



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:37 AM EDT

PDB ID : 8STD / pdb\_00008std  
Title : S127A variant of LarB, a carboxylase/hydrolase involved in synthesis of the cofactor for lactate racemase, in complex with authentic substrate NaAD and soaked with CS2  
Authors : Chatterjee, S.; Rankin, J.A.; Hu, J.; Hausinger, R.P.  
Deposited on : 2023-05-10  
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

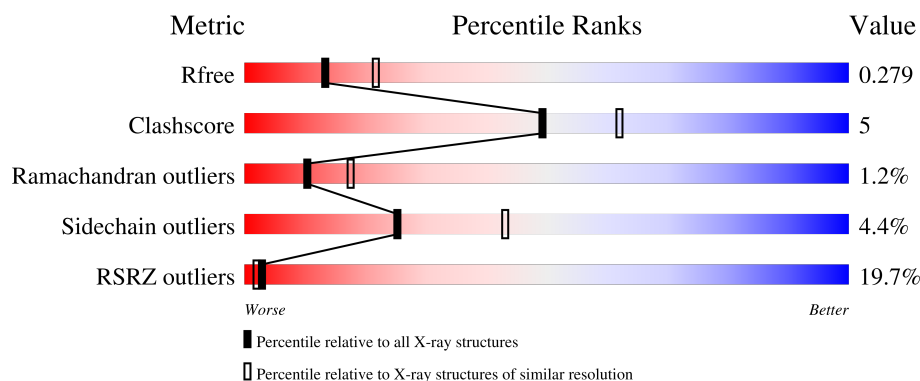
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	256	
1	B	256	
1	C	256	
1	D	256	

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Mol	Chain	Length	Quality of chain
1	E	256	<div><div></div><div>21%</div><div></div><div>74%</div><div></div><div>9%</div><div></div><div>15%</div></div>
1	F	256	<div><div></div><div>24%</div><div></div><div>65%</div><div></div><div>12%</div><div></div><div>23%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8620 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 Pyridinium-3,5-biscarboxylic acid mononucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	6	0
			1435	906	246	274	9			
1	B	202	Total	C	N	O	S	0	1	0
			1406	891	242	265	8			
1	C	202	Total	C	N	O	S	0	0	0
			1405	895	238	265	7			
1	D	204	Total	C	N	O	S	0	0	0
			1387	877	241	261	8			
1	E	217	Total	C	N	O	S	0	0	0
			1448	916	250	276	6			
1	F	198	Total	C	N	O	S	0	0	0
			1320	836	225	251	8			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	SER	conflict	UNP F9UST0
A	247	ALA	-	expression tag	UNP F9UST0
A	248	SER	-	expression tag	UNP F9UST0
A	249	TRP	-	expression tag	UNP F9UST0
A	250	SER	-	expression tag	UNP F9UST0
A	251	HIS	-	expression tag	UNP F9UST0
A	252	PRO	-	expression tag	UNP F9UST0
A	253	GLN	-	expression tag	UNP F9UST0
A	254	PHE	-	expression tag	UNP F9UST0
A	255	GLU	-	expression tag	UNP F9UST0
A	256	LYS	-	expression tag	UNP F9UST0
B	127	ALA	SER	conflict	UNP F9UST0
B	247	ALA	-	expression tag	UNP F9UST0
B	248	SER	-	expression tag	UNP F9UST0
B	249	TRP	-	expression tag	UNP F9UST0
B	250	SER	-	expression tag	UNP F9UST0
B	251	HIS	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	252	PRO	-	expression tag	UNP F9UST0
B	253	GLN	-	expression tag	UNP F9UST0
B	254	PHE	-	expression tag	UNP F9UST0
B	255	GLU	-	expression tag	UNP F9UST0
B	256	LYS	-	expression tag	UNP F9UST0
C	127	ALA	SER	conflict	UNP F9UST0
C	247	ALA	-	expression tag	UNP F9UST0
C	248	SER	-	expression tag	UNP F9UST0
C	249	TRP	-	expression tag	UNP F9UST0
C	250	SER	-	expression tag	UNP F9UST0
C	251	HIS	-	expression tag	UNP F9UST0
C	252	PRO	-	expression tag	UNP F9UST0
C	253	GLN	-	expression tag	UNP F9UST0
C	254	PHE	-	expression tag	UNP F9UST0
C	255	GLU	-	expression tag	UNP F9UST0
C	256	LYS	-	expression tag	UNP F9UST0
D	127	ALA	SER	conflict	UNP F9UST0
D	247	ALA	-	expression tag	UNP F9UST0
D	248	SER	-	expression tag	UNP F9UST0
D	249	TRP	-	expression tag	UNP F9UST0
D	250	SER	-	expression tag	UNP F9UST0
D	251	HIS	-	expression tag	UNP F9UST0
D	252	PRO	-	expression tag	UNP F9UST0
D	253	GLN	-	expression tag	UNP F9UST0
D	254	PHE	-	expression tag	UNP F9UST0
D	255	GLU	-	expression tag	UNP F9UST0
D	256	LYS	-	expression tag	UNP F9UST0
E	127	ALA	SER	conflict	UNP F9UST0
E	247	ALA	-	expression tag	UNP F9UST0
E	248	SER	-	expression tag	UNP F9UST0
E	249	TRP	-	expression tag	UNP F9UST0
E	250	SER	-	expression tag	UNP F9UST0
E	251	HIS	-	expression tag	UNP F9UST0
E	252	PRO	-	expression tag	UNP F9UST0
E	253	GLN	-	expression tag	UNP F9UST0
E	254	PHE	-	expression tag	UNP F9UST0
E	255	GLU	-	expression tag	UNP F9UST0
E	256	LYS	-	expression tag	UNP F9UST0
F	127	ALA	SER	conflict	UNP F9UST0
F	247	ALA	-	expression tag	UNP F9UST0
F	248	SER	-	expression tag	UNP F9UST0
F	249	TRP	-	expression tag	UNP F9UST0

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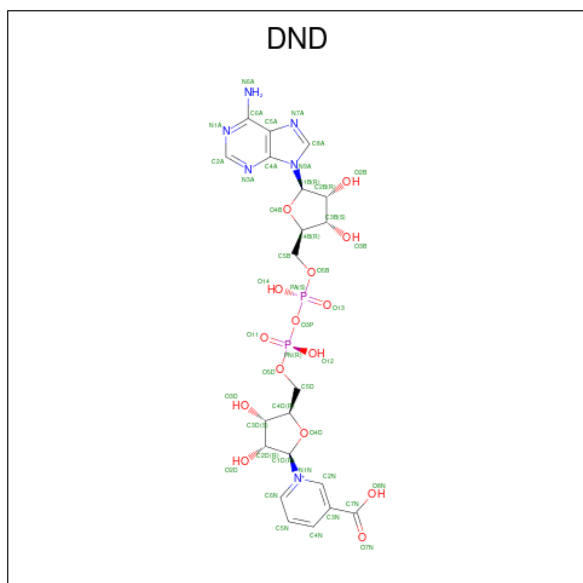
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Chain	Residue	Modelled	Actual	Comment	Reference
F	250	SER	-	expression tag	UNP F9UST0
F	251	HIS	-	expression tag	UNP F9UST0
F	252	PRO	-	expression tag	UNP F9UST0
F	253	GLN	-	expression tag	UNP F9UST0
F	254	PHE	-	expression tag	UNP F9UST0
F	255	GLU	-	expression tag	UNP F9UST0
F	256	LYS	-	expression tag	UNP F9UST0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is NICOTINIC ACID ADENINE DINUCLEOTIDE (CCD ID: DND) (formula:  $C_{21}H_{27}N_6O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).

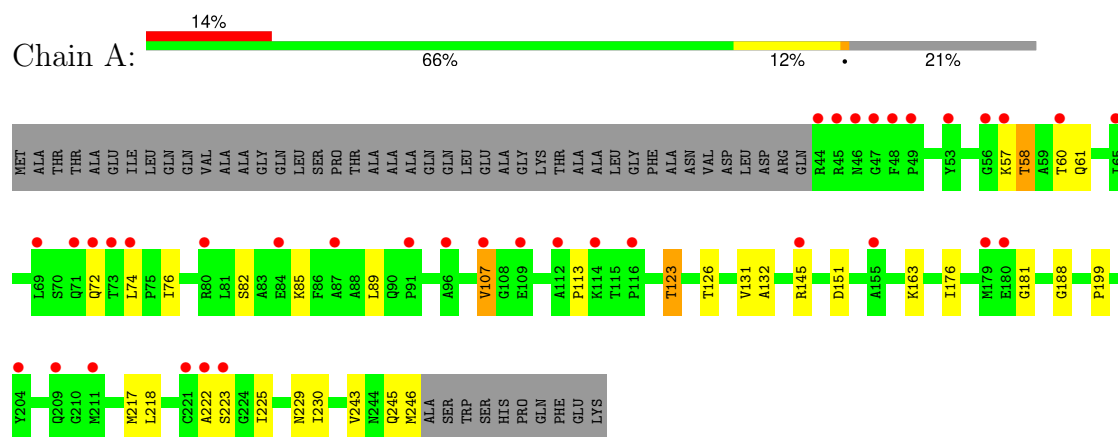


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	B	1	Total	C	N	O	P	0	0
			26	11	1	12	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	D	1	Total	C	N	O	P	0	0
			26	11	1	12	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	F	1	Total	C	N	O	P	0	0
			26	11	1	12	2		

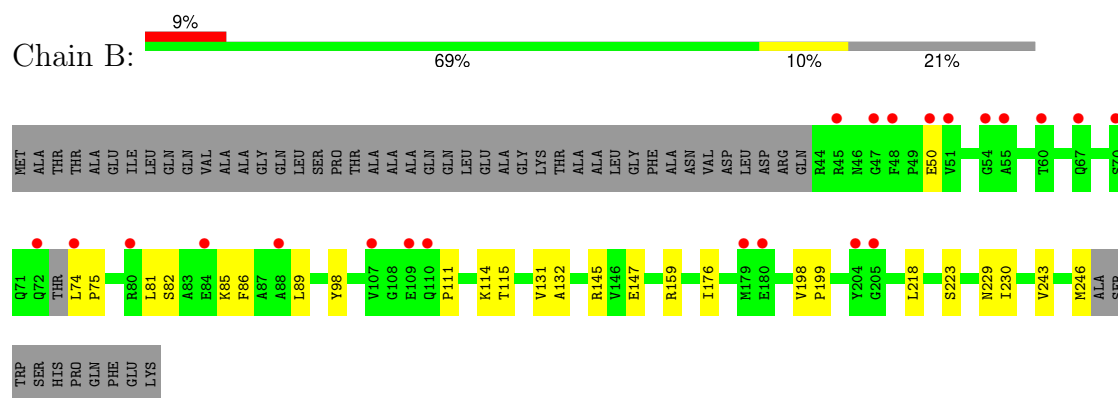
### 3 Residue-property plots

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.

