

wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 02:47 PM JST

PDB ID : 7VB3

Title : Crystal structure of hydroxynitrile lyase from Linum usitatissimum

Authors: Zheng, D.; Nakabayashi, M.; Asano, Y.

Deposited on : 2021-08-30

Resolution : 1.48 Å(reported)

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

We welcome your comments at 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

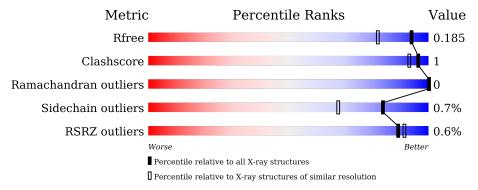
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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 >=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 <=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	443	88%	•	8%
1	В	443	91%		7%
1	С	443	89%		8%
1	D	443	90%		8%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14555 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 Aliphatic (R)-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	408	Total	С	N	О	S	0	6	0
1	A	400	3142	1993	525	599	25	U	0	
1	В	414	Total	С	N	О	S	0	5	0
1	Б	414	3176	2011	528	612	25	U	9	0
1	C	400	Total	al C I	N	О	S	0	1	0
1		409	3115	1971	520	599	25	U	1	
1	D	408	Total	С	N	О	S	0	3	0
1	ע	400	3122	1980	521	597	24	U)	

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P93243
A	-19	GLY	-	expression tag	UNP P93243
A	-18	SER	-	expression tag	UNP P93243
A	-17	SER	-	expression tag	UNP P93243
A	-16	HIS	-	expression tag	UNP P93243
A	-15	HIS	-	expression tag	UNP P93243
A	-14	HIS	-	expression tag	UNP P93243
A	-13	HIS	-	expression tag	UNP P93243
A	-12	HIS	-	expression tag	UNP P93243
A	-11	HIS	-	expression tag	UNP P93243
A	-10	SER	-	expression tag	UNP P93243
A	-9	SER	-	expression tag	UNP P93243
A	-8	GLY	-	expression tag	UNP P93243
A	-7	LEU	-	expression tag	UNP P93243
A	-6	VAL	-	expression tag	UNP P93243
A	-5	PRO	-	expression tag	UNP P93243
A	-4	ARG	-	expression tag	UNP P93243
A	-3	GLY	-	expression tag	UNP P93243
A	-2	SER		expression tag	UNP P93243
A	-1	HIS	-	expression tag	UNP P93243
A	0	MET	-	expression tag	UNP P93243



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B -20 MET - initiating methionine UNITION B -19 GLY - expression tag UNITION B -18 SER - expression tag UNITION B -17 SER - expression tag UNITION B -16 HIS - expression tag UNITION B -15 HIS - expression tag UNITION B -14 HIS - expression tag UNITION B -13 HIS - expression tag UNITION B -12 HIS - expression tag UNITION B -11 HIS - expression tag UNITION B -10 SER - expression tag UNITION B -9 SER - expression tag UNITION B -8 GLY - expression tag UNITION	P P93243
B -19 GLY - expression tag UNITOR B -18 SER - expression tag UNITOR B -17 SER - expression tag UNITOR B -16 HIS - expression tag UNITOR B -15 HIS - expression tag UNITOR B -14 HIS - expression tag UNITOR B -13 HIS - expression tag UNITOR B -12 HIS - expression tag UNITOR B -10 SER - expression tag UNITOR B -9 SER - expression tag UNITOR B -8 GLY - expression tag UNITOR B -6 VAL - expression tag UNITOR B -6 VAL - expression tag UNITOR B	P P93243
B	P P93243
B -17 SER - expression tag UNIT B -16 HIS - expression tag UNIT B -15 HIS - expression tag UNIT B -14 HIS - expression tag UNIT B -13 HIS - expression tag UNIT B -12 HIS - expression tag UNIT B -11 HIS - expression tag UNIT B -10 SER - expression tag UNIT B -9 SER - expression tag UNIT B -8 GLY - expression tag UNIT B -7 LEU - expression tag UNIT B -6 VAL - expression tag UNIT B -6 VAL - expression tag UNIT B -6	P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243
B	P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243
B -15 HIS - expression tag UNIDAR B -14 HIS - expression tag UNIDAR B -13 HIS - expression tag UNIDAR B -12 HIS - expression tag UNIDAR B -11 HIS - expression tag UNIDAR B -10 SER - expression tag UNIDAR B -9 SER - expression tag UNIDAR B -8 GLY - expression tag UNIDAR B -7 LEU - expression tag UNIDAR B -6 VAL - expression tag UNIDAR B -6 VAL - expression tag UNIDAR B -5 PRO - expression tag UNIDAR	P P93243 P P93243 P P93243 P P93243 P P93243 P P93243 P P93243
B -14 HIS - expression tag UNIDAR B -13 HIS - expression tag UNIDAR B -12 HIS - expression tag UNIDAR B -11 HIS - expression tag UNIDAR B -10 SER - expression tag UNIDAR B -9 SER - expression tag UNIDAR B -8 GLY - expression tag UNIDAR B -7 LEU - expression tag UNIDAR B -6 VAL - expression tag UNIDAR B -5 PRO - expression tag UNIDAR	P P93243 P P93243 P P93243 P P93243 P P93243 P P93243
B -13 HIS - expression tag UN B -12 HIS - expression tag UN B -11 HIS - expression tag UN B -10 SER - expression tag UN B -9 SER - expression tag UN B -8 GLY - expression tag UN B -7 LEU - expression tag UN B -6 VAL - expression tag UN B -5 PRO - expression tag UN	P P93243 P P93243 P P93243 P P93243 P P93243
B -12 HIS - expression tag UNIDAR B -11 HIS - expression tag UNIDAR B -10 SER - expression tag UNIDAR B -9 SER - expression tag UNIDAR B -8 GLY - expression tag UNIDAR B -7 LEU - expression tag UNIDAR B -6 VAL - expression tag UNIDAR B -5 PRO - expression tag UNIDAR	P P93243 P P93243 P P93243 P P93243
B -11 HIS - expression tag UNIT B -10 SER - expression tag UNIT B -9 SER - expression tag UNIT B -8 GLY - expression tag UNIT B -7 LEU - expression tag UNIT B -6 VAL - expression tag UNIT B -5 PRO - expression tag UNIT	P P93243 P P93243 P P93243 P P93243
B -10 SER - expression tag UNI B -9 SER - expression tag UNI B -8 GLY - expression tag UNI B -7 LEU - expression tag UNI B -6 VAL - expression tag UNI B -5 PRO - expression tag UNI	P P93243 P P93243 P P93243
B -9 SER - expression tag UNI B -8 GLY - expression tag UNI B -7 LEU - expression tag UNI B -6 VAL - expression tag UNI B -5 PRO - expression tag UNI	P P93243 P P93243
B -8 GLY - expression tag UNID B -7 LEU - expression tag UNID B -6 VAL - expression tag UNID B -5 PRO - expression tag UNID	P P93243
B -7 LEU - expression tag UND B -6 VAL - expression tag UND B -5 PRO - expression tag UND	
B -6 VAL - expression tag UNI B -5 PRO - expression tag UNI	
B -5 PRO - expression tag UN	P P93243
	P P93243
D 4 ADC	P P93243
B -4 ARG - expression tag UN	P P93243
B -3 GLY - expression tag UN	P P93243
B -2 SER - expression tag UN	P P93243
B -1 HIS - expression tag UN	P P93243
B 0 MET - expression tag UN	P P93243
B 117 THR VAL conflict UN	P P93243
C -20 MET - initiating methionine UN	P P93243
C -19 GLY - expression tag UN	P P93243
C -18 SER - expression tag UN	P P93243
C -17 SER - expression tag UN	P P93243
	P P93243
C -15 HIS - expression tag UN	P P93243
C -14 HIS - expression tag UN	P P93243
C -13 HIS - expression tag UN	P P93243
C -12 HIS - expression tag UN	P P93243
C -11 HIS - expression tag UN	P P93243
C -10 SER - expression tag UN	P P93243
C -9 SER - expression tag UN	P P93243
C -8 GLY - expression tag UN	P P93243
C -7 LEU - expression tag UN	P P93243
C -6 VAL - expression tag UN	P P93243
C -5 PRO - expression tag UN	P P93243
C -4 ARG - expression tag UN	P P93243
C -3 GLY - expression tag UN	P P93243
C -2 SER - expression tag UN	P P93243

