



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 24, 2025 – 03:19 pm GMT

PDB ID : 8S2R  
Title : BzdNO in partially coenzyme A - free state  
Authors : Ermler, U.; Boll, M.; Fuchs, J.; Demmer, U.  
Deposited on : 2024-02-19  
Resolution : 1.60 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](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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

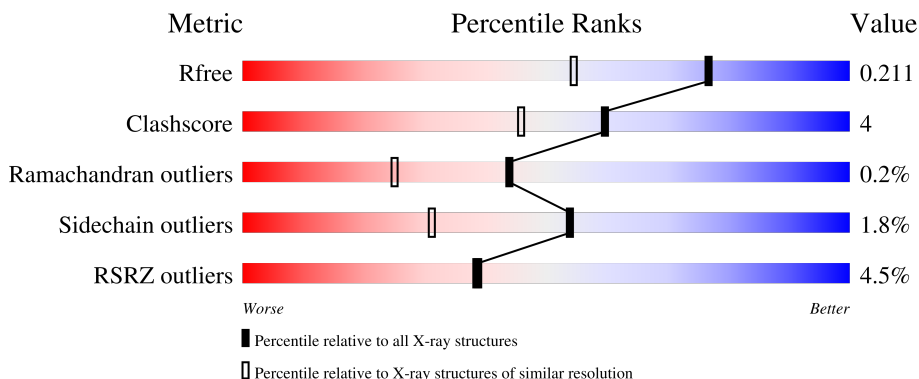
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	447	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	C	447	<div> <div>7%</div> <div>85%</div> <div>10%</div> <div>..</div> </div>
2	B	379	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>..</div> </div>
2	D	379	<div> <div>6%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>

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
4	GOL	A	502	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14200 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 BzdO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	8	0
			3603	2296	619	662	26			
1	C	429	Total	C	N	O	S	0	1	0
			3472	2216	590	641	25			

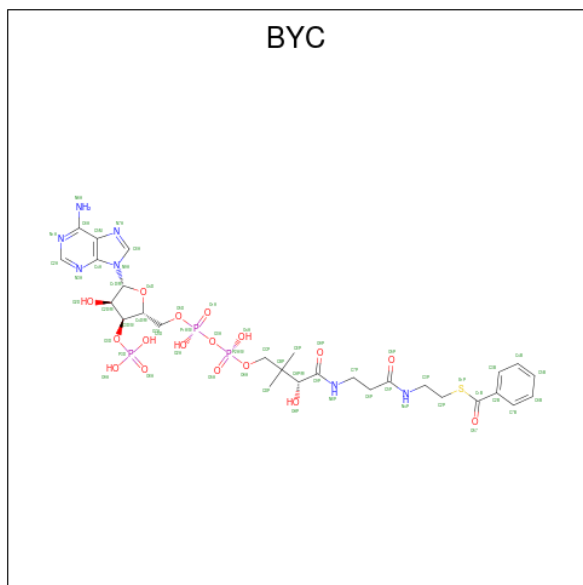
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP Q68VL9
A	439	ALA	-	expression tag	UNP Q68VL9
A	440	TRP	-	expression tag	UNP Q68VL9
A	441	SER	-	expression tag	UNP Q68VL9
A	442	HIS	-	expression tag	UNP Q68VL9
A	443	PRO	-	expression tag	UNP Q68VL9
A	444	GLN	-	expression tag	UNP Q68VL9
A	445	PHE	-	expression tag	UNP Q68VL9
A	446	GLU	-	expression tag	UNP Q68VL9
A	447	LYS	-	expression tag	UNP Q68VL9
C	438	SER	-	expression tag	UNP Q68VL9
C	439	ALA	-	expression tag	UNP Q68VL9
C	440	TRP	-	expression tag	UNP Q68VL9
C	441	SER	-	expression tag	UNP Q68VL9
C	442	HIS	-	expression tag	UNP Q68VL9
C	443	PRO	-	expression tag	UNP Q68VL9
C	444	GLN	-	expression tag	UNP Q68VL9
C	445	PHE	-	expression tag	UNP Q68VL9
C	446	GLU	-	expression tag	UNP Q68VL9
C	447	LYS	-	expression tag	UNP Q68VL9

- Molecule 2 is a protein called BzdN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	5	0
			3064	1943	532	569	20			
2	D	375	Total	C	N	O	S	0	5	0
			3061	1940	531	571	19			

- Molecule 3 is benzoyl coenzyme A (three-letter code: BYC) (formula:  $C_{28}H_{40}N_7O_{17}P_3S$ ).



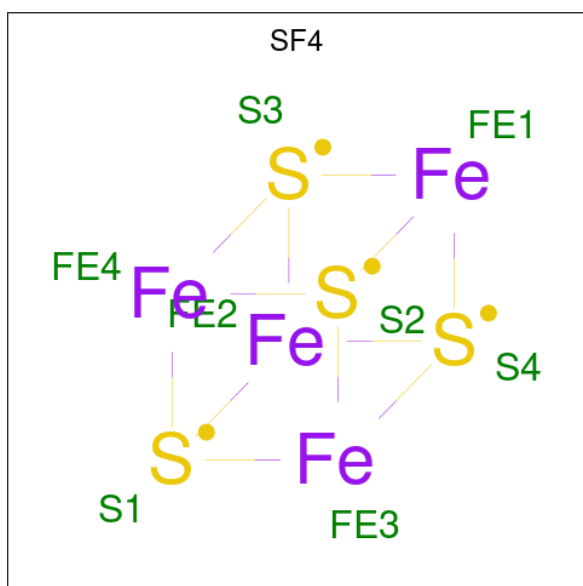
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