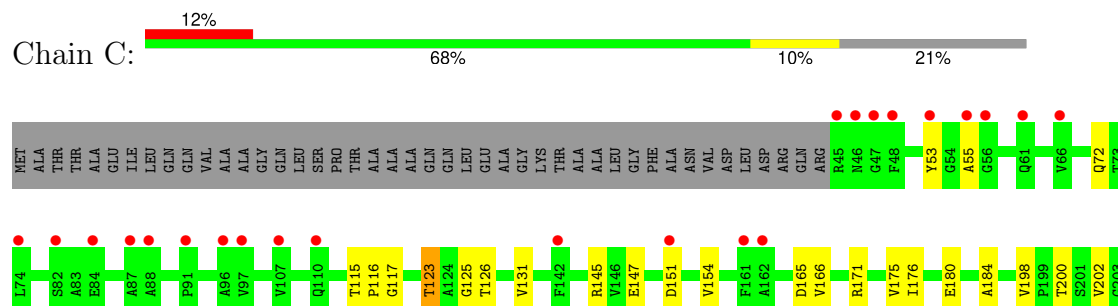
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



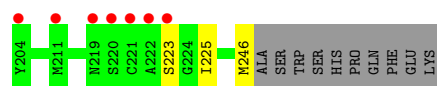
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



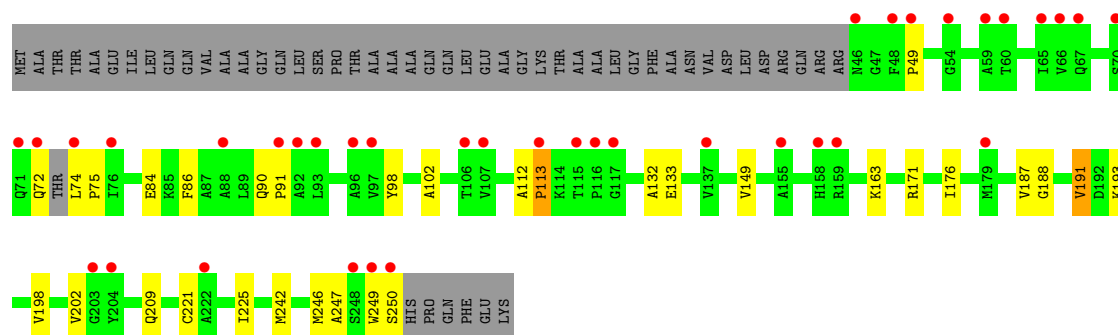
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



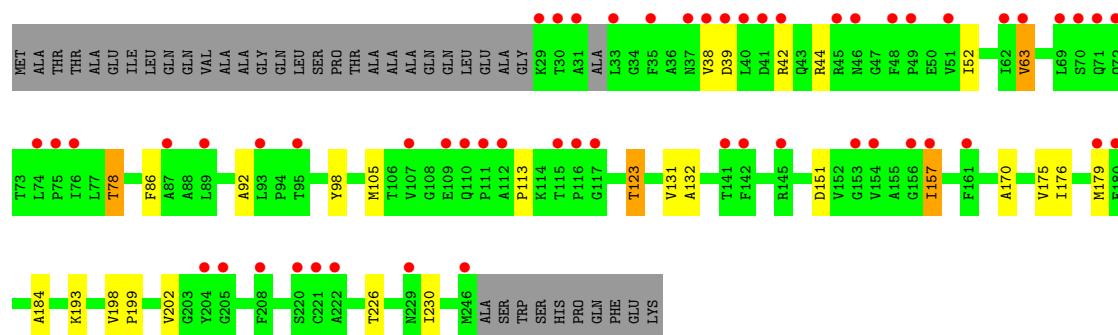
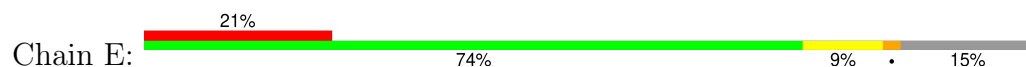




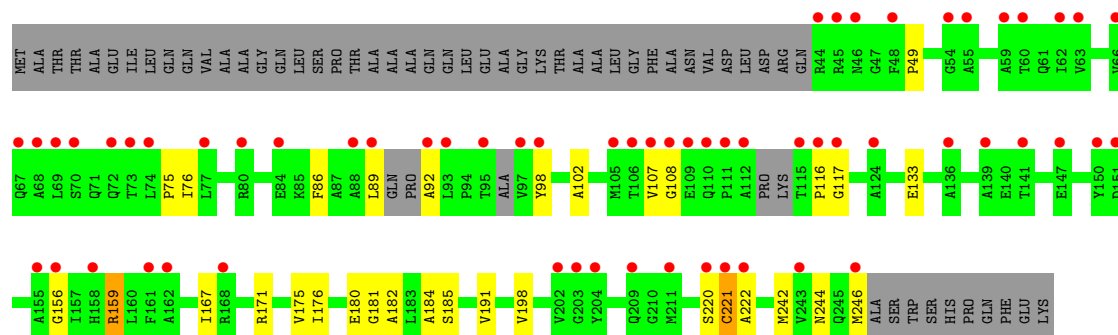
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.84Å 118.84Å 211.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.96 – 2.65 78.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (78.96-2.65) 99.4 (78.96-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, $R_{free}$	0.242 , 0.273 0.244 , 0.279	Depositor DCC
$R_{free}$ test set	2245 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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: DND, 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	0.16	0/1460	0.38	0/1999
1	B	0.19	0/1425	0.42	0/1946
1	C	0.23	0/1427	0.45	0/1955
1	D	0.19	0/1409	0.42	0/1931
1	E	0.15	0/1470	0.34	0/2019
1	F	0.19	0/1335	0.38	0/1826
All	All	0.19	0/8526	0.40	0/11676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1435	0	1401	19	0
1	B	1406	0	1408	15	0
1	C	1405	0	1400	18	0
1	D	1387	0	1325	18	0
1	E	1448	0	1353	14	0
1	F	1320	0	1259	16	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	44	0	24	1	0
3	B	26	0	12	0	0
3	C	44	0	25	2	0
3	D	26	0	12	0	0
3	E	44	0	24	1	0
3	F	26	0	12	0	0
All	All	8620	0	8255	91	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 (91) 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:E:123:THR:HG22	1:E:151:ASP:H	1.39	0.88
1:C:123:THR:HG22	1:C:151:ASP:H	1.36	0.86
1:A:123:THR:HG22	1:A:151:ASP:H	1.39	0.84
1:F:156:GLY:O	1:F:159:ARG:HG3	1.83	0.78
1:A:76:ILE:HB	1:A:107:VAL:HG13	1.65	0.77
1:F:221:CYS:SG	1:F:222:ALA:N	2.60	0.75
1:C:171:ARG:NH1	1:D:247:ALA:O	2.22	0.73
1:A:58:THR:HG22	1:A:61:GLN:HG3	1.72	0.71
1:A:199:PRO:HD3	1:A:217:MET:HE1	1.76	0.68
1:C:116:PRO:HA	1:C:145:ARG:HH21	1.58	0.67
1:C:125:GLY:HA3	3:C:303:DND:H3	1.80	0.63
1:C:126:THR:HG23	1:C:151:ASP:OD2	2.00	0.62
1:F:76:ILE:H	1:F:107:VAL:HG22	1.66	0.61
1:A:199:PRO:HG2	1:A:230:ILE:HA	1.83	0.60
1:C:126:THR:CG2	1:C:151:ASP:OD2	2.49	0.60
1:A:58:THR:HG23	1:A:60:THR:H	1.67	0.58
1:A:57:LYS:O	1:A:85:LYS:NZ	2.33	0.57
1:E:170:ALA:O	1:E:193:LYS:HD3	2.05	0.56
1:F:49:PRO:HB3	1:F:75:PRO:HD2	1.87	0.56
1:E:63:VAL:HG21	1:E:92:ALA:HB3	1.89	0.54
1:D:187:VAL:O	1:D:191:VAL:HG13	2.09	0.53
1:E:78:THR:HG21	1:E:105:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PRO:CD	1:A:217:MET:HE1	2.37	0.53
1:B:111:PRO:HG2	1:D:250:SER:HA	1.89	0.53
1:B:86:PHE:CZ	1:B:98:TYR:HB2	2.43	0.53
1:A:229[A]:ASN:OD1	1:A:230:ILE:N	2.42	0.52
1:B:81:LEU:HA	1:B:85[B]:LYS:HE2	1.91	0.52
1:B:82:SER:OG	1:B:85[B]:LYS:HG2	2.09	0.52
1:D:132:ALA:HA	1:D:176:ILE:HD13	1.92	0.52
1:A:132:ALA:HA	1:A:176:ILE:HD13	1.92	0.51
1:E:52:ILE:HB	1:E:78:THR:HB	1.92	0.51
1:F:176:ILE:HG12	1:F:198:VAL:HB	1.93	0.50
1:F:86:PHE:CE1	1:F:98:TYR:HB2	2.47	0.49
1:B:145:ARG:HH12	1:C:165:ASP:HB3	1.77	0.49
1:D:191:VAL:HG23	1:D:193:LYS:H	1.76	0.49
1:F:89:LEU:HA	1:F:92:ALA:HB3	1.96	0.48
1:A:113:PRO:HB3	1:A:145:ARG:HG3	1.96	0.48
1:F:180:GLU:O	1:F:182:ALA:N	2.47	0.48
1:B:132:ALA:HA	1:B:176:ILE:HD13	1.94	0.48
1:A:229[A]:ASN:HB2	1:B:218:LEU:O	2.14	0.47
1:D:188:GLY:HA3	1:D:225:ILE:HD11	1.96	0.47
1:A:222[B]:ALA:O	1:A:223[B]:SER:OG	2.26	0.47
1:C:176:ILE:HG12	1:C:198:VAL:HB	1.96	0.47
1:F:175:VAL:HG11	1:F:184:ALA:HA	1.96	0.47
1:B:176:ILE:HG12	1:B:198:VAL:HB	1.96	0.47
1:E:175:VAL:HG11	1:E:184:ALA:HA	1.97	0.47
1:F:167:ILE:HG22	1:F:191:VAL:HG11	1.96	0.46
1:D:149:VAL:HG13	1:D:163:LYS:HD2	1.97	0.46
1:D:72:GLN:O	1:D:74:LEU:N	2.49	0.46
1:B:199:PRO:HG2	1:B:230:ILE:HA	1.99	0.45
1:D:102:ALA:HB2	1:D:133:GLU:HB3	1.98	0.45
1:C:223:SER:C	1:C:225:ILE:H	2.25	0.44
1:E:42:ARG:C	1:E:44:ARG:H	2.24	0.44
1:C:147:GLU:HG2	1:C:166:VAL:HG11	1.99	0.44
1:B:114:LYS:HE2	1:D:250:SER:C	2.43	0.44
1:B:145:ARG:NH2	1:C:166:VAL:HG22	2.32	0.44
1:C:246:MET:HE1	1:D:171:ARG:HB3	1.99	0.44
1:A:126:THR:N	3:A:303:DND:O11	2.50	0.44
1:E:176:ILE:HG12	1:E:198:VAL:HB	1.98	0.44
1:C:147:GLU:HG2	1:C:166:VAL:CG1	2.48	0.44
1:F:102:ALA:HB2	1:F:133:GLU:HB3	2.00	0.44
1:F:171:ARG:NH1	1:F:244:ASN:O	2.51	0.44
1:E:86:PHE:CZ	1:E:98:TYR:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:MET:O	1:F:246:MET:HG3	2.18	0.44
1:E:199:PRO:HG2	1:E:230:ILE:HA	2.00	0.43
1:F:185:SER:HB3	1:F:221:CYS:SG	2.58	0.43
1:E:179:MET:HE2	3:E:302:DND:O4D	2.18	0.43
1:C:126:THR:HG22	1:C:151:ASP:OD2	2.18	0.43
1:A:243:VAL:HG13	1:B:243:VAL:HG13	2.01	0.43
1:E:157:ILE:H	1:E:157:ILE:HG13	1.58	0.43
1:D:49:PRO:HB3	1:D:75:PRO:O	2.18	0.43
1:D:176:ILE:HG12	1:D:198:VAL:HB	2.01	0.43
1:D:90:GLN:N	1:D:91:PRO:HD2	2.34	0.42
1:C:175:VAL:HG11	1:C:184:ALA:HA	2.00	0.42
1:D:221:CYS:HA	1:D:225:ILE:HB	2.00	0.42
1:B:145:ARG:NH1	1:C:165:ASP:HB3	2.34	0.42
1:A:218:LEU:O	1:B:229:ASN:HB2	2.19	0.42
1:C:200:THR:OG1	1:C:202:VAL:HG22	2.20	0.42
1:F:117:GLY:HA3	1:F:171:ARG:CD	2.50	0.41
1:D:112:ALA:O	1:D:113:PRO:C	2.63	0.41
1:C:53:TYR:CZ	1:C:55:ALA:HB3	2.55	0.41
1:E:78:THR:HG23	1:E:105:MET:HB3	2.03	0.41
1:A:217:MET:HE2	1:A:217:MET:HB2	1.91	0.41
1:B:74:LEU:HB3	1:B:75:PRO:CD	2.51	0.41
1:D:86:PHE:CZ	1:D:98:TYR:HB2	2.56	0.40
1:A:188:GLY:HA3	1:A:225:ILE:HD11	2.03	0.40
1:D:242:MET:O	1:D:246:MET:HG3	2.22	0.40
1:F:159:ARG:HG3	1:F:159:ARG:H	1.58	0.40
3:C:303:DND:H25	3:C:303:DND:H21	1.90	0.40
1:E:132:ALA:HA	1:E:176:ILE:HD13	2.02	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	207/256 (81%)	196 (95%)	8 (4%)	3 (1%)	9	14
1	B	199/256 (78%)	188 (94%)	10 (5%)	1 (0%)	24	39
1	C	200/256 (78%)	186 (93%)	12 (6%)	2 (1%)	12	20
1	D	200/256 (78%)	190 (95%)	8 (4%)	2 (1%)	12	20
1	E	213/256 (83%)	193 (91%)	17 (8%)	3 (1%)	9	14
1	F	190/256 (74%)	174 (92%)	12 (6%)	4 (2%)	5	9
All	All	1209/1536 (79%)	1127 (93%)	67 (6%)	15 (1%)	10	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	PRO
1	E	38	VAL
1	F	181	GLY
1	A	181	GLY
1	C	72	GLN
1	F	220	SER
1	A	74	LEU
1	F	116	PRO
1	B	223	SER
1	A	72	GLN
1	D	249	TRP
1	E	39	ASP
1	E	113	PRO
1	C	117	GLY
1	F	108	GLY

