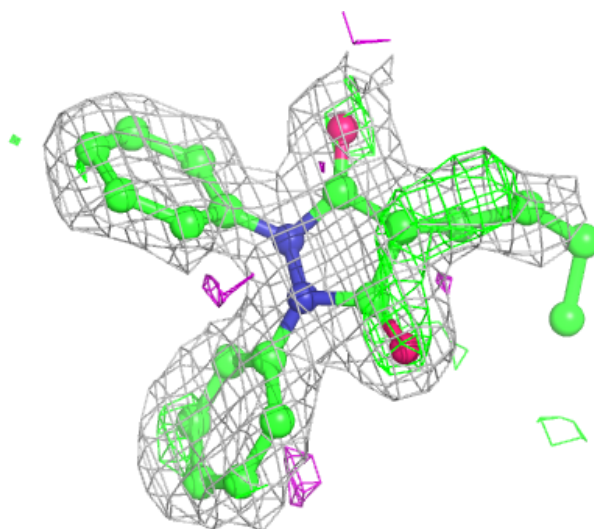
**Electron density around P1Z B 1359:**

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



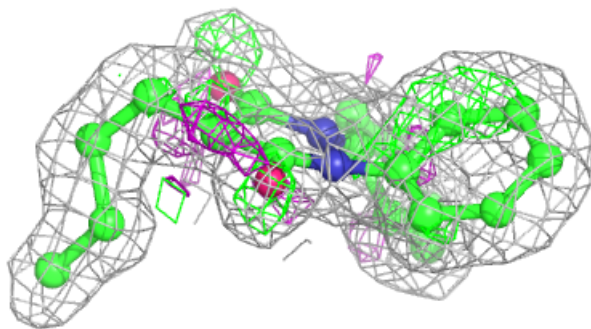
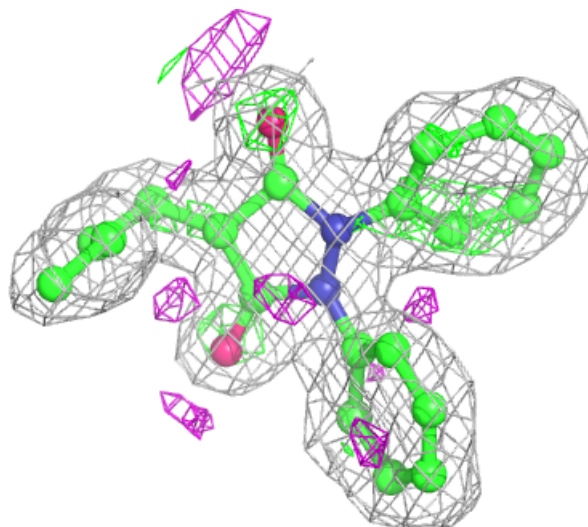
**Electron density around P1Z A 1352:**

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and green (positive)



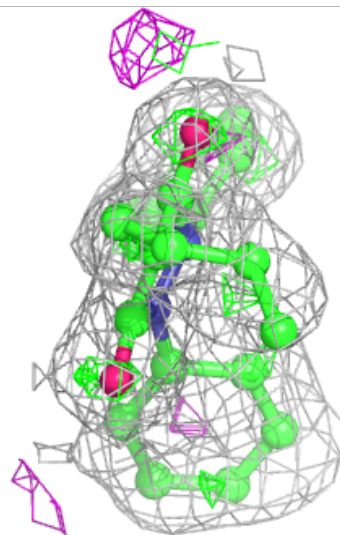
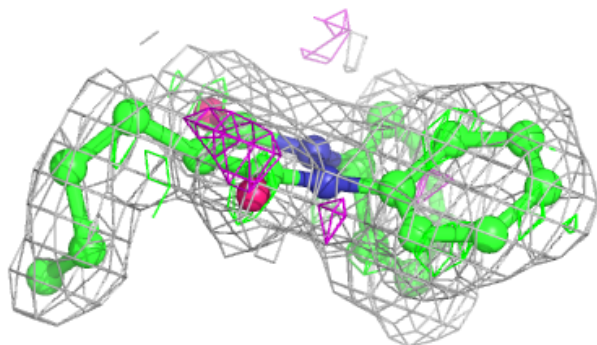
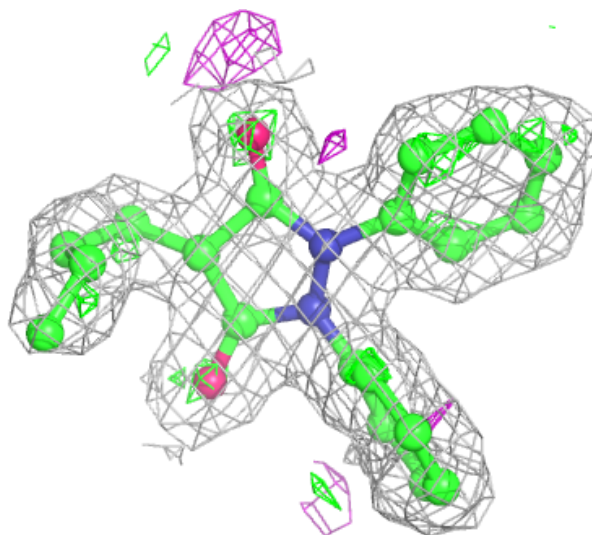
**Electron density around P1Z B 1356:**