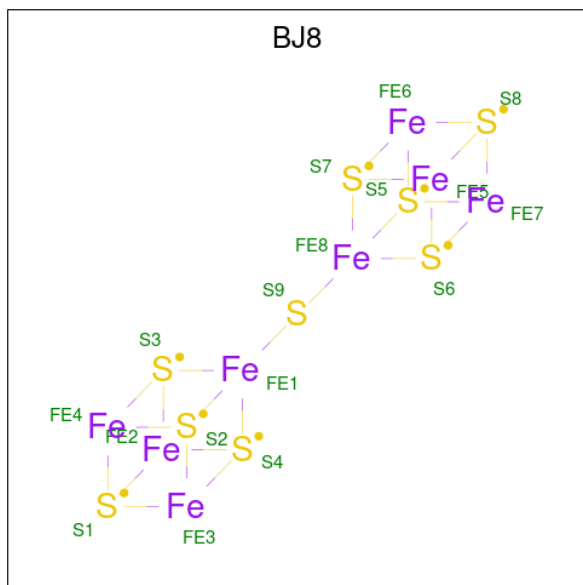
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



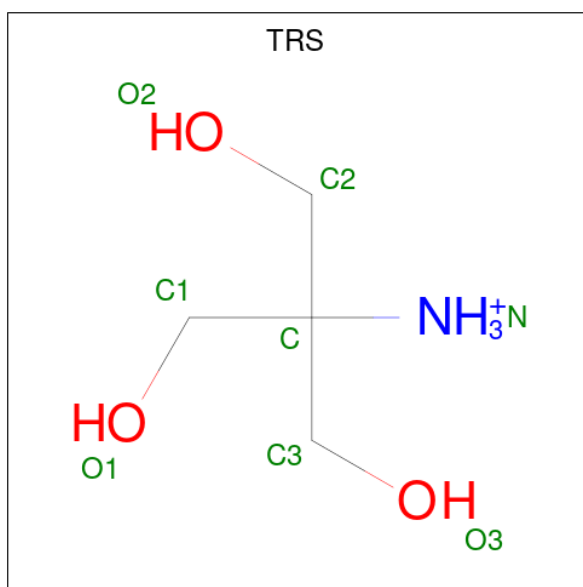
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is Double cubane cluster (three-letter code: BJ8) (formula:  $\text{Fe}_8\text{S}_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			17	8	9		
6	D	1	Total	Fe	S	0	0
			17	8	9		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $\text{C}_4\text{H}_{12}\text{NO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

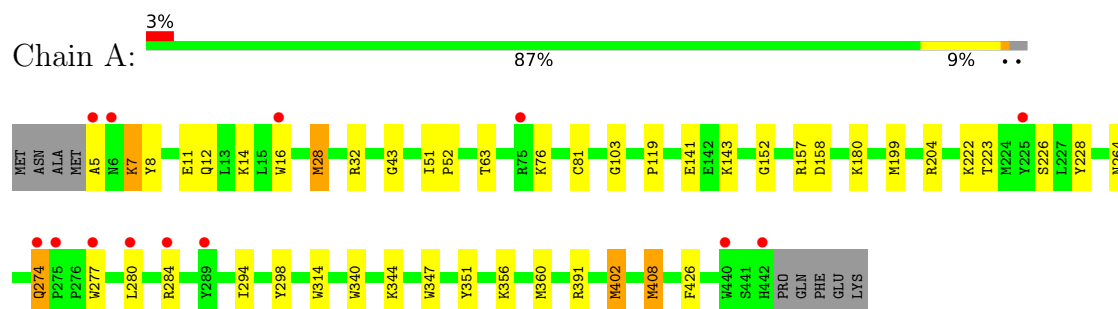
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	257	Total	O	0	1
			258	258		
8	B	161	Total	O	0	1
			162	162		
8	C	219	Total	O	0	2
			221	221		
8	D	156	Total	O	0	1
			157	157		



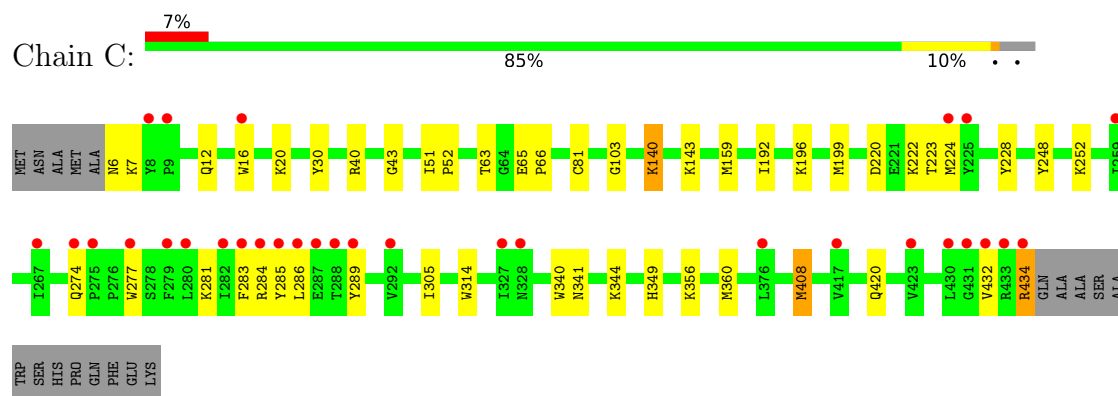
### 3 Residue-property plots [i](#)

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.