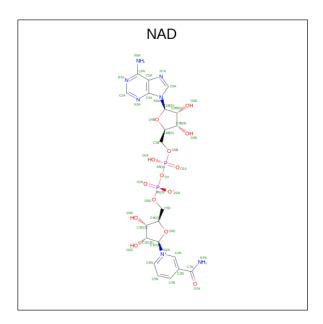


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Chain	Residue	Modelled	Actual	Comment	Reference
С	-1	HIS	-	expression tag	UNP P93243
С	0	MET	-	expression tag	UNP P93243
С	117	THR	VAL	conflict	UNP P93243
D	-20	MET	-	initiating methionine	UNP P93243
D	-19	GLY	-	expression tag	UNP P93243
D	-18	SER	-	expression tag	UNP P93243
D	-17	SER	-	expression tag	UNP P93243
D	-16	HIS	-	expression tag	UNP P93243
D	-15	HIS	-	expression tag	UNP P93243
D	-14	HIS	-	expression tag	UNP P93243
D	-13	HIS	-	expression tag	UNP P93243
D	-12	HIS	-	expression tag	UNP P93243
D	-11	HIS	-	expression tag	UNP P93243
D	-10	SER	-	expression tag	UNP P93243
D	-9	SER	-	expression tag	UNP P93243
D	-8	GLY	-	expression tag	UNP P93243
D	-7	LEU	-	expression tag	UNP P93243
D	-6	VAL	-	expression tag	UNP P93243
D	-5	PRO	-	expression tag	UNP P93243
D	-4	ARG	-	expression tag	UNP P93243
D	-3	GLY	-	expression tag	UNP P93243
D	-2	SER	-	expression tag	UNP P93243
D	-1	HIS	-	expression tag	UNP P93243
D	0	MET	-	expression tag	UNP P93243
D	117	THR	VAL	conflict	UNP P93243

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).





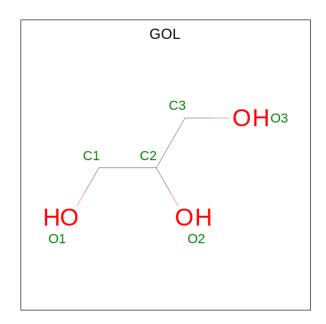
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	٨	1	Total	С	N	О	Р	0	0	
2	A	1	44	21	7	14	2	U	U	
9	В	1	Total	С	N	О	Р	0	0	
2	Б	1	44	21	7	14	2	U		
9	C	1	Total	С	N	О	Р	0	0	
2	$\begin{array}{c c} 2 & C \end{array}$	1	44	21	7	14	2	U	U	
2	D	1	Total	С	N	О	Р	0	0	
2	ש	1	44	21	7	14	2	U	U	

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0
3	В	2	Total Zn 2 2	0	0
3	С	2	Total Zn 2 2	0	0
3	D	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0
4	С	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

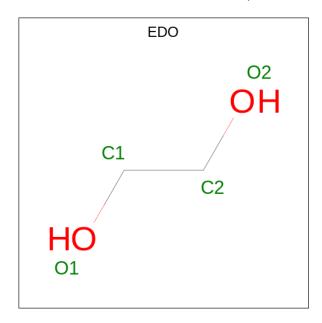
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

 \bullet Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



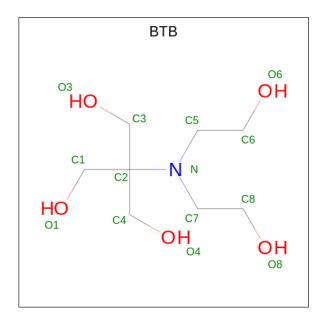
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	В	1	Total C O 4 2 2	0	0
6	В	1	Total C O 4 2 2	0	0
6	В	1	Total C O 4 2 2	0	0
6	В	1	Total C O 4 2 2	0	0
6	С	1	Total C O 4 2 2	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	D	1	Total 4	C 2	O 2	0	0

• Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	В	1	Total C N O 14 8 1 5	0	0

• Molecule 8 is water.

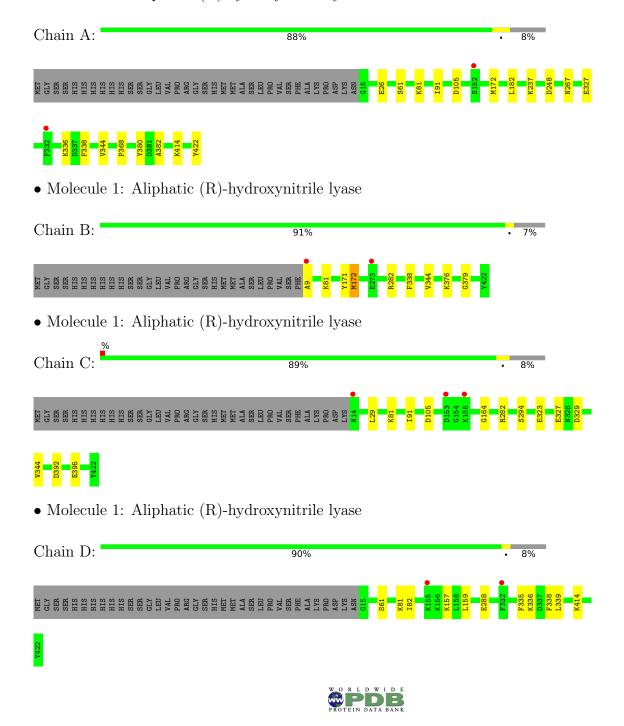
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	474	Total O 474 474	0	0
8	В	478	Total O 478 478	0	0
8	С	346	Total O 346 346	0	0
8	D	370	Total O 370 370	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aliphatic (R)-hydroxynitrile lyase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	94.12Å 52.18Å 168.51Å	Donositor
a, b, c, α , β , γ	90.00° 95.01° 90.00°	Depositor
Resolution (Å)	84.07 - 1.48	Depositor
Resolution (A)	83.93 - 1.48	EDS
% Data completeness	99.5 (84.07-1.48)	Depositor
(in resolution range)	99.5 (83.93-1.48)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	2.54 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.156 , 0.183	Depositor
R, R_{free}	0.158 , 0.185	DCC
R_{free} test set	13630 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 43.6	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14555	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: NAD, ZN, EDO, MG, GOL, BTB, SNC

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).

Mal	Chain	Bo	nd lengths	Bond angles		
IVIOI	Mol Chain		# Z > 5	RMSZ	# Z >5	
1	A	0.82	$2/3206 \ (0.1\%)$	0.90	1/4330 (0.0%)	
1	В	0.78	0/3237	0.92	3/4373 (0.1%)	
1	С	0.77	1/3163~(0.0%)	0.90	$2/4275 \ (0.0\%)$	
1	D	0.75	$1/3177 \ (0.0\%)$	0.86	0/4294	
All	All	0.78	$4/12783 \ (0.0\%)$	0.90	6/17272 (0.0%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	327	GLU	CD-OE2	6.97	1.33	1.25
1	A	26	GLU	CD-OE1	-6.38	1.18	1.25
1	D	288	GLU	CD-OE2	6.13	1.32	1.25
1	С	294	SER	CA-CB	-5.01	1.45	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
1	В	282	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	С	282	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	С	282	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	422	TYR	CB-CG-CD1	5.86	124.51	121.00
1	В	172	MET	CG-SD-CE	-5.28	91.75	100.20

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	3142	0	3176	9	0
1	В	3176	0	3201	5	0
1	С	3115	0	3130	10	0
1	D	3122	0	3146	7	0
2	A	44	0	26	0	0
2	В	44	0	26	0	0
2	С	44	0	26	0	0
2	D	44	0	26	0	0
3	A	2	0	0	0	0
3	В	2	0	0	0	0
3	С	2	0	0	0	0
3	D	2	0	0	0	0
4	A	24	0	32	1	0
4	В	24	0	32	0	0
4	С	6	0	8	0	0
4	D	12	0	16	0	0
5	A	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	18	1	0
6	В	16	0	24	2	0
6	С	4	0	6	0	0
6	D	4	0	6	0	0
7	A	28	0	38	1	0
7	В	14	0	19	0	0
8	A	474	0	0	1	0
8	В	478	0	0	1	0
8	С	346	0	0	1	0
8	D	370	0	0	1	0
All	All	14555	0	12956	26	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 1.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:344:VAL:HG12	1:D:338:PHE:HZ	1.51	0.75
6:B:511:EDO:H12	8:B:855:HOH:O	1.90	0.72
1:C:344:VAL:HG12	1:D:338:PHE:CZ	2.34	0.59
1:C:327:GLU:HA	1:C:327:GLU:OE1	2.03	0.57
1:A:338:PHE:HZ	1:B:344:VAL:HG12	1.69	0.56