### 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	138/190 (73%)	129 (94%)	9 (6%)	15	27
1	B	137/190 (72%)	130 (95%)	7 (5%)	21	36
1	C	136/190 (72%)	131 (96%)	5 (4%)	30	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	126/190 (66%)	122 (97%)	4 (3%)	34	55
1	E	126/190 (66%)	119 (94%)	7 (6%)	19	32
1	F	119/190 (63%)	117 (98%)	2 (2%)	53	73
All	All	782/1140 (69%)	748 (96%)	34 (4%)	25	44

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

Mol	Chain	Res	Type
1	A	58	THR
1	A	82	SER
1	A	89	LEU
1	A	107	VAL
1	A	123	THR
1	A	131	VAL
1	A	163	LYS
1	A	245	GLN
1	A	246	MET
1	B	50	GLU
1	B	89	LEU
1	B	115	THR
1	B	131	VAL
1	B	147	GLU
1	B	159	ARG
1	B	246	MET
1	C	115	THR
1	C	123	THR
1	C	131	VAL
1	C	154	VAL
1	C	180	GLU
1	D	84	GLU
1	D	191	VAL
1	D	202	VAL
1	D	209	GLN
1	E	63	VAL
1	E	78	THR
1	E	123	THR
1	E	131	VAL
1	E	157	ILE
1	E	202	VAL
1	E	226	THR
1	F	159	ARG

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Mol	Chain	Res	Type
1	F	221	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	158	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	DND	A	303	2	46,48,48	2.74	15 (32%)	64,73,73	2.53	20 (31%)
3	DND	D	302	-	24,27,48	3.08	9 (37%)	33,41,73	2.10	8 (24%)
3	DND	C	303	2	46,48,48	2.86	16 (34%)	64,73,73	2.45	15 (23%)
3	DND	B	303	2	24,27,48	3.01	9 (37%)	33,41,73	2.08	8 (24%)
3	DND	F	302	2	24,27,48	3.05	9 (37%)	33,41,73	2.06	7 (21%)
3	DND	E	302	2	46,48,48	2.79	15 (32%)	64,73,73	2.50	16 (25%)

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	DND	A	303	2	-	9/30/62/62	0/5/5/5
3	DND	D	302	-	-	0/20/36/62	0/2/2/5
3	DND	C	303	2	-	4/30/62/62	0/5/5/5
3	DND	B	303	2	-	7/20/36/62	0/2/2/5
3	DND	F	302	2	-	7/20/36/62	0/2/2/5
3	DND	E	302	2	-	9/30/62/62	0/5/5/5