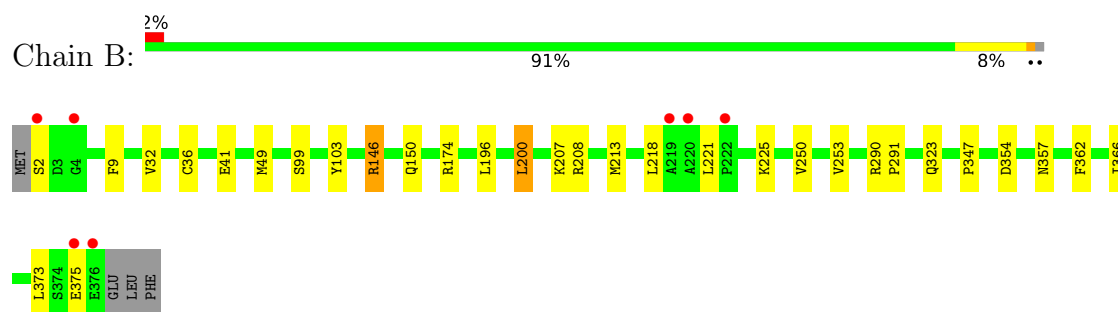
#### • Molecule 1: BzdO



#### • Molecule 1: BzdO

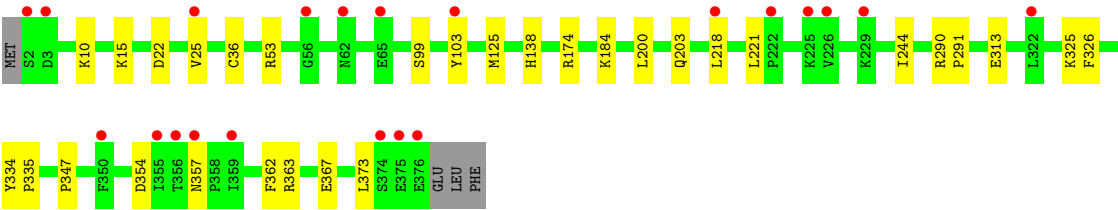


#### • Molecule 2: BzdN



#### • Molecule 2: BzdN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.17Å 102.71Å 86.90Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	48.45 – 1.60 48.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.1 (48.45-1.60) 86.1 (48.45-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.183 , 0.211 0.184 , 0.211	Depositor DCC
$R_{free}$ test set	11748 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.5	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	0.96	EDS
Total number of atoms	14200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% 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: BYC, DOD, BJ8, TRS, SF4, GOL

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	0.80	1/3697 (0.0%)	0.85	0/4992
1	C	0.76	0/3563	0.82	0/4815
2	B	0.71	0/3140	0.82	0/4251
2	D	0.70	0/3137	0.80	0/4249
All	All	0.75	1/13537 (0.0%)	0.82	0/18307

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLN	C-N	7.71	1.48	1.34

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	3603	0	3485	42	0
1	C	3472	0	3357	35	0
2	B	3064	0	2969	15	0
2	D	3061	0	2959	17	0
3	A	56	0	36	4	0
3	C	56	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	8	9	0
4	C	18	0	24	3	0
5	A	8	0	0	0	0
5	C	8	0	0	0	0
6	B	17	0	0	0	0
6	D	17	0	0	0	0
7	B	8	0	12	1	0
7	D	8	0	12	0	0
8	A	258	0	0	5	0
8	B	162	0	0	1	0
8	C	221	0	0	0	0
8	D	157	0	0	1	0
All	All	14200	0	12898	111	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 4.

The worst 5 of 111 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:28[B]:MET:HE3	1:A:32:ARG:HH11	1.22	1.04
1:A:344:LYS:HG3	8:A:631:HOH:O	1.74	0.88
1:A:274:GLN:HB2	8:A:609:HOH:O	1.73	0.87
1:C:434:ARG:O	1:C:434:ARG:HG2	1.85	0.76
1:A:274:GLN:O	1:A:274:GLN:HG2	1.87	0.75

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	444/447 (99%)	432 (97%)	12 (3%)	0	100	100
1	C	428/447 (96%)	419 (98%)	9 (2%)	0	100	100
2	B	378/379 (100%)	368 (97%)	7 (2%)	3 (1%)	16	5
2	D	378/379 (100%)	367 (97%)	8 (2%)	3 (1%)	16	5
All	All	1628/1652 (98%)	1586 (97%)	36 (2%)	6 (0%)	44	14

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	36	CYS
2	D	99[A]	SER
2	D	99[B]	SER
2	B	36	CYS
2	B	99[A]	SER

### 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	371/371 (100%)	361 (97%)	10 (3%)	40	17
1	C	359/371 (97%)	350 (98%)	9 (2%)	42	19
2	B	326/325 (100%)	319 (98%)	7 (2%)	48	25
2	D	326/325 (100%)	324 (99%)	2 (1%)	84	74
All	All	1382/1392 (99%)	1354 (98%)	28 (2%)	54	26