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	Perce	ntiles
1	A	411/443~(93%)	402 (98%)	9 (2%)	0	100	100
1	В	416/443~(94%)	407 (98%)	9 (2%)	0	100	100
1	С	407/443~(92%)	397 (98%)	10 (2%)	0	100	100
1	D	408/443~(92%)	397 (97%)	11 (3%)	0	100	100
All	All	1642/1772~(93%)	1603 (98%)	39 (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	343/367~(94%)	339 (99%)	4 (1%)	71 46
1	В	347/367 (95%)	344 (99%)	3 (1%)	78 59



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	С	339/367~(92%)	338 (100%)	1 (0%)	92 84
1	D	340/367~(93%)	338 (99%)	2 (1%)	86 72
All	All	$1369/1468 \; (93\%)$	1359 (99%)	10 (1%)	84 68

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	81	LYS
1	D	81	LYS
1	D	336	LYS
1	A	336	LYS
1	В	81	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	Trmo	Chain	Pos	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SNC	D	265	1	4,7,8	0.81	0	1,7,9	0.96	0
1	SNC	С	265	1	4,7,8	0.68	0	1,7,9	0.85	0
1	SNC	В	265	1	4,7,8	0.92	0	1,7,9	0.24	0
1	SNC	A	265	1	4,7,8	0.60	0	1,7,9	0.49	0

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SNC	D	265	1	-	0/0/6/8	-
1	SNC	С	265	1	-	0/0/6/8	-
1	SNC	В	265	1	-	0/0/6/8	-
1	SNC	A	265	1	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 39 ligands modelled in this entry, 12 are monoatomic - leaving 27 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	Trino	Chain	Res	Link	Во	Bond lengths			ond ang	cles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	510	-	3,3,3	0.24	0	2,2,2	0.16	0
6	EDO	В	509	-	3,3,3	0.15	0	2,2,2	0.46	0
6	EDO	В	512	-	3,3,3	0.07	0	2,2,2	0.45	0
2	NAD	С	501	-	42,48,48	0.83	2 (4%)	50,73,73	0.82	2 (4%)
7	BTB	В	513	-	13,13,13	1.40	3 (23%)	7,16,16	0.48	0
4	GOL	D	504	-	5,5,5	0.18	0	5,5,5	0.13	0
6	EDO	A	509	-	3,3,3	0.58	0	2,2,2	0.42	0
6	EDO	В	511	-	3,3,3	0.36	0	2,2,2	0.08	0



Mol	Type	Chain	Res	Link	Во	ond leng	ths	В	ond ang	eles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	511	-	3,3,3	0.27	0	2,2,2	0.44	0
6	EDO	В	510	-	3,3,3	0.11	0	2,2,2	0.25	0
6	EDO	С	506	-	3,3,3	0.28	0	2,2,2	0.38	0
4	GOL	В	505	-	5,5,5	0.14	0	5,5,5	0.43	0
7	BTB	A	512	_	13,13,13	1.37	3 (23%)	7,16,16	0.45	0
7	ВТВ	A	513	-	13,13,13	1.36	3 (23%)	7,16,16	0.95	1 (14%)
4	GOL	С	504	-	5,5,5	0.19	0	5,5,5	0.31	0
2	NAD	A	501	-	42,48,48	0.69	1 (2%)	50,73,73	1.06	4 (8%)
4	GOL	A	505	-	5,5,5	0.45	0	5,5,5	0.73	0
4	GOL	В	506	-	5,5,5	0.13	0	5,5,5	0.36	0
4	GOL	A	507	-	5,5,5	0.18	0	5,5,5	0.44	0
4	GOL	A	504	_	5,5,5	0.25	0	5, 5, 5	0.24	0
4	GOL	D	505	-	5,5,5	0.10	0	5, 5, 5	0.28	0
6	EDO	D	507	_	3,3,3	0.24	0	2,2,2	0.46	0
2	NAD	В	501	-	42,48,48	0.74	0	50,73,73	0.87	2 (4%)
4	GOL	В	504	-	5,5,5	0.29	0	5,5,5	0.32	0
4	GOL	В	507	-	5,5,5	0.20	0	5,5,5	0.44	0
2	NAD	D	501	-	42,48,48	0.80	1 (2%)	50,73,73	0.92	1 (2%)
4	GOL	A	506	-	5,5,5	0.11	0	5,5,5	0.34	0

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
6	EDO	A	510	-	-	1/1/1/1	-
6	EDO	В	509	-	-	0/1/1/1	-
6	EDO	В	512	-	-	0/1/1/1	-
2	NAD	С	501	-	-	5/26/62/62	0/5/5/5
7	BTB	В	513	-	-	3/21/21/21	-
4	GOL	D	504	-	-	0/4/4/4	-
6	EDO	A	509	-	-	0/1/1/1	-
6	EDO	В	511	-	-	0/1/1/1	-
6	EDO	A	511	-	-	0/1/1/1	-
6	EDO	В	510	-	-	1/1/1/1	-
6	EDO	С	506	-	-	0/1/1/1	-
4	GOL	В	505	-	-	0/4/4/4	-
7	BTB	A	512	-	-	4/21/21/21	_
7	BTB	A	513		-	4/21/21/21	
4	GOL	С	504	-	-	0/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
4	GOL	A	505	-	-	4/4/4/4	-
4	GOL	В	506	-	-	0/4/4/4	-
4	GOL	A	507	-	-	4/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-
6	EDO	D	507	-	-	0/1/1/1	-
2	NAD	В	501	-	-	4/26/62/62	0/5/5/5
4	GOL	В	504	_	-	0/4/4/4	-
4	GOL	В	507	-	-	2/4/4/4	-
2	NAD	D	501	_	-	4/26/62/62	0/5/5/5
4	GOL	A	506	-	-	1/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
7	A	513	BTB	C2-N	3.40	1.55	1.48
7	A	512	BTB	C2-N	3.31	1.55	1.48
7	В	513	BTB	C5-N	2.97	1.52	1.48
7	В	513	BTB	C2-N	2.74	1.54	1.48
7	В	513	BTB	C7-N	2.74	1.51	1.48

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	501	NAD	C6N-N1N-C2N	-2.95	119.29	121.97
2	С	501	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
2	В	501	NAD	C5A-C6A-N6A	2.54	124.22	120.35
2	С	501	NAD	C5A-C6A-N6A	2.41	124.02	120.35
2	A	501	NAD	O7N-C7N-N7N	2.37	125.94	122.58

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	В	501	NAD	O4D-C1D-N1N-C2N



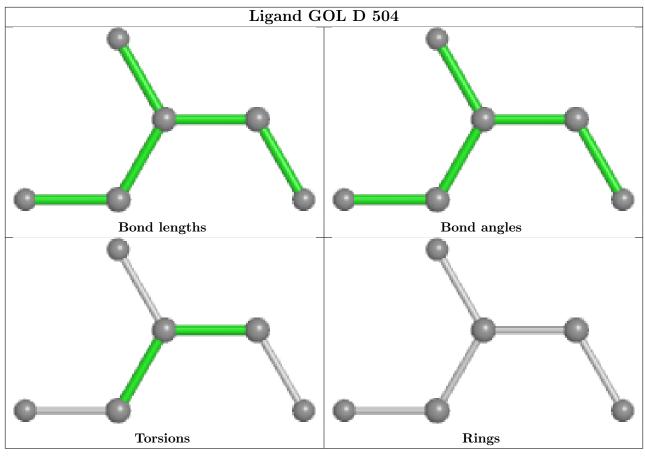
There are no ring outliers.