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	DND	O4D-C1D	8.59	1.52	1.40
3	D	302	DND	O4D-C1D	8.19	1.51	1.40
3	A	303	DND	O4D-C1D	8.18	1.51	1.40
3	B	303	DND	O4D-C1D	8.11	1.51	1.40
3	F	302	DND	O4D-C1D	8.07	1.51	1.40
3	E	302	DND	O4D-C1D	7.89	1.51	1.40
3	D	302	DND	PN-O3P	6.79	1.66	1.59
3	F	302	DND	PN-O3P	6.73	1.66	1.59
3	E	302	DND	PA-O3P	6.42	1.66	1.59
3	C	303	DND	PA-O3P	6.41	1.66	1.59
3	E	302	DND	PN-O3P	6.23	1.66	1.59
3	C	303	DND	PN-O3P	6.21	1.66	1.59
3	B	303	DND	PN-O3P	6.20	1.66	1.59
3	A	303	DND	PN-O3P	5.84	1.65	1.59
3	A	303	DND	PA-O3P	5.77	1.65	1.59
3	C	303	DND	C8A-N9A	-5.33	1.28	1.37
3	B	303	DND	PA-O13	5.30	1.66	1.50
3	D	302	DND	PA-O13	5.29	1.66	1.50
3	E	302	DND	C8A-N9A	-5.27	1.28	1.37
3	A	303	DND	C8A-N9A	-5.26	1.28	1.37
3	F	302	DND	PA-O13	5.20	1.66	1.50
3	C	303	DND	C6A-N6A	4.86	1.46	1.34
3	E	302	DND	C4A-N9A	-4.85	1.27	1.37
3	A	303	DND	C6A-N6A	4.85	1.46	1.34
3	E	302	DND	C6A-N6A	4.80	1.46	1.34
3	D	302	DND	PN-O11	4.77	1.67	1.50
3	C	303	DND	PA-O13	4.77	1.67	1.50
3	C	303	DND	C4A-N9A	-4.74	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302	DND	PN-O11	4.74	1.67	1.50
3	B	303	DND	PN-O11	4.73	1.67	1.50
3	A	303	DND	PA-O13	4.72	1.67	1.50
3	E	302	DND	PA-O13	4.71	1.67	1.50
3	A	303	DND	C4A-N9A	-4.49	1.28	1.37
3	A	303	DND	O4B-C1B	4.26	1.51	1.42
3	C	303	DND	O4B-C1B	4.22	1.51	1.42
3	E	302	DND	O4B-C1B	4.10	1.51	1.42
3	B	303	DND	PA-O14	3.38	1.67	1.54
3	D	302	DND	PA-O14	3.36	1.67	1.54
3	F	302	DND	PA-O14	3.33	1.67	1.54
3	C	303	DND	O4D-C4D	3.10	1.51	1.45
3	C	303	DND	O4B-C4B	3.07	1.51	1.45
3	C	303	DND	C2D-C3D	-2.99	1.45	1.53
3	E	302	DND	O4B-C4B	2.96	1.51	1.45
3	A	303	DND	O4B-C4B	2.95	1.51	1.45
3	A	303	DND	O4D-C4D	2.90	1.51	1.45
3	D	302	DND	C2D-C3D	-2.88	1.45	1.53
3	E	302	DND	C2B-C3B	-2.88	1.45	1.53
3	F	302	DND	C2D-C3D	-2.84	1.45	1.53
3	B	303	DND	C2D-C3D	-2.83	1.45	1.53
3	C	303	DND	C2B-C3B	-2.83	1.45	1.53
3	B	303	DND	O4D-C4D	2.82	1.51	1.45
3	F	302	DND	O4D-C4D	2.79	1.51	1.45
3	A	303	DND	C2D-C3D	-2.77	1.45	1.53
3	E	302	DND	C2D-C3D	-2.73	1.46	1.53
3	E	302	DND	O4D-C4D	2.73	1.51	1.45
3	D	302	DND	O4D-C4D	2.71	1.51	1.45
3	C	303	DND	PN-O12	2.59	1.67	1.55
3	A	303	DND	PN-O12	2.57	1.67	1.55
3	E	302	DND	PN-O12	2.54	1.67	1.55
3	A	303	DND	C2B-C3B	-2.54	1.46	1.53
3	C	303	DND	C8A-N7A	2.50	1.36	1.31
3	E	302	DND	C8A-N7A	2.42	1.36	1.31
3	B	303	DND	C3N-C7N	2.39	1.54	1.49
3	A	303	DND	C8A-N7A	2.37	1.36	1.31
3	A	303	DND	C3N-C7N	2.35	1.54	1.49
3	C	303	DND	C3N-C7N	2.30	1.54	1.49
3	B	303	DND	PA-O5B	-2.28	1.46	1.54
3	F	302	DND	PA-O5B	-2.25	1.46	1.54
3	F	302	DND	C3N-C7N	2.23	1.54	1.49
3	D	302	DND	PA-O5B	-2.23	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	DND	C3N-C7N	2.19	1.54	1.49
3	D	302	DND	C3N-C7N	2.15	1.54	1.49
3	C	303	DND	C3D-C4D	-2.03	1.47	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	DND	C4A-N9A-C8A	9.32	115.53	105.74
3	C	303	DND	C4A-N9A-C8A	8.98	115.17	105.74
3	A	303	DND	C4A-N9A-C8A	8.57	114.74	105.74
3	A	303	DND	C4D-O4D-C1D	-8.10	102.51	109.92
3	E	302	DND	C4D-O4D-C1D	-7.29	103.25	109.92
3	B	303	DND	C4D-O4D-C1D	-7.27	103.27	109.92
3	D	302	DND	C4D-O4D-C1D	-7.03	103.48	109.92
3	F	302	DND	C4D-O4D-C1D	-6.91	103.60	109.92
3	C	303	DND	C4D-O4D-C1D	-6.64	103.85	109.92
3	E	302	DND	O8N-C7N-O7N	6.13	136.53	123.35
3	D	302	DND	O8N-C7N-O7N	6.09	136.45	123.35
3	F	302	DND	O8N-C7N-O7N	6.04	136.33	123.35
3	A	303	DND	O8N-C7N-O7N	5.99	136.24	123.35
3	C	303	DND	O8N-C7N-O7N	5.96	136.16	123.35
3	E	302	DND	N1A-C2A-N3A	-5.89	119.67	128.58
3	B	303	DND	O8N-C7N-O7N	5.72	135.66	123.35
3	A	303	DND	N1A-C2A-N3A	-5.71	119.94	128.58
3	C	303	DND	N1A-C2A-N3A	-5.67	119.99	128.58
3	E	302	DND	N9A-C8A-N7A	-5.55	106.06	113.94
3	C	303	DND	N9A-C8A-N7A	-5.33	106.37	113.94
3	A	303	DND	C5A-C4A-N3A	-5.13	119.65	126.72
3	A	303	DND	N9A-C8A-N7A	-4.89	107.00	113.94
3	C	303	DND	C5A-C4A-N3A	-4.83	120.06	126.72
3	E	302	DND	C5A-C4A-N3A	-4.42	120.63	126.72
3	A	303	DND	N3A-C4A-N9A	4.33	134.54	127.17
3	C	303	DND	N3A-C4A-N9A	3.94	133.87	127.17
3	C	303	DND	C4A-C5A-N7A	-3.84	106.19	110.58
3	E	302	DND	O7N-C7N-C3N	-3.80	111.49	121.46
3	D	302	DND	O7N-C7N-C3N	-3.79	111.53	121.46
3	E	302	DND	N3A-C4A-N9A	3.75	133.55	127.17
3	A	303	DND	O7N-C7N-C3N	-3.74	111.66	121.46
3	E	302	DND	C4A-C5A-N7A	-3.64	106.42	110.58
3	B	303	DND	O7N-C7N-C3N	-3.64	111.92	121.46
3	C	303	DND	O7N-C7N-C3N	-3.59	112.04	121.46
3	F	302	DND	O7N-C7N-C3N	-3.59	112.04	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	DND	C2A-N3A-C4A	3.47	120.31	111.83
3	A	303	DND	C4A-C5A-N7A	-3.43	106.66	110.58
3	C	303	DND	C2A-N3A-C4A	3.40	120.14	111.83
3	E	302	DND	C4B-O4B-C1B	-3.32	102.14	109.47
3	E	302	DND	C2A-N3A-C4A	3.28	119.83	111.83
3	A	303	DND	C4B-O4B-C1B	-3.08	102.67	109.47
3	A	303	DND	O4B-C1B-N9A	2.96	113.77	108.09
3	E	302	DND	C2D-C3D-C4D	2.81	108.05	102.61
3	A	303	DND	C2B-C3B-C4B	2.74	107.90	102.61
3	F	302	DND	C2D-C3D-C4D	2.73	107.88	102.61
3	A	303	DND	C1B-N9A-C8A	-2.68	121.14	127.09
3	C	303	DND	C6N-N1N-C2N	-2.66	119.62	121.88
3	C	303	DND	C4B-O4B-C1B	-2.64	103.64	109.47
3	B	303	DND	O14-PA-O3P	2.59	113.32	104.64
3	A	303	DND	C3B-C2B-C1B	2.56	106.31	101.46
3	E	302	DND	C4A-N9A-C1B	-2.47	120.86	126.63
3	D	302	DND	C2D-C3D-C4D	2.45	107.34	102.61
3	A	303	DND	C2D-C3D-C4D	2.41	107.27	102.61
3	D	302	DND	C6N-N1N-C2N	-2.41	119.83	121.88
3	C	303	DND	O14-PA-O13	-2.38	101.39	112.44
3	C	303	DND	O12-PN-O11	-2.34	101.56	112.44
3	B	303	DND	C2D-C3D-C4D	2.33	107.11	102.61
3	E	302	DND	O14-PA-O13	-2.33	101.63	112.44
3	D	302	DND	O12-PN-O11	-2.28	101.83	112.44
3	A	303	DND	O14-PA-O13	-2.23	102.06	112.44
3	F	302	DND	O12-PN-O11	-2.23	102.06	112.44
3	A	303	DND	C6N-N1N-C2N	-2.21	119.99	121.88
3	A	303	DND	O12-PN-O11	-2.20	102.21	112.44
3	B	303	DND	C6N-N1N-C2N	-2.19	120.01	121.88
3	F	302	DND	O14-PA-O3P	2.16	111.88	104.64
3	E	302	DND	O12-PN-O11	-2.15	102.45	112.44
3	D	302	DND	O5B-PA-O3P	2.11	111.72	104.64
3	B	303	DND	C5D-C4D-C3D	-2.10	107.67	115.21
3	B	303	DND	O12-PN-O11	-2.09	102.72	112.44
3	F	302	DND	C6N-N1N-C2N	-2.07	120.11	121.88
3	E	302	DND	O4B-C1B-N9A	2.03	111.99	108.09
3	A	303	DND	C6A-C5A-C4A	2.03	119.94	117.18
3	C	303	DND	C1B-N9A-C8A	-2.02	122.61	127.09
3	D	302	DND	O14-PA-O3P	2.01	111.38	104.64

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	DND	C5D-O5D-PN-O12
3	B	303	DND	PN-O3P-PA-O14
3	C	303	DND	O4D-C1D-N1N-C2N
3	F	302	DND	C5D-O5D-PN-O12
3	F	302	DND	C5D-O5D-PN-O3P
3	C	303	DND	C3B-C4B-C5B-O5B
3	A	303	DND	C4N-C3N-C7N-O8N
3	A	303	DND	C4N-C3N-C7N-O7N
3	C	303	DND	O4B-C4B-C5B-O5B
3	A	303	DND	O4B-C1B-N9A-C4A
3	A	303	DND	C2N-C3N-C7N-O8N
3	A	303	DND	C2N-C3N-C7N-O7N
3	E	302	DND	C4N-C3N-C7N-O8N
3	E	302	DND	C4N-C3N-C7N-O7N
3	E	302	DND	C2N-C3N-C7N-O7N
3	A	303	DND	O4B-C1B-N9A-C8A
3	F	302	DND	C4N-C3N-C7N-O8N
3	E	302	DND	C2B-C1B-N9A-C8A
3	A	303	DND	PA-O3P-PN-O11
3	E	302	DND	PA-O3P-PN-O11
3	F	302	DND	C4N-C3N-C7N-O7N
3	E	302	DND	C2N-C3N-C7N-O8N
3	F	302	DND	C2N-C3N-C7N-O8N
3	B	303	DND	C5D-O5D-PN-O3P
3	F	302	DND	C2N-C3N-C7N-O7N
3	E	302	DND	C2B-C1B-N9A-C4A
3	C	303	DND	C4B-C5B-O5B-PA
3	B	303	DND	C3D-C4D-C5D-O5D
3	B	303	DND	PN-O3P-PA-O5B
3	A	303	DND	C2B-C1B-N9A-C8A
3	E	302	DND	PN-O3P-PA-O14
3	B	303	DND	O4D-C4D-C5D-O5D
3	E	302	DND	O4B-C1B-N9A-C8A
3	B	303	DND	PA-O3P-PN-O12
3	F	302	DND	PA-O3P-PN-O12
3	A	303	DND	O4D-C4D-C5D-O5D

There are no ring outliers.