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	323[A]	GLN
2	D	103	TYR
1	C	6	ASN
1	C	432	VAL
2	B	375	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	328	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	BJ8	D	401	2	0,26,26	-	-	-		
5	SF4	C	504	1,8	0,12,12	-	-	-		
4	GOL	C	502	-	5,5,5	1.85	2 (40%)	5,5,5	0.76	0
6	BJ8	B	401	2	0,26,26	-	-	-		
7	TRS	D	402	-	7,7,7	0.67	0	9,9,9	1.02	0
5	SF4	A	503	1,8	0,12,12	-	-	-		
3	BYC	A	501	-	51,59,59	1.65	7 (13%)	64,87,87	2.01	17 (26%)
4	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.32	0
3	BYC	C	501	-	51,59,59	1.57	5 (9%)	64,87,87	1.79	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	503[B]	-	5,5,5	1.43	2 (40%)	5,5,5	0.70	0
4	GOL	C	503[A]	-	5,5,5	0.09	0	5,5,5	0.32	0
7	TRS	B	402	-	7,7,7	0.17	0	9,9,9	0.68	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	BJ8	D	401	2	-	-	0/12/10/10
5	SF4	C	504	1,8	-	-	0/6/5/5
4	GOL	C	502	-	-	2/4/4/4	-
6	BJ8	B	401	2	-	-	0/12/10/10
7	TRS	D	402	-	-	2/9/9/9	-
5	SF4	A	503	1,8	-	-	0/6/5/5
3	BYC	A	501	-	-	20/51/71/71	0/4/4/4
4	GOL	A	502	-	-	0/4/4/4	-
3	BYC	C	501	-	-	17/51/71/71	0/4/4/4
4	GOL	C	503[B]	-	-	2/4/4/4	-
4	GOL	C	503[A]	-	-	4/4/4/4	-
7	TRS	B	402	-	-	2/9/9/9	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	BYC	C5P-N4P	6.33	1.47	1.33
3	C	501	BYC	C9P-N8P	6.18	1.47	1.33
3	A	501	BYC	C9P-N8P	5.65	1.46	1.33
3	C	501	BYC	C5P-N4P	5.38	1.45	1.33
3	A	501	BYC	C2B-C1B	-3.69	1.42	1.49

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	BYC	N3A-C2A-N1A	-6.65	118.29	128.68
3	A	501	BYC	N3A-C2A-N1A	-6.49	118.54	128.68
3	A	501	BYC	C1D-N9A-C4A	-4.43	118.86	126.64
3	A	501	BYC	C3P-N4P-C5P	4.37	130.95	122.84
3	A	501	BYC	C2P-S1P-C1B	4.19	105.06	99.80



There are no chirality outliers.

5 of 49 torsion outliers are listed below:

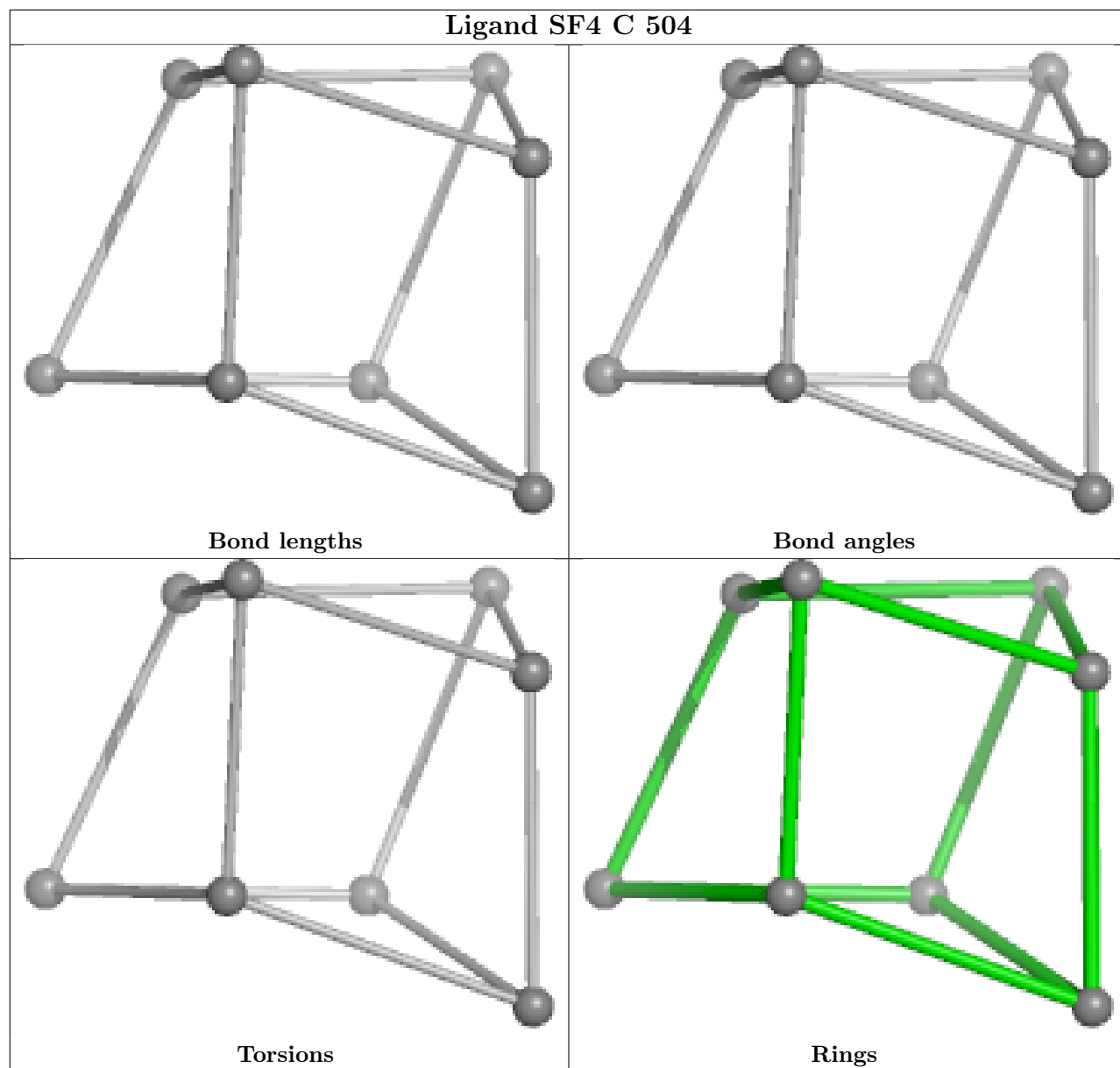
Mol	Chain	Res	Type	Atoms
3	A	501	BYC	C3P-C2P-S1P-C1B
3	A	501	BYC	CCP-O6A-P2A-O3A
3	A	501	BYC	CCP-O6A-P2A-O5A
3	A	501	BYC	C9P-CAP-CBP-CCP
3	A	501	BYC	C9P-CAP-CBP-CDP