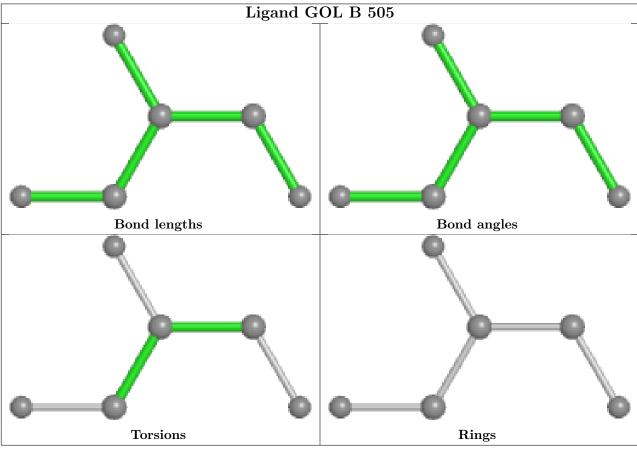
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	512	EDO	1	0
6	В	511	EDO	1	0
6	A	511	EDO	1	0
7	A	513	BTB	1	0
4	A	505	GOL	1	0

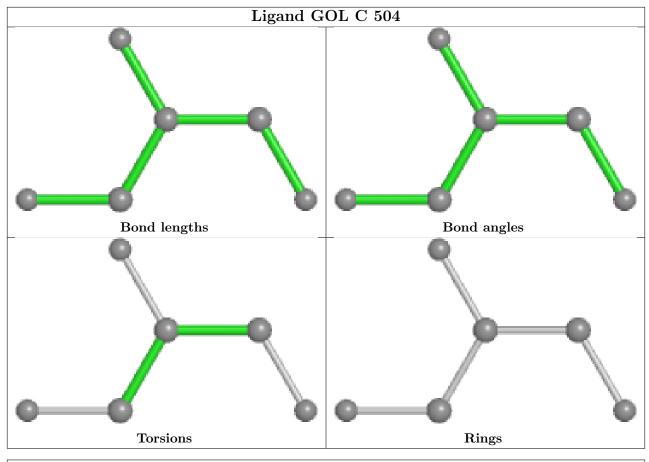
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