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



**Electron density around P1Z A 1351:**

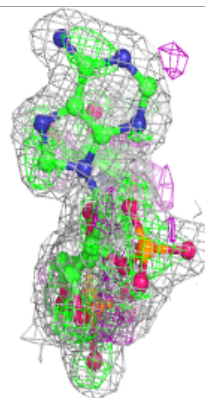
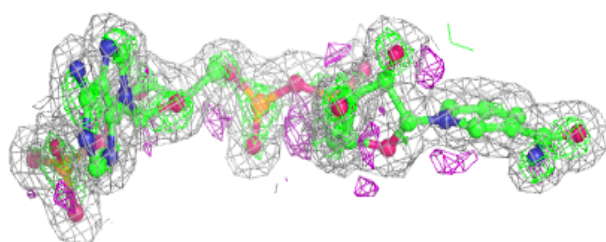
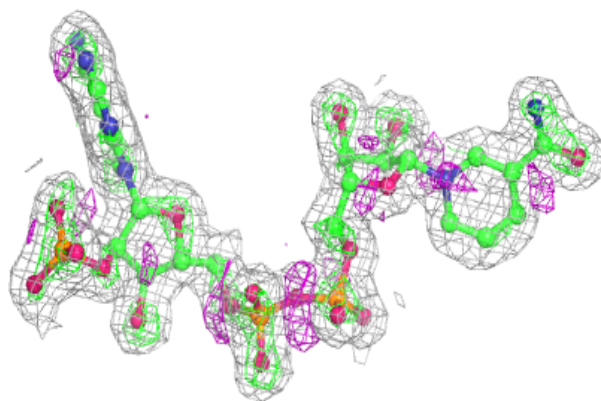
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



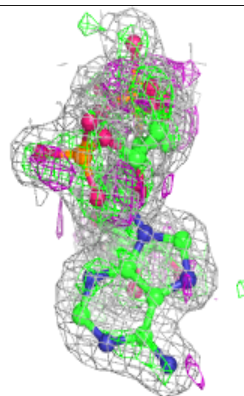
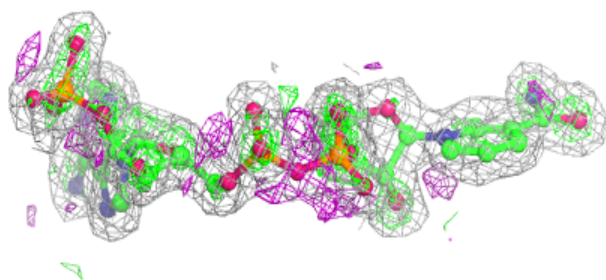
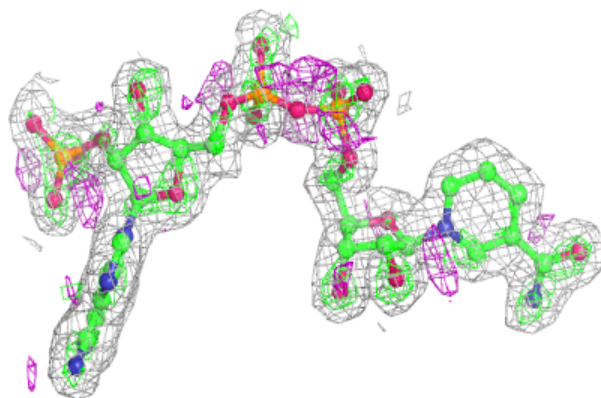


**Electron density around NAP A 1350:**

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

**Electron density around NAP B 1355:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.