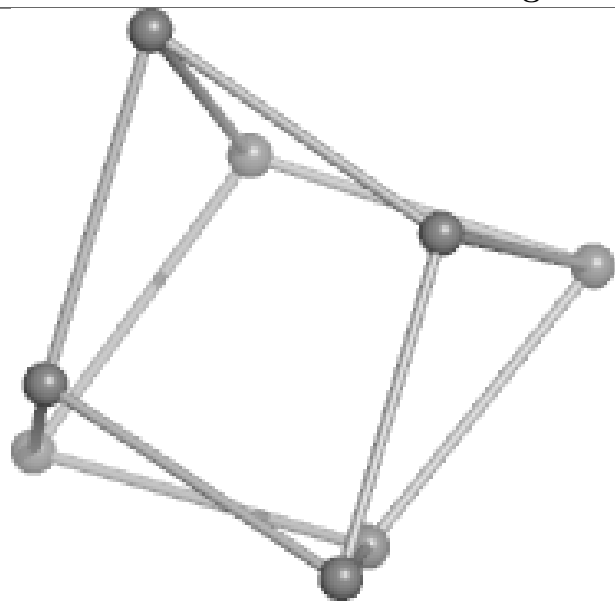
There are no ring outliers.

5 monomers are involved in 22 short contacts:

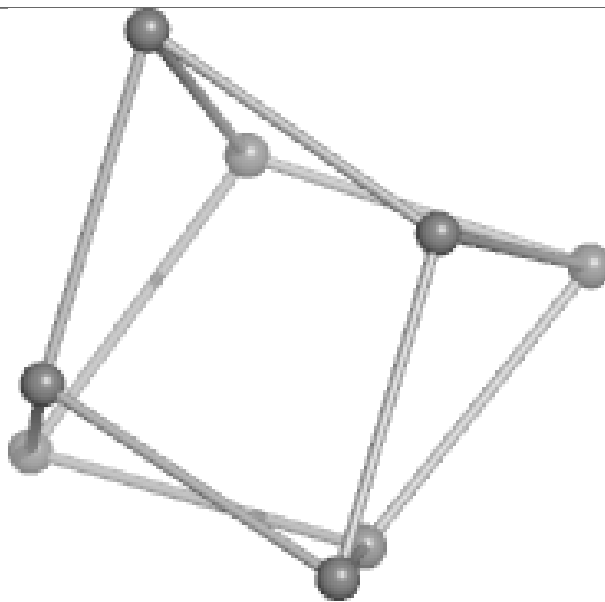
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	GOL	3	0
3	A	501	BYC	4	0
4	A	502	GOL	9	0
3	C	501	BYC	5	0
7	B	402	TRS	1	0

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.