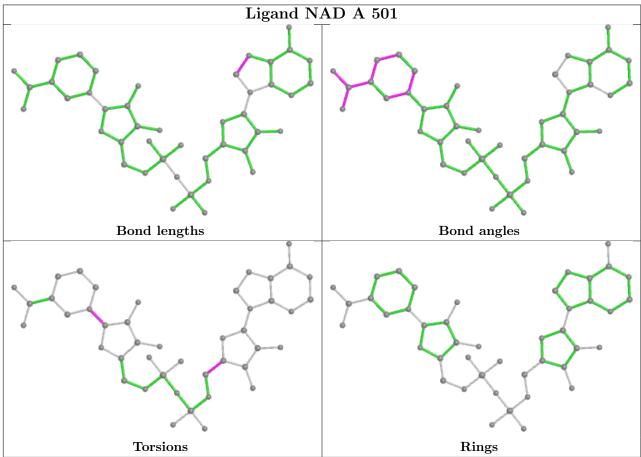




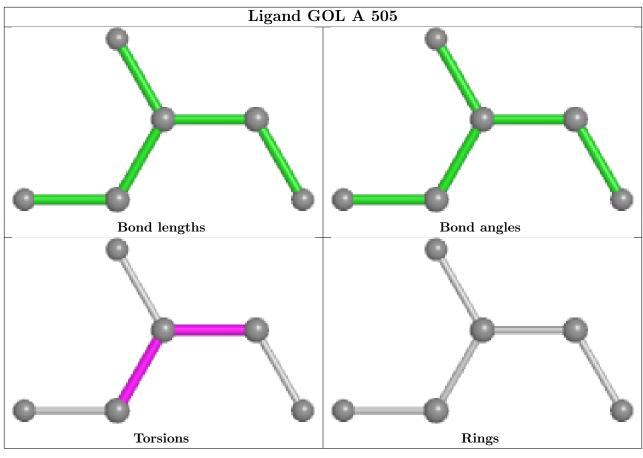


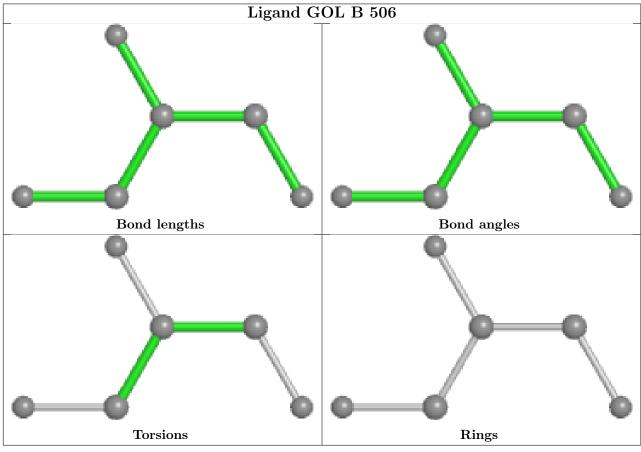




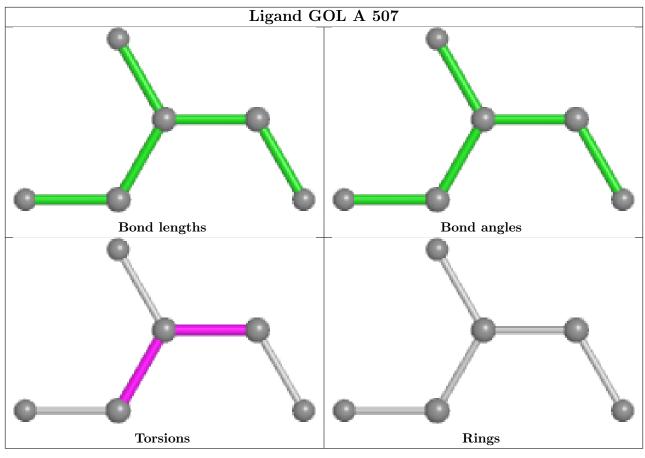


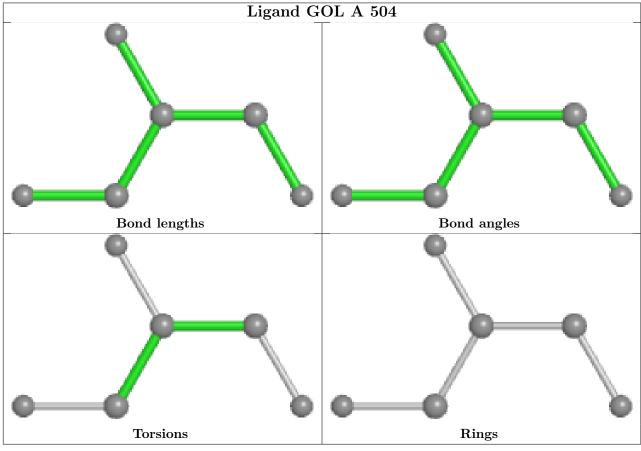




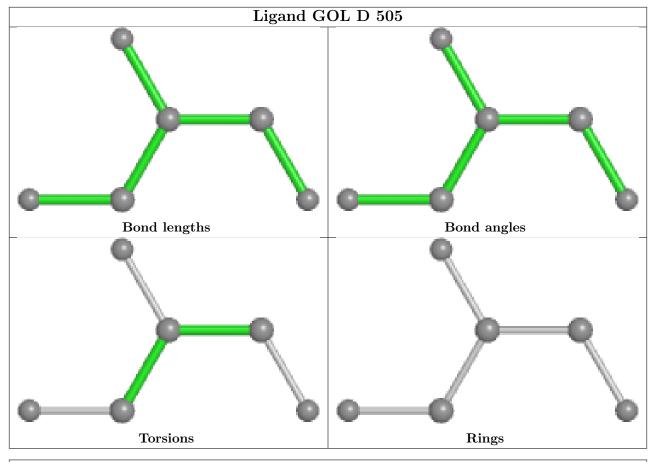


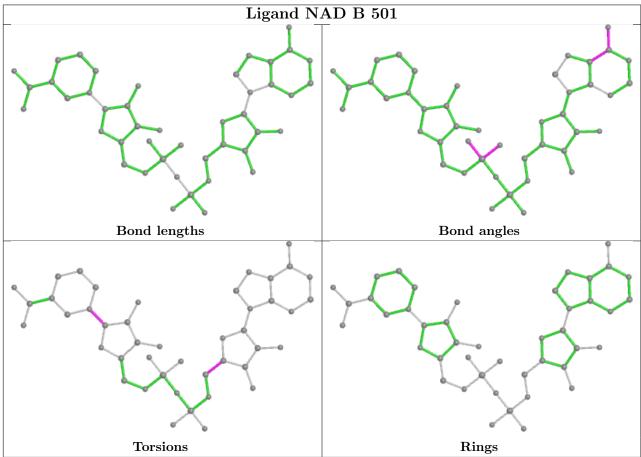




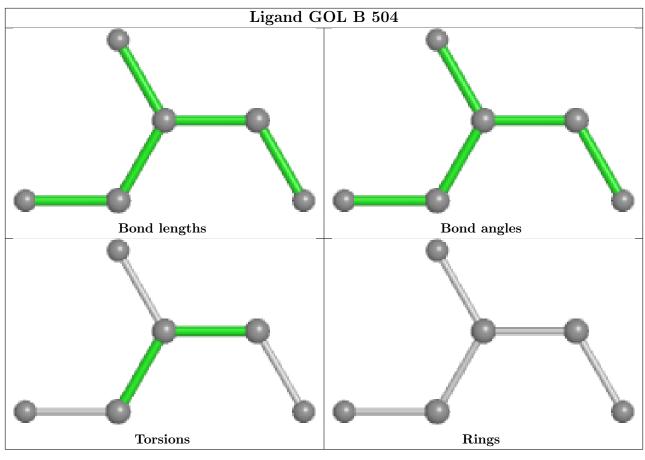


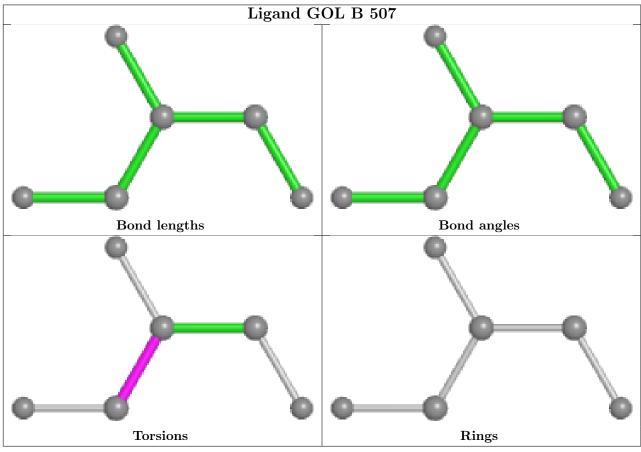




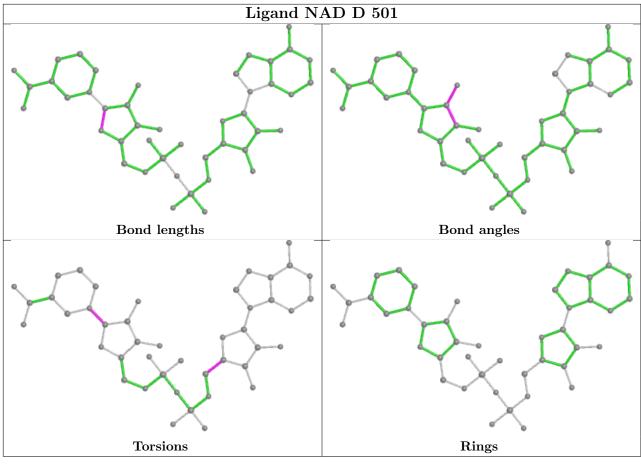


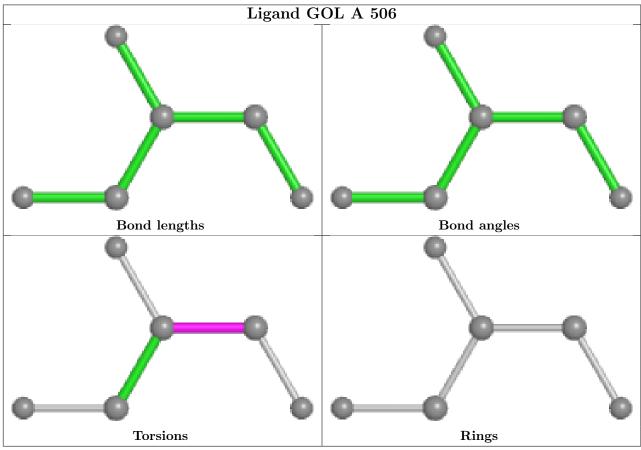














5.7 Other polymers (i)

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^{th} 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>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	407/443 (91%)	-0.28	2 (0%) 91 93	9, 13, 22, 54	0
1	В	413/443 (93%)	-0.25	2 (0%) 91 93	9, 13, 26, 49	0
1	С	408/443 (92%)	-0.11	3 (0%) 87 90	13, 19, 33, 57	0
1	D	407/443 (91%)	-0.13	2 (0%) 91 93	12, 18, 30, 52	0
All	All	$1635/1772 \ (92\%)$	-0.19	9 (0%) 89 91	9, 16, 29, 57	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	D	332[A]	PHE	3.3	
1	В	273	GLU	3.3	
1	С	153	ASP	3.2	
1	A	332[A]	PHE	3.0	
1	С	155	LYS	2.9	

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	SNC	С	265	8/9	0.91	0.10	18,20,24,32	0
1	SNC	В	265	8/9	0.95	0.07	13,15,26,33	0
1	SNC	D	265	8/9	0.95	0.08	14,17,19,24	0
1	SNC	A	265	8/9	0.96	0.08	12,13,18,29	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

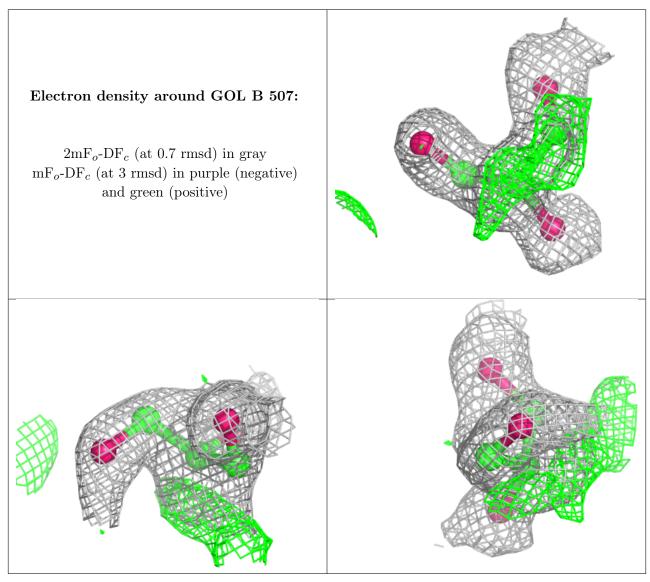
4 7	GOL	В						Q<0.9
	COL	D	507	6/6	0.68	0.15	34,40,43,46	0
7	GOL	A	507	6/6	0.75	0.30	34,37,40,43	0
' '	BTB	A	513	14/14	0.75	0.28	37,51,66,68	0
6	EDO	С	506	4/4	0.78	0.11	32,35,39,40	0
4	GOL	A	505	6/6	0.78	0.18	22,32,37,42	0
6	EDO	A	511	4/4	0.80	0.26	35,35,36,42	0
7	BTB	A	512	14/14	0.81	0.21	24,31,34,34	0
6	EDO	В	509	4/4	0.81	0.11	28,31,36,38	0
4	GOL	A	506	6/6	0.82	0.17	41,43,48,50	0
6	EDO	D	507	4/4	0.83	0.12	36,37,40,44	0
4	GOL	В	506	6/6	0.85	0.17	25,36,38,39	0
4	GOL	D	505	6/6	0.85	0.22	34,43,45,46	0
7	BTB	В	513	14/14	0.85	0.16	22,29,34,34	0
6	EDO	A	510	4/4	0.87	0.20	33,34,36,40	0
6	EDO	В	511	4/4	0.88	0.19	22,30,34,35	0
6	EDO	Α	509	4/4	0.88	0.11	19,25,26,32	0
4	GOL	В	505	6/6	0.88	0.13	27,28,29,29	0
6	EDO	В	512	4/4	0.90	0.28	36,37,37,45	0
4	GOL	С	504	6/6	0.93	0.09	22,25,26,27	0
4	GOL	В	504	6/6	0.94	0.08	16,19,20,22	0
6	EDO	В	510	4/4	0.94	0.11	22,29,32,35	0
4	GOL	D	504	6/6	0.94	0.08	23,26,28,30	0
4	GOL	A	504	6/6	0.96	0.07	19,21,21,22	0
2	NAD	D	501	44/44	0.97	0.07	12,15,17,18	0
5	MG	D	506	1/1	0.97	0.06	16,16,16,16	0
2	NAD	В	501	44/44	0.98	0.06	8,11,13,15	0
2	NAD	С	501	44/44	0.98	0.06	12,15,18,19	0
2	NAD	A	501	44/44	0.98	0.07	8,10,12,15	0
3	ZN	С	503	1/1	0.99	0.06	13,13,13,13	1
3	ZN	D	502	1/1	0.99	0.08	14,14,14,14	1
3	ZN	D	503	1/1	0.99	0.06	14,14,14,14	1
5	MG	A	508	1/1	1.00	0.14	9,9,9,9	0