3 monomers are involved in 4 short contacts:

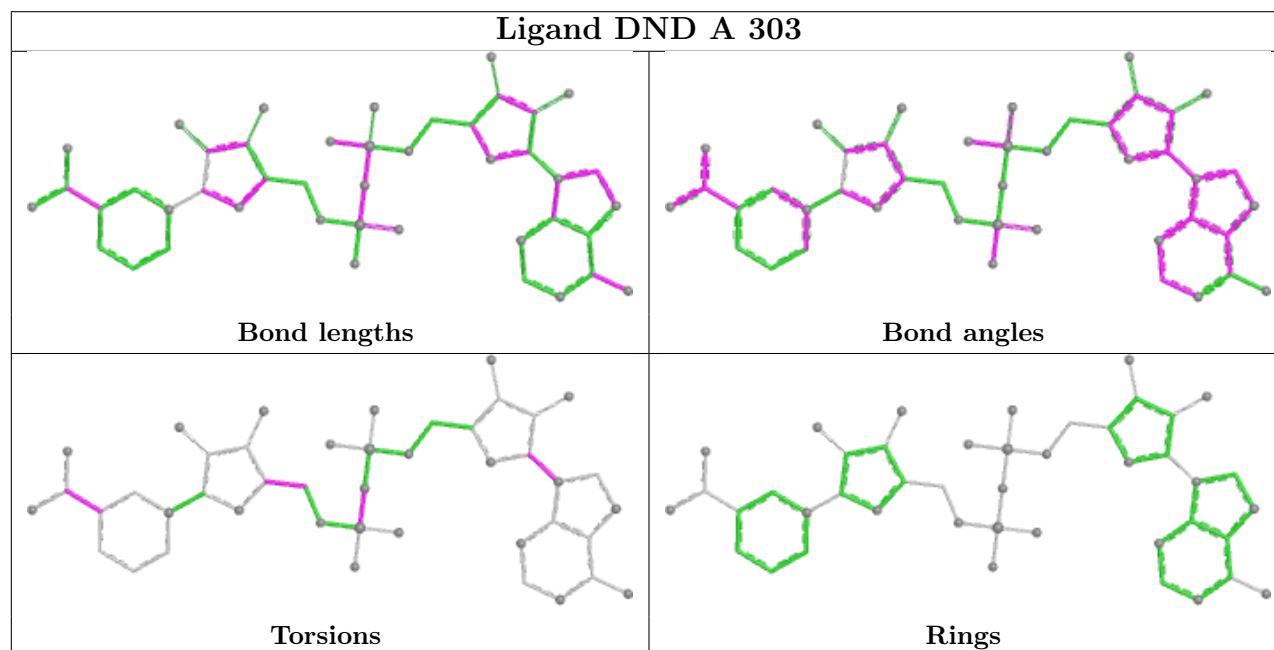
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	DND	1	0
3	C	303	DND	2	0

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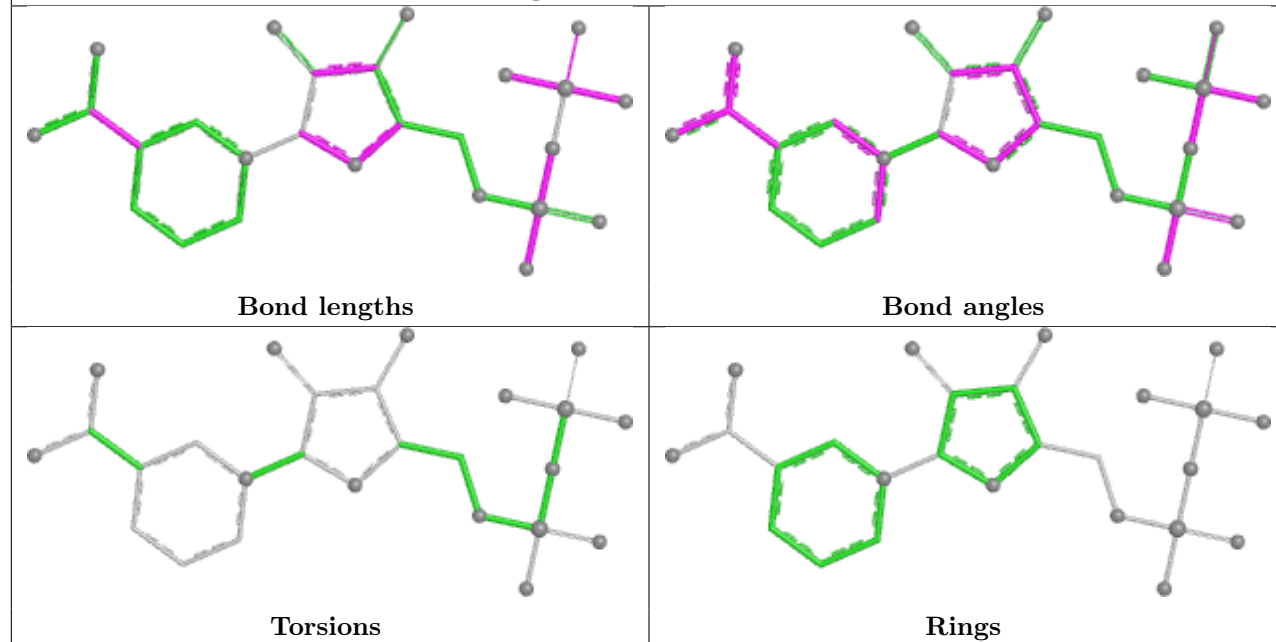
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	DND	1	0

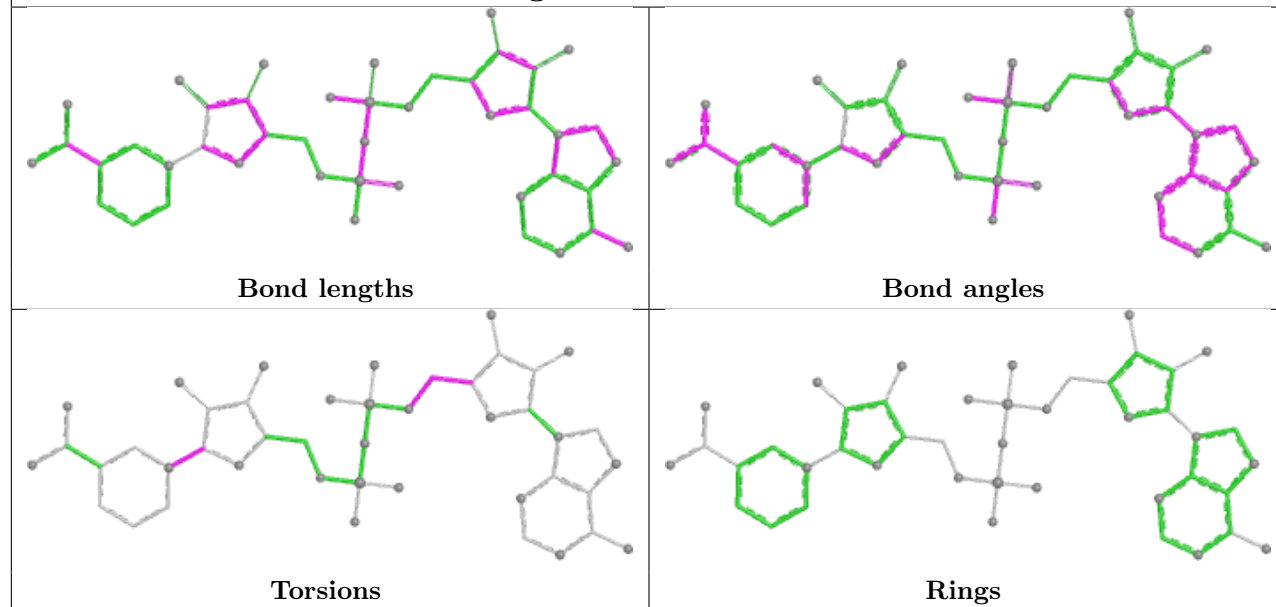
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