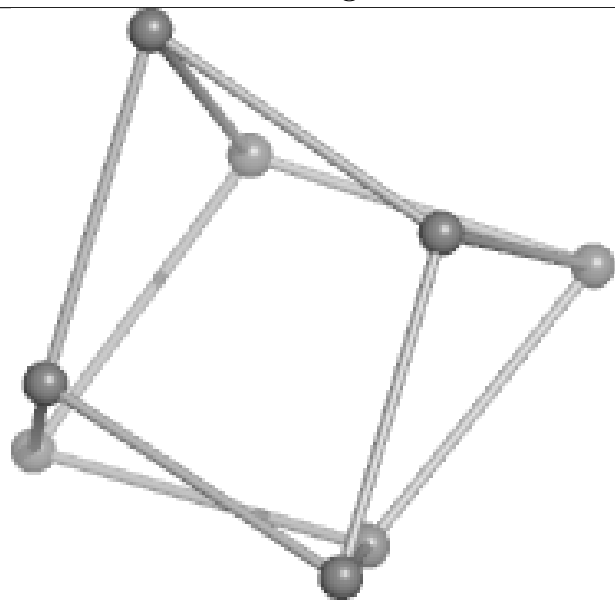


**Ligand SF4 A 503**

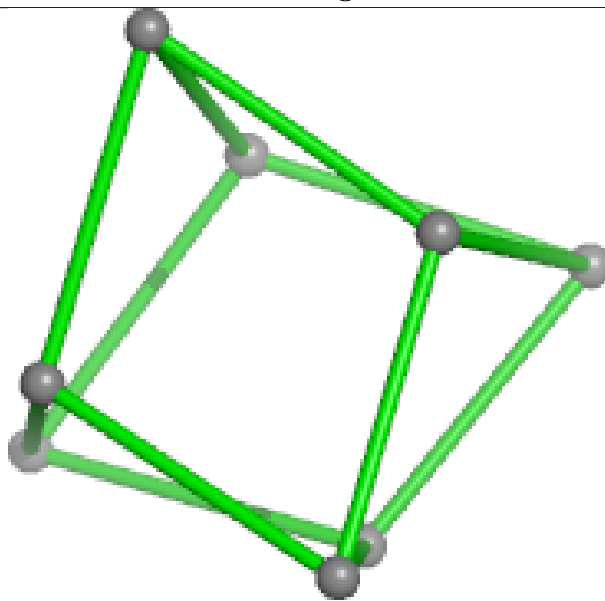
Bond lengths



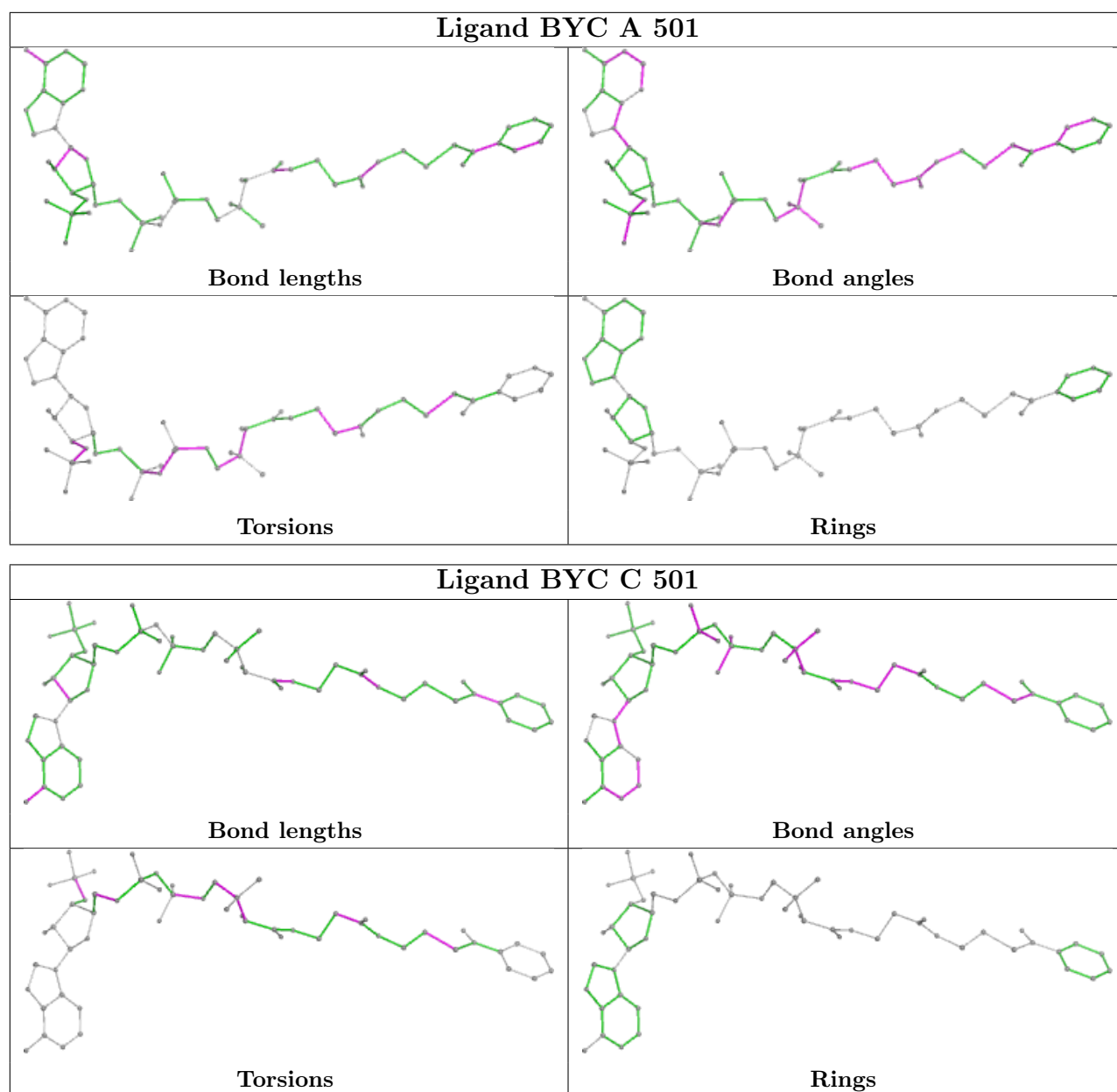
Bond angles



Torsions



Rings



## 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	438/447 (97%)	0.25	13 (2%) 52 53	12, 25, 40, 90	8 (1%)
1	C	429/447 (95%)	0.48	31 (7%) 23 22	16, 28, 54, 107	1 (0%)
2	B	375/379 (98%)	0.42	7 (1%) 66 68	11, 29, 46, 94	5 (1%)
2	D	375/379 (98%)	0.53	21 (5%) 31 30	11, 30, 50, 92	5 (1%)
All	All	1617/1652 (97%)	0.41	72 (4%) 39 38	11, 28, 48, 107	19 (1%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	TRP	5.0
1	C	280	LEU	4.9
1	A	274	GLN	4.3
1	C	283	PHE	4.3
1	C	431	GLY	4.2