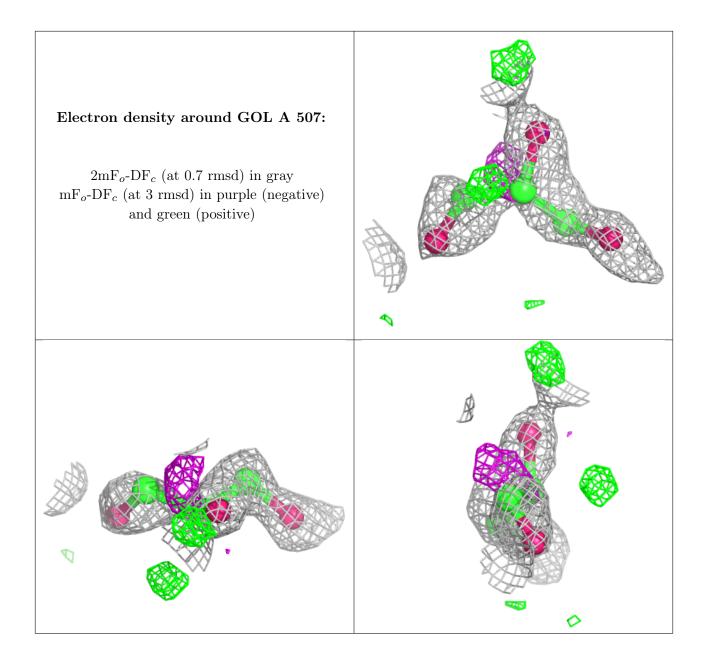
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	MG	В	508	1/1	1.00	0.09	10,10,10,10	0
5	MG	С	505	1/1	1.00	0.07	17,17,17,17	0
3	ZN	С	502	1/1	1.00	0.05	16,16,16,16	0
3	ZN	A	502	1/1	1.00	0.07	12,12,12,12	0
3	ZN	A	503	1/1	1.00	0.07	10,10,10,10	1
3	ZN	В	502	1/1	1.00	0.07	12,12,12,12	0
3	ZN	В	503	1/1	1.00	0.05	11,11,11,11	0

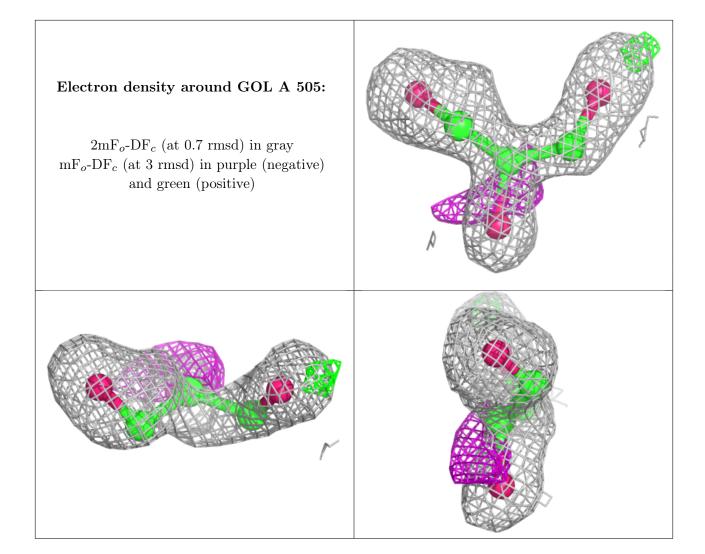
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