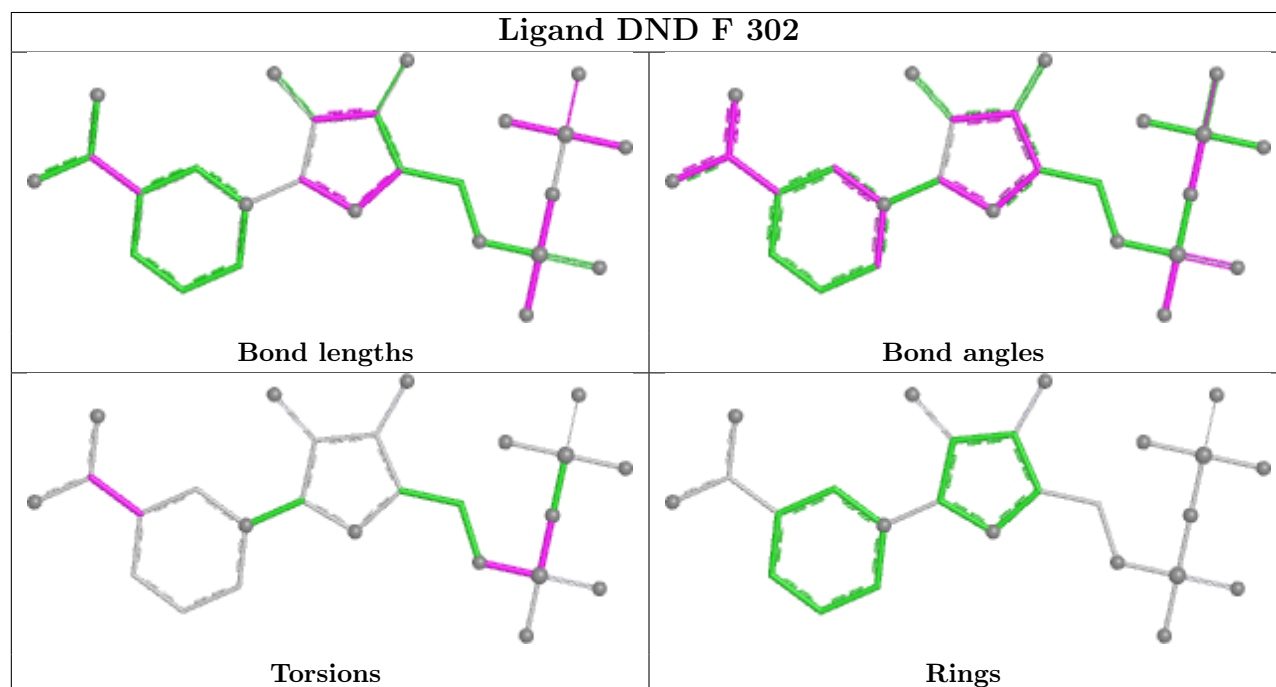
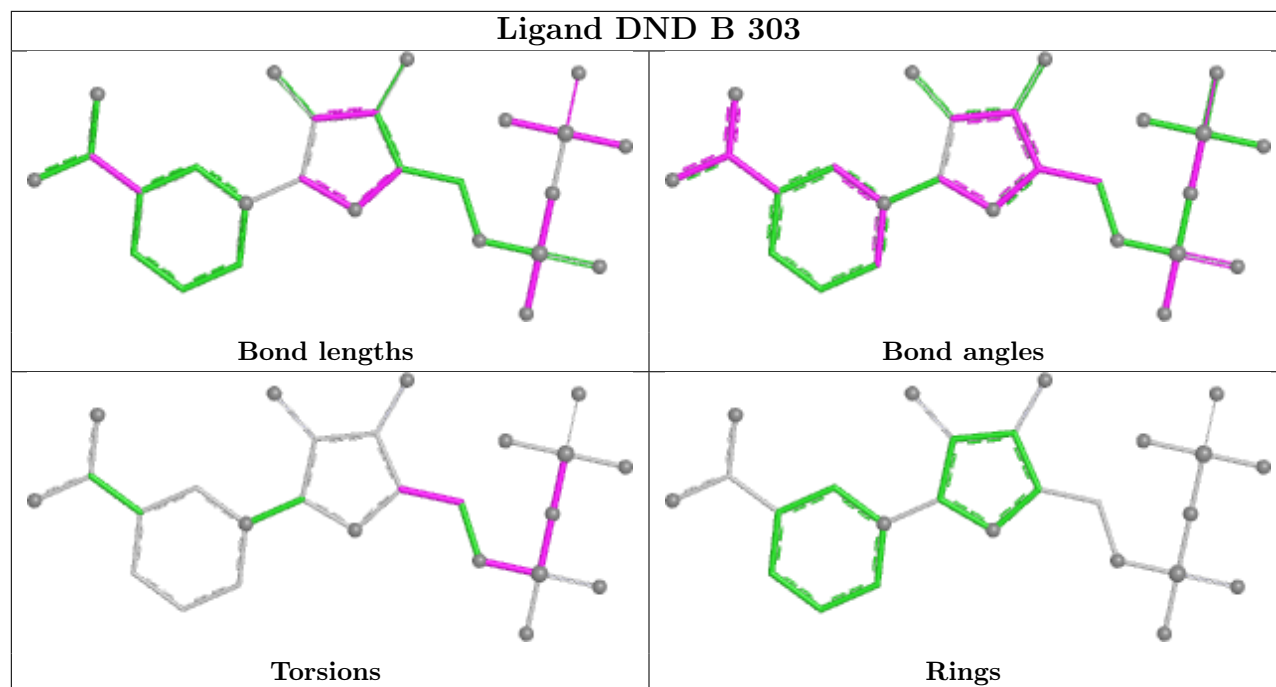
## Ligand DND D 302