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

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

### 6.3 Carbohydrates [i](#)

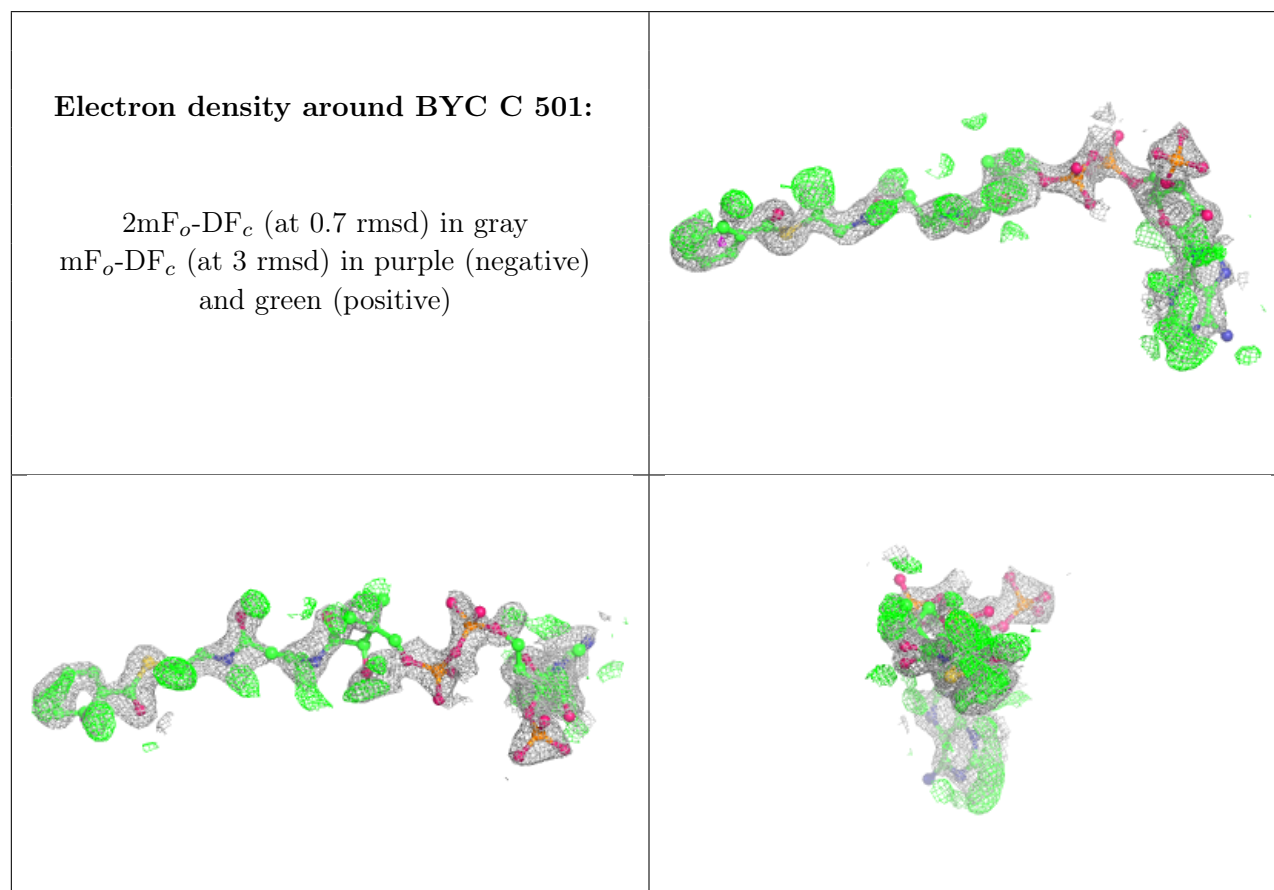
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

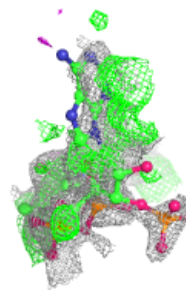
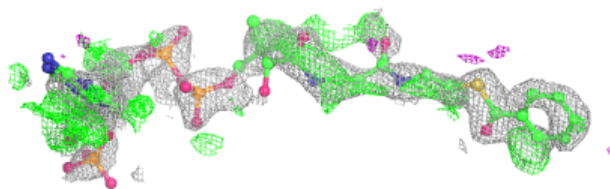
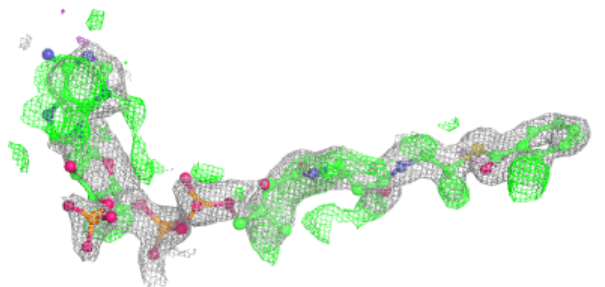
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BYC	C	501	56/56	0.68	0.27	17,43,52,61	56
3	BYC	A	501	56/56	0.69	0.28	15,40,50,56	56
4	GOL	C	502	6/6	0.82	0.13	41,44,45,51	0
4	GOL	A	502	6/6	0.83	0.12	36,37,40,44	0
4	GOL	C	503[A]	6/6	0.87	0.12	27,28,31,34	6
4	GOL	C	503[B]	6/6	0.87	0.12	25,31,34,34	6
7	TRS	D	402	8/8	0.88	0.11	27,28,29,31	0
7	TRS	B	402	8/8	0.90	0.09	26,27,31,42	0
6	BJ8	B	401	17/17	0.99	0.04	21,24,26,27	0
6	BJ8	D	401	17/17	0.99	0.03	23,24,27,28	0
5	SF4	A	503	8/8	0.99	0.03	19,20,21,23	0
5	SF4	C	504	8/8	0.99	0.03	21,21,23,25	0