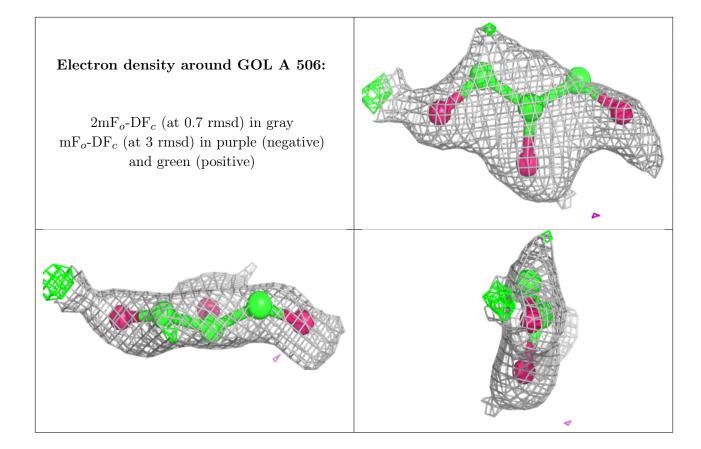




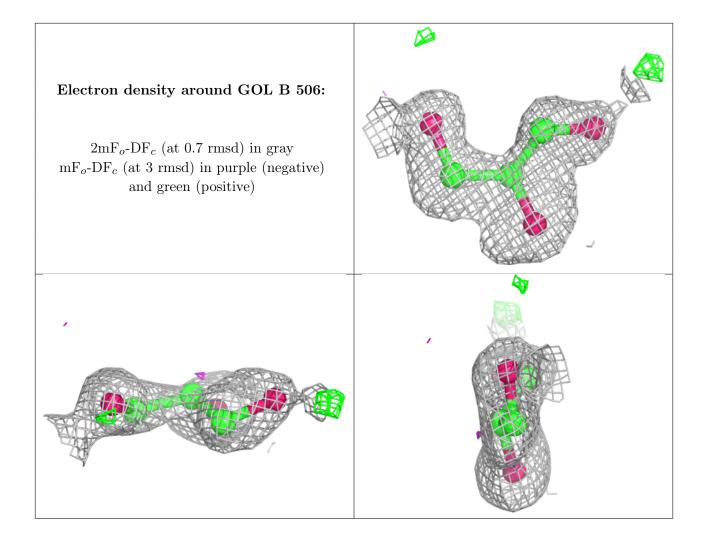




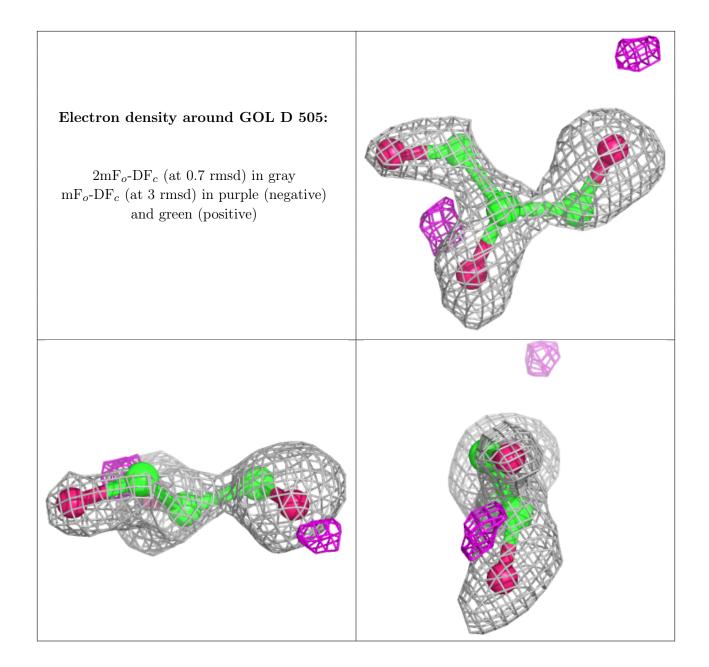




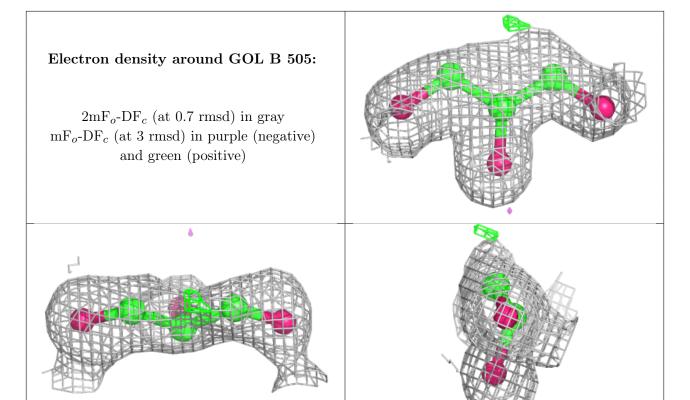




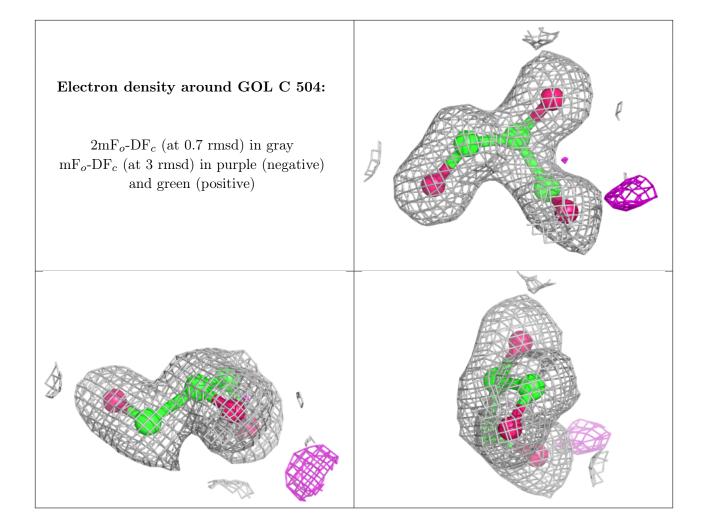




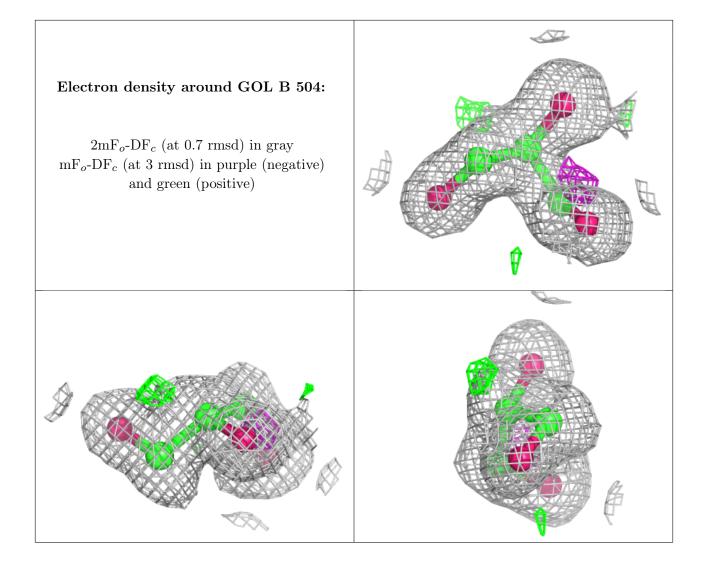




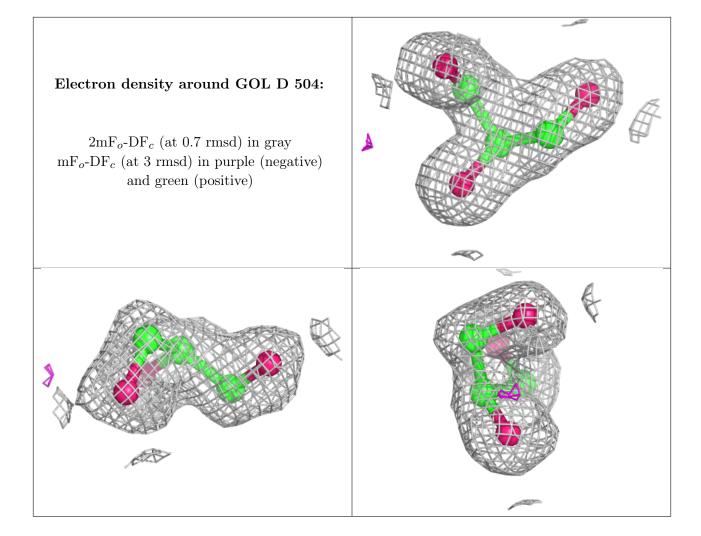




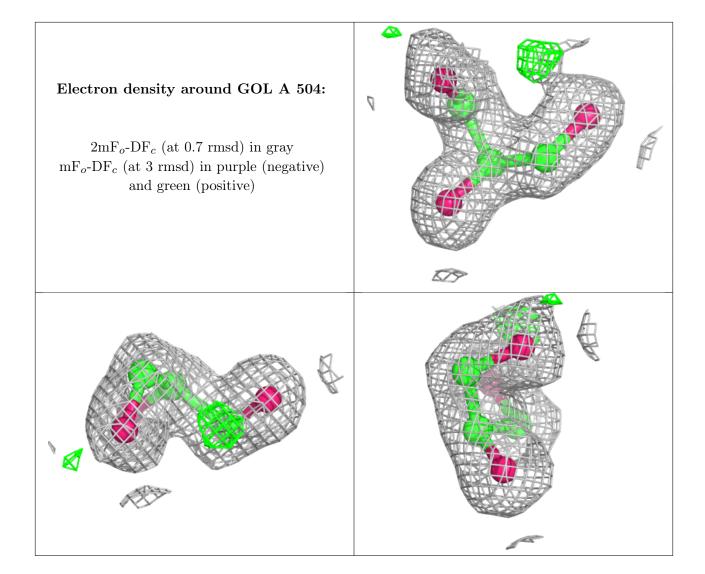








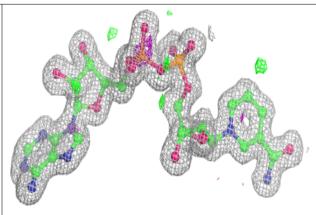


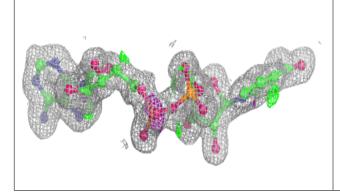


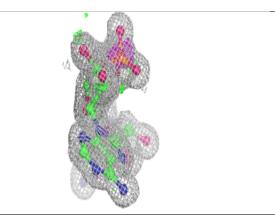


Electron density around NAD D 501:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

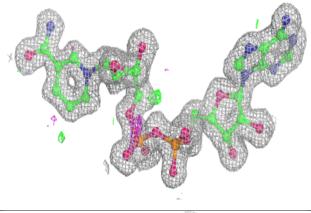


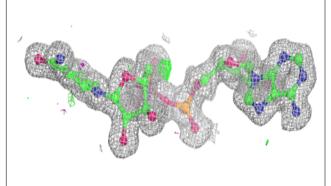


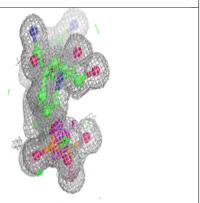


Electron density around NAD B 501:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