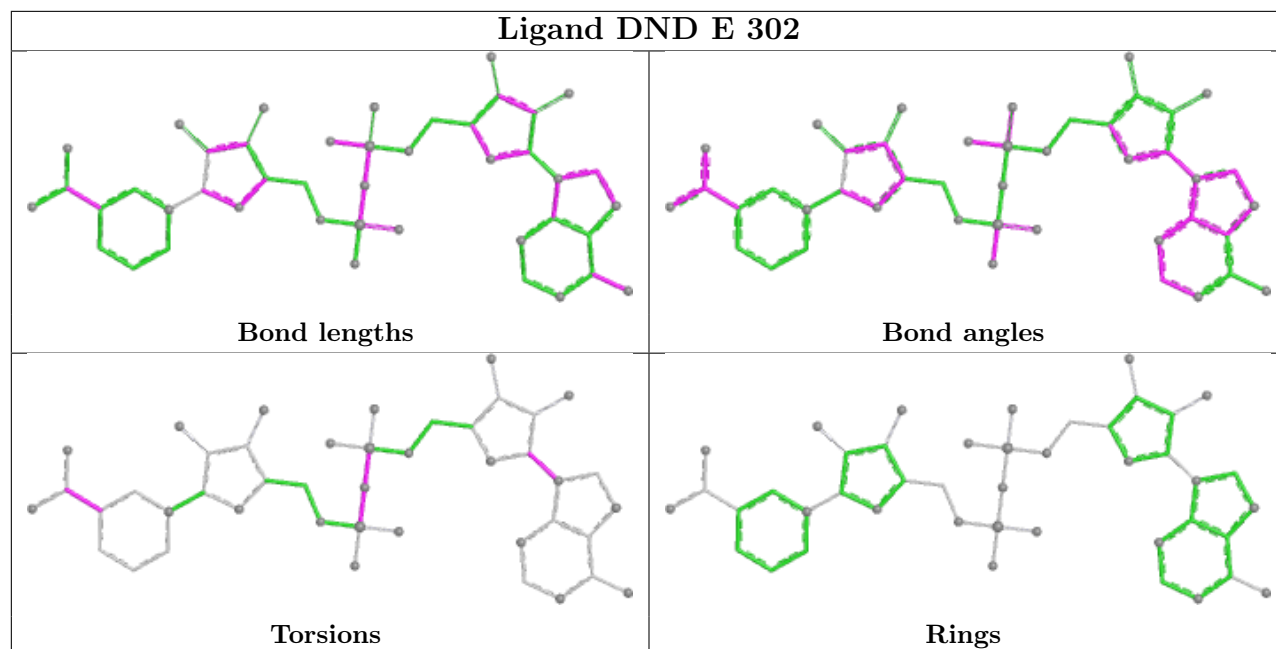


## Ligand DND C 303









## 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	203/256 (79%)	0.92	36 (17%) <b>4</b> <b>2</b>	18, 65, 137, 187	6 (2%)
1	B	202/256 (78%)	0.63	22 (10%) <b>10</b> <b>9</b>	32, 58, 110, 152	1 (0%)
1	C	202/256 (78%)	0.82	30 (14%) <b>5</b> <b>4</b>	30, 58, 129, 168	0
1	D	204/256 (79%)	0.99	37 (18%) <b>3</b> <b>2</b>	35, 72, 152, 191	0
1	E	217/256 (84%)	1.32	55 (25%) <b>1</b> <b>1</b>	47, 88, 152, 181	0
1	F	198/256 (77%)	1.53	62 (31%) <b>1</b> <b>0</b>	58, 94, 150, 190	0
All	All	1226/1536 (79%)	1.04	242 (19%) <b>3</b> <b>2</b>	18, 76, 143, 191	7 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221[A]	CYS	16.4
1	E	35	PHE	6.5
1	C	221	CYS	6.0
1	F	112	ALA	6.0
1	E	221	CYS	5.7
1	C	223	SER	5.6
1	A	116	PRO	5.5
1	F	155	ALA	5.4
1	F	66	VAL	5.3
1	F	221	CYS	5.3
1	E	39	ASP	5.1
1	C	46	ASN	4.9
1	D	60	THR	4.9
1	D	249	TRP	4.8
1	F	67	GLN	4.6
1	F	115	THR	4.5
1	A	73	THR	4.3
1	C	56	GLY	4.2
1	A	222[A]	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	4.2
1	E	49	PRO	4.1
1	F	111	PRO	4.1
1	E	38	VAL	4.1
1	E	246	MET	4.1
1	D	46	ASN	4.1
1	D	204	TYR	4.0
1	F	116	PRO	4.0
1	E	70	SER	4.0
1	B	204	TYR	3.8
1	E	48	PHE	3.8
1	D	107	VAL	3.8
1	B	45	ARG	3.8
1	A	112	ALA	3.7
1	D	248	SER	3.7
1	E	63	VAL	3.7
1	E	107	VAL	3.7
1	F	73	THR	3.7
1	F	88	ALA	3.7
1	B	48	PHE	3.7
1	F	95	THR	3.6
1	C	74	LEU	3.6
1	A	49	PRO	3.6
1	A	114	LYS	3.6
1	F	72	GLN	3.5
1	E	33	LEU	3.5
1	E	29	LYS	3.5
1	E	154	VAL	3.5
1	E	40	LEU	3.5
1	C	107	VAL	3.5
1	F	44	ARG	3.5
1	F	54	GLY	3.4
1	F	220	SER	3.4
1	F	246	MET	3.4
1	E	30	THR	3.4
1	D	72	GLN	3.4
1	B	180	GLU	3.3
1	E	89	LEU	3.3
1	C	162	ALA	3.3
1	E	75	PRO	3.3
1	B	54	GLY	3.3
1	C	219	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	63	VAL	3.3
1	F	107	VAL	3.3
1	E	157	ILE	3.3
1	D	106	THR	3.2
1	B	51	VAL	3.2
1	F	69	LEU	3.2
1	B	47	GLY	3.2
1	E	71	GLN	3.2
1	A	74	LEU	3.1
1	D	92	ALA	3.1
1	A	179	MET	3.1
1	F	162	ALA	3.1
1	C	161	PHE	3.1
1	A	48	PHE	3.1
1	A	109	GLU	3.0
1	E	31	ALA	3.0
1	E	153	GLY	3.0
1	D	48	PHE	3.0
1	E	161	PHE	3.0
1	E	180	GLU	2.9
1	A	204	TYR	2.9
1	C	211	MET	2.9
1	F	136	ALA	2.9
1	F	117	GLY	2.9
1	F	59	ALA	2.9
1	F	60	THR	2.9
1	F	92	ALA	2.9
1	B	74	LEU	2.9
1	B	107	VAL	2.9
1	D	76	ILE	2.9
1	E	41	ASP	2.9
1	D	66	VAL	2.9
1	F	93	LEU	2.9
1	A	44	ARG	2.8
1	D	250	SER	2.8
1	E	76	ILE	2.8
1	E	74	LEU	2.8
1	D	59	ALA	2.8
1	E	95	THR	2.8
1	F	147	GLU	2.8
1	D	116	PRO	2.8
1	E	42	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLN	2.8
1	E	142	PHE	2.8
1	E	204	TYR	2.8
1	F	84	GLU	2.8
1	E	205	GLY	2.8
1	B	109	GLU	2.7
1	E	116	PRO	2.7
1	A	84	GLU	2.7
1	B	80	ARG	2.7
1	A	53	TYR	2.7
1	F	46	ASN	2.7
1	D	97	VAL	2.7
1	A	80	ARG	2.7
1	E	51	VAL	2.7
1	D	113	PRO	2.7
1	F	89	LEU	2.6
1	A	145	ARG	2.6
1	B	67	GLN	2.6
1	F	110	GLN	2.6
1	C	48	PHE	2.6
1	F	97	VAL	2.6
1	F	202	VAL	2.6
1	C	91	PRO	2.6
1	F	204	TYR	2.6
1	F	108	GLY	2.6
1	C	97	VAL	2.6
1	D	179	MET	2.6
1	E	179	MET	2.6
1	E	69	LEU	2.6
1	D	91	PRO	2.6
1	B	70	SER	2.5
1	B	179	MET	2.5
1	C	151	ASP	2.5
1	D	88	ALA	2.5
1	D	222	ALA	2.5
1	A	46	ASN	2.5
1	E	220	SER	2.5
1	F	151	ASP	2.5
1	F	168	ARG	2.5
1	D	117	GLY	2.5
1	F	55	ALA	2.5
1	F	139	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	115	THR	2.5
1	C	220	SER	2.5
1	A	45	ARG	2.5
1	E	62	ILE	2.5
1	C	88	ALA	2.5
1	E	46	ASN	2.5
1	F	70	SER	2.5
1	D	71	GLN	2.5
1	F	161	PHE	2.5
1	E	37	ASN	2.4
1	E	145	ARG	2.4
1	F	109	GLU	2.4
1	C	87	ALA	2.4
1	D	96	ALA	2.4
1	E	112	ALA	2.4
1	F	45	ARG	2.4
1	A	56	GLY	2.4
1	E	222	ALA	2.4
1	F	222	ALA	2.4
1	D	158	HIS	2.4
1	A	69	LEU	2.4
1	F	77	LEU	2.4
1	E	111	PRO	2.4
1	E	72	GLN	2.4
1	A	87	ALA	2.4
1	C	53	TYR	2.3
1	E	93	LEU	2.3
1	F	62	ILE	2.3
1	E	141	THR	2.3
1	B	50	GLU	2.3
1	A	223[A]	SER	2.3
1	F	74	LEU	2.3
1	D	65	ILE	2.3
1	B	84	GLU	2.3
1	C	84	GLU	2.3
1	E	156	GLY	2.3
1	D	67	GLN	2.3
1	F	48	PHE	2.3
1	A	96	ALA	2.3
1	D	115	THR	2.3
1	F	105	MET	2.3
1	C	82	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	70	SER	2.3
1	C	96	ALA	2.2
1	F	141	THR	2.2
1	C	61	GLN	2.2
1	B	205	GLY	2.2
1	A	65	ILE	2.2
1	C	142	PHE	2.2
1	A	211	MET	2.2
1	C	222	ALA	2.2
1	C	47	GLY	2.2
1	A	155	ALA	2.2
1	B	55	ALA	2.2
1	D	49	PRO	2.2
1	A	209	GLN	2.2
1	F	209	GLN	2.2
1	D	54	GLY	2.2
1	F	203	GLY	2.2
1	E	109	GLU	2.2
1	F	106	THR	2.2
1	D	159	ARG	2.2
1	E	229	ASN	2.2
1	A	60	THR	2.1
1	B	60	THR	2.1
1	A	71	GLN	2.1
1	F	243	VAL	2.1
1	E	208	PHE	2.1
1	F	80	ARG	2.1
1	C	204	TYR	2.1
1	D	93	LEU	2.1
1	C	66	VAL	2.1
1	F	124	ALA	2.1
1	A	72	GLN	2.1
1	F	158	HIS	2.1
1	A	180	GLU	2.1
1	C	45	ARG	2.1
1	A	91	PRO	2.1
1	F	211	MET	2.1
1	B	72	GLN	2.1
1	E	110	GLN	2.1
1	D	74	LEU	2.1
1	A	47	GLY	2.1
1	E	117	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	150	TYR	2.1
1	D	137	VAL	2.1
1	D	155	ALA	2.0
1	F	68	ALA	2.0
1	D	203	GLY	2.0
1	F	98	TYR	2.0
1	E	45	ARG	2.0
1	A	57	LYS	2.0
1	C	55	ALA	2.0
1	E	87	ALA	2.0
1	C	110	GLN	2.0
1	F	156	GLY	2.0
1	A	107	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

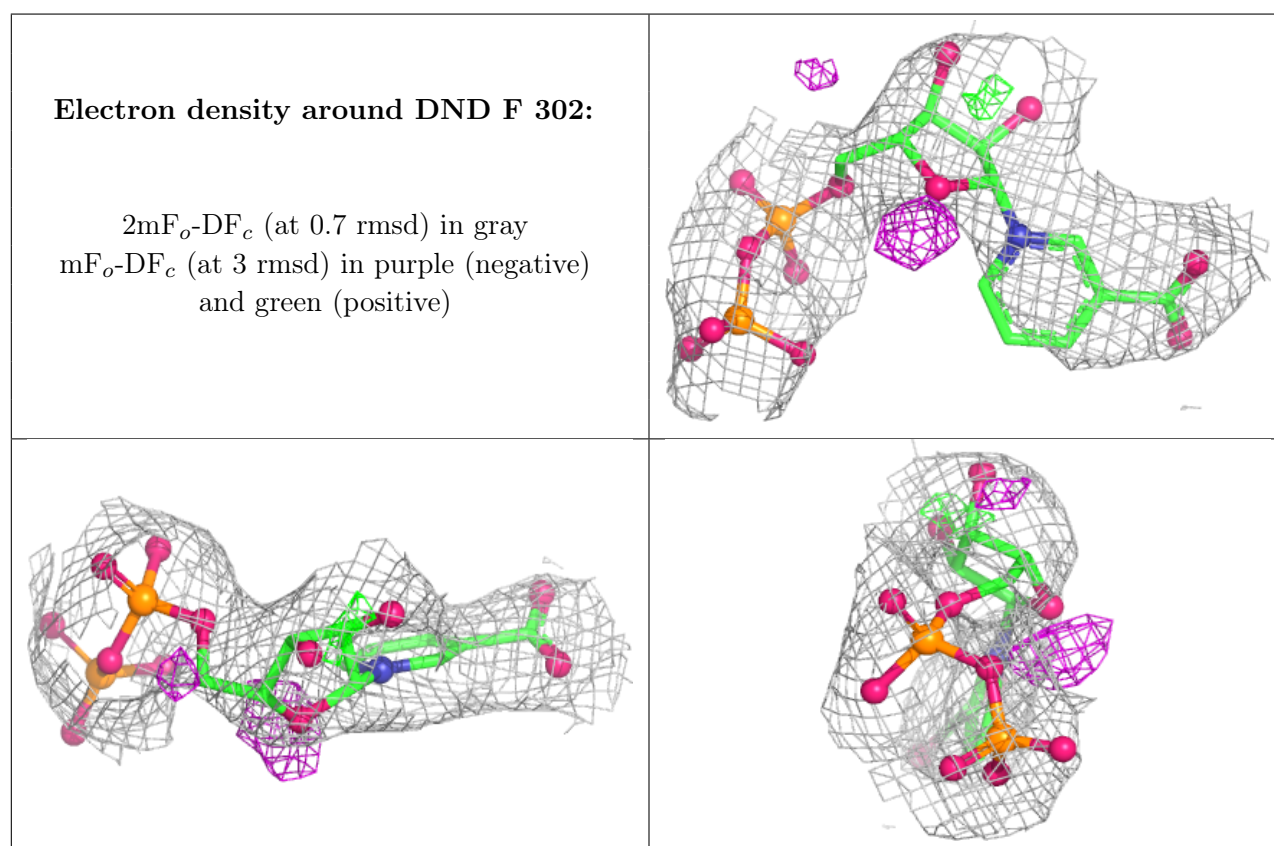
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	F	301	1/1	0.52	0.15	120,120,120,120	0
2	MG	C	302	1/1	0.82	0.09	93,93,93,93	0
3	DND	F	302	26/44	0.82	0.17	110,115,133,136	0
2	MG	D	301	1/1	0.83	0.22	87,87,87,87	0
3	DND	C	303	44/44	0.84	0.19	103,110,130,134	0
3	DND	A	303	44/44	0.85	0.16	85,100,119,123	0
3	DND	B	303	26/44	0.88	0.14	71,72,85,95	0
3	DND	E	302	44/44	0.90	0.13	84,95,107,116	0
2	MG	A	301	1/1	0.90	0.13	68,68,68,68	0
3	DND	D	302	26/44	0.91	0.13	74,83,93,96	0