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



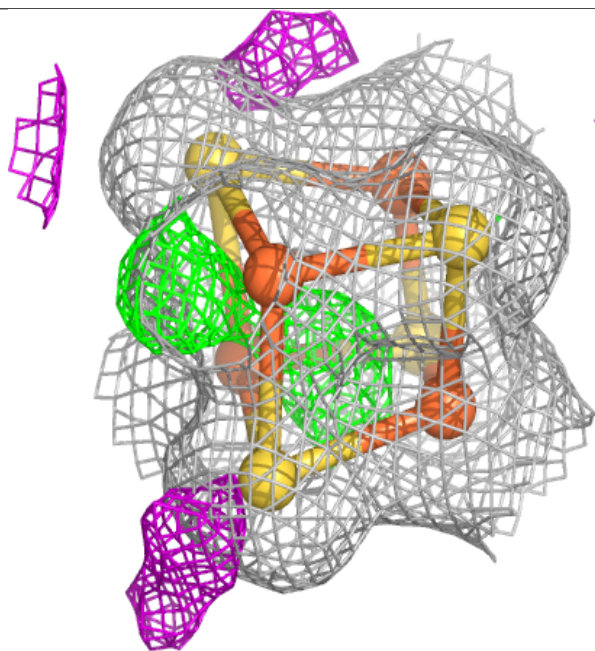
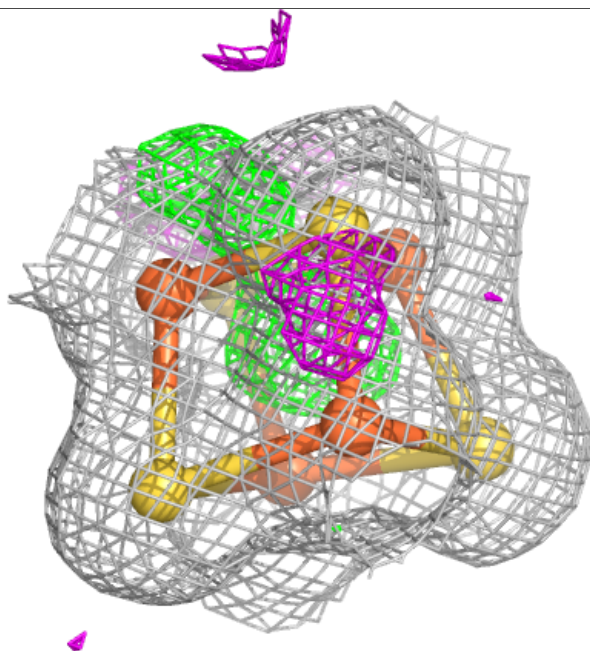
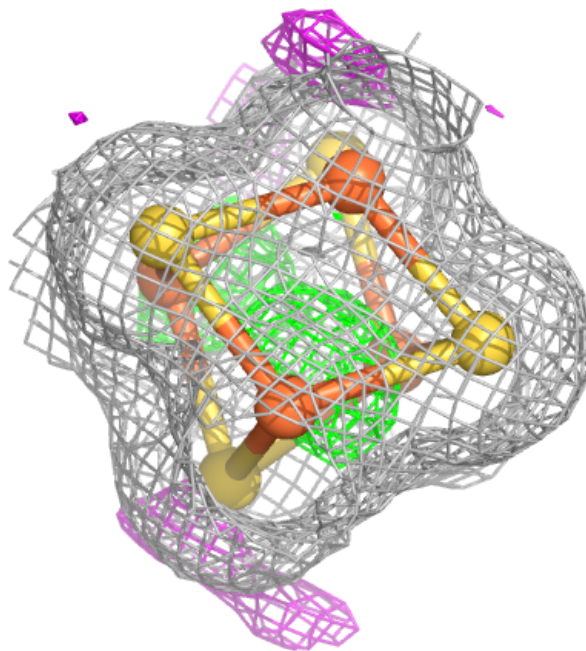
**Electron density around BYC A 501:**

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



**Electron density around SF4 A 503:**

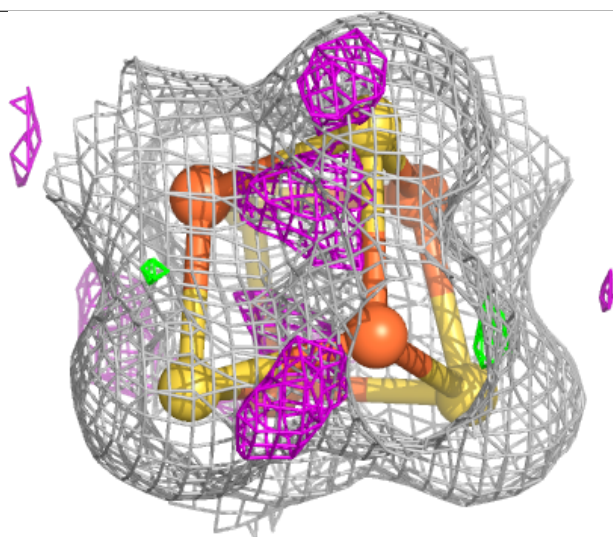
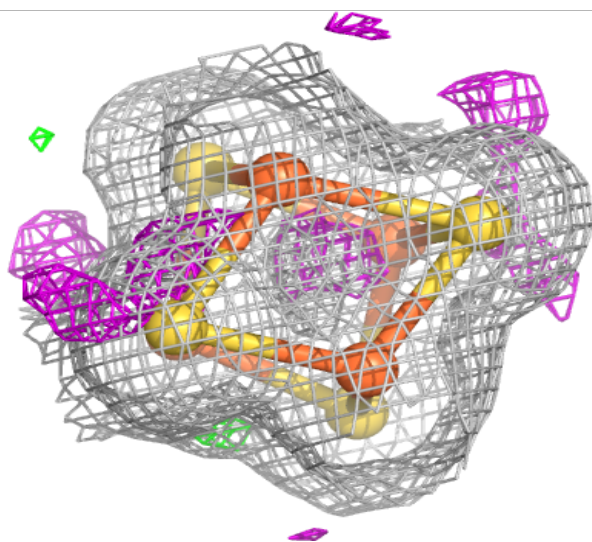