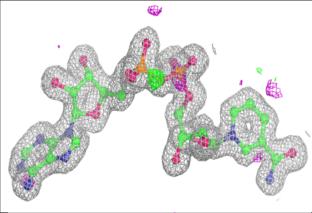


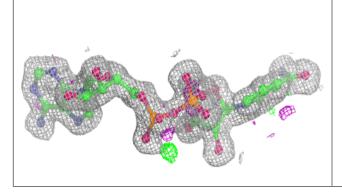


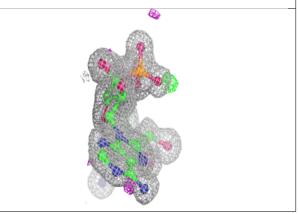


Electron density around NAD C 501:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

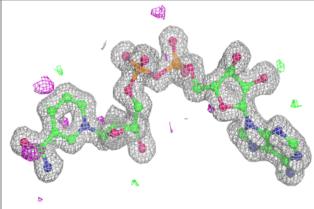


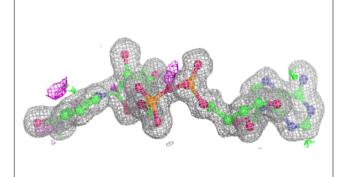


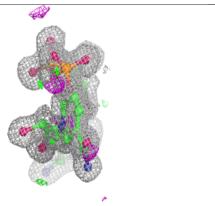


Electron density around NAD A 501:

 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



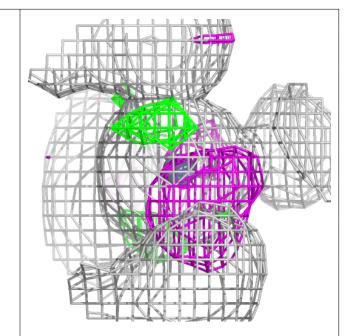


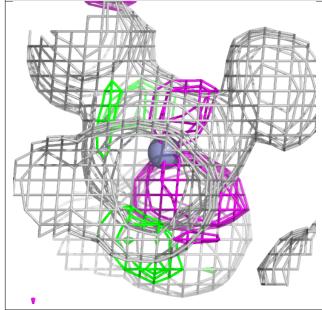


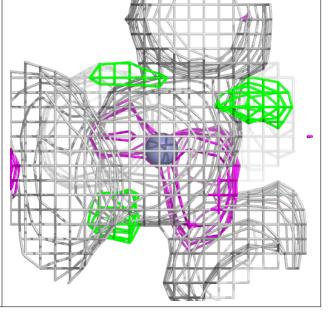


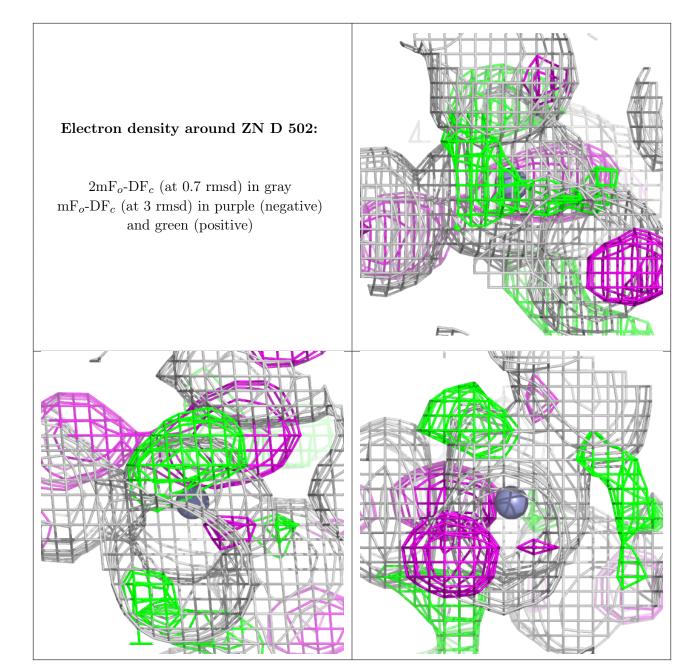
Electron density around ZN C 503:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





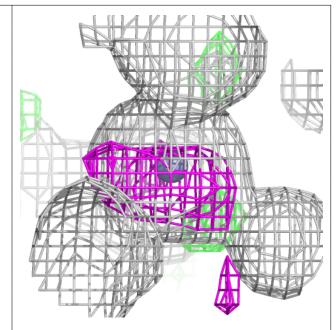


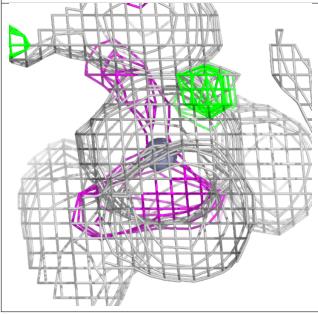


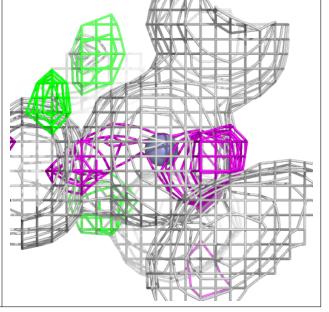


Electron density around ZN D 503:

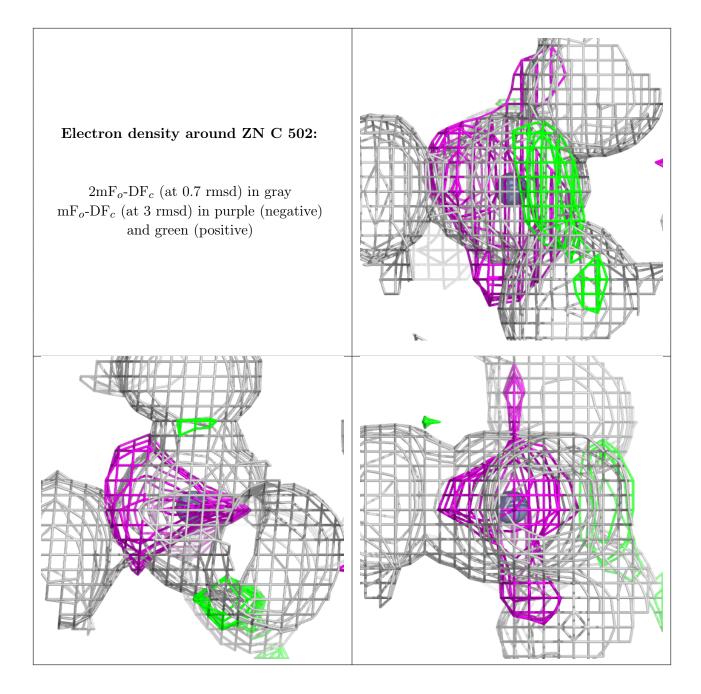
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











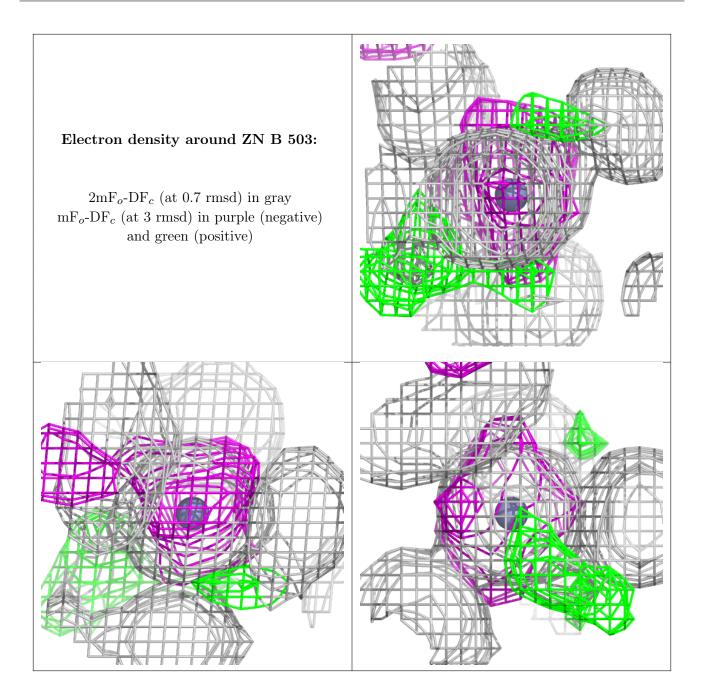




Electron density around ZN A 503: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.