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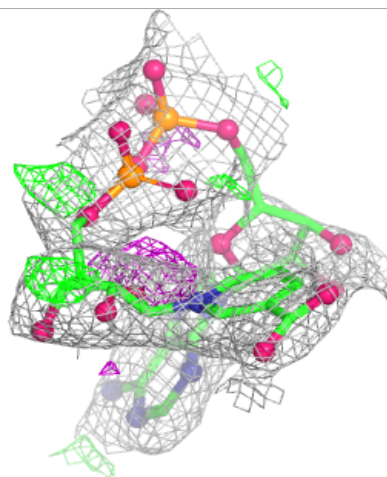
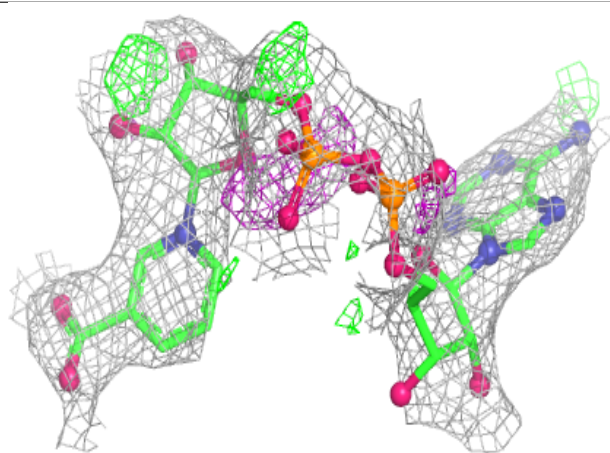
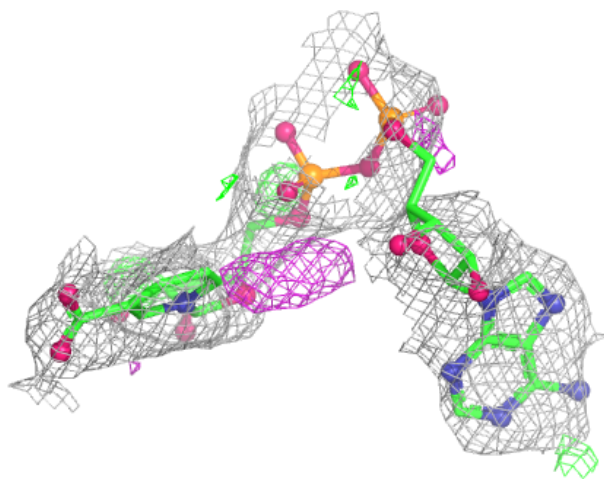
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	302	1/1	0.91	0.08	91,91,91,91	0
2	MG	C	301	1/1	0.91	0.11	70,70,70,70	0
2	MG	A	302	1/1	0.93	0.07	32,32,32,32	1
2	MG	E	301	1/1	0.94	0.07	98,98,98,98	0
2	MG	B	301	1/1	0.94	0.10	61,61,61,61	0

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.



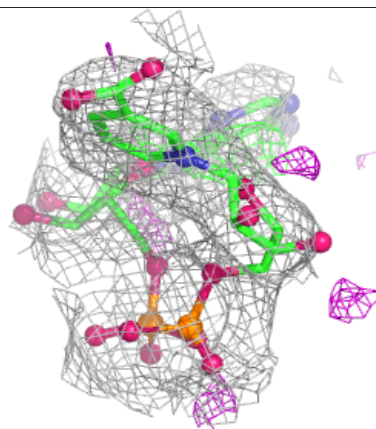
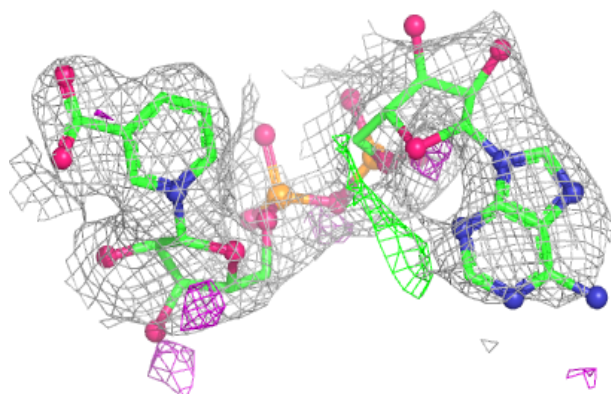
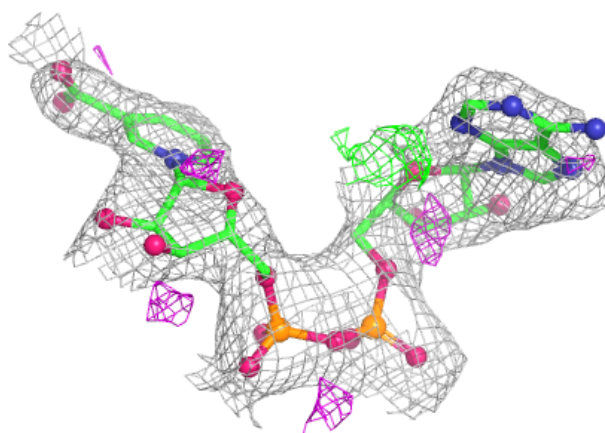
**Electron density around DND C 303:**

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

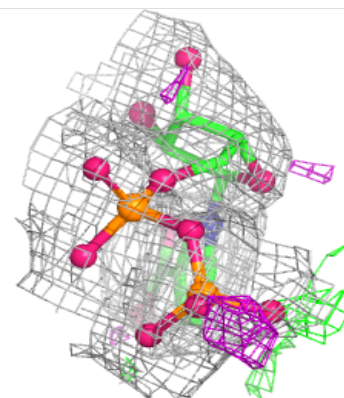
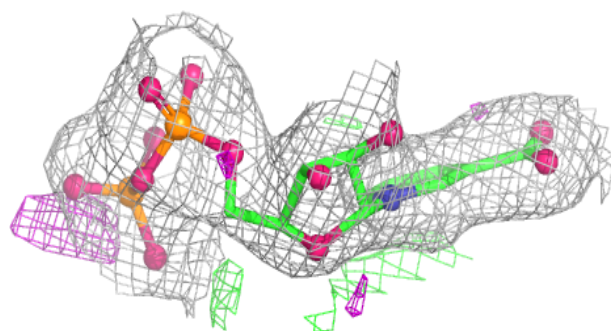
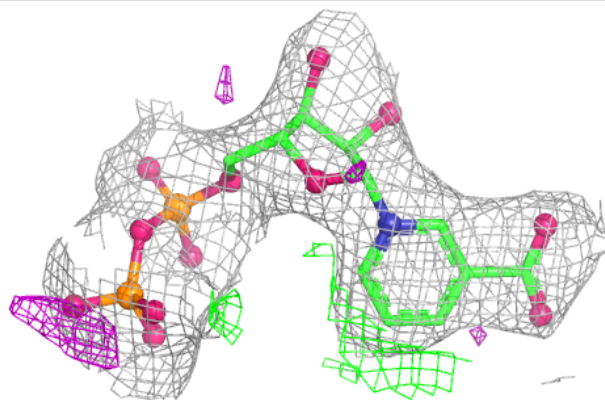


**Electron density around DND A 303:**

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

**Electron density around DND B 303:**

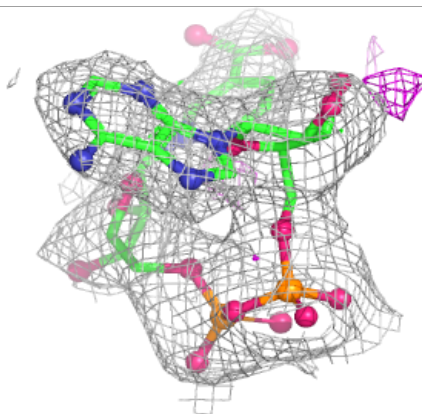
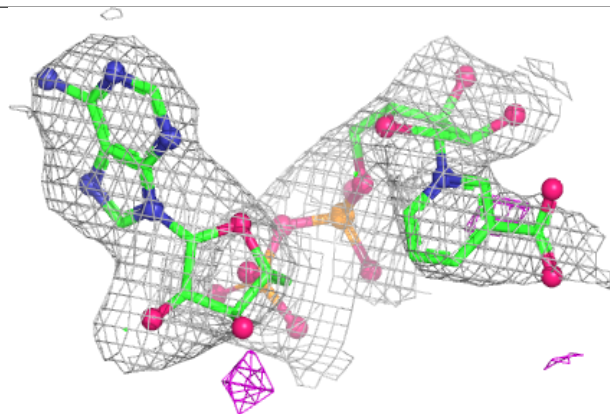
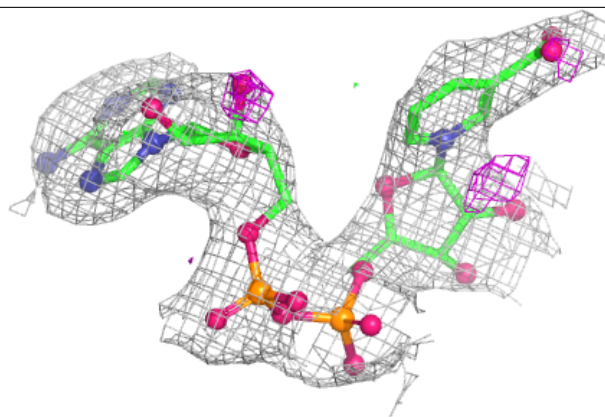
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



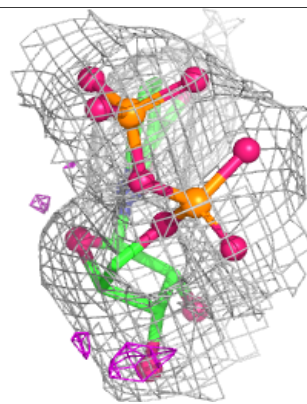
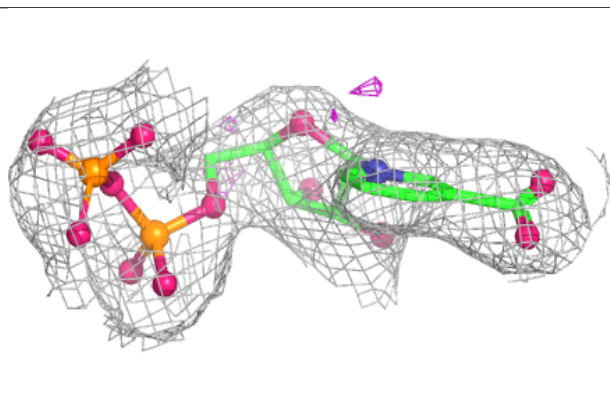
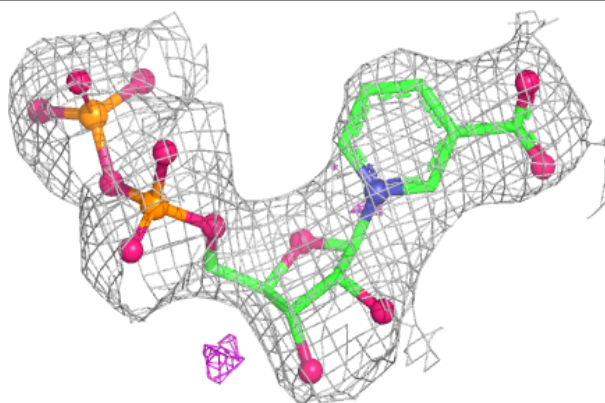


**Electron density around DND E 302:**

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

**Electron density around DND D 302:**

$2mF_o-DF_c$  (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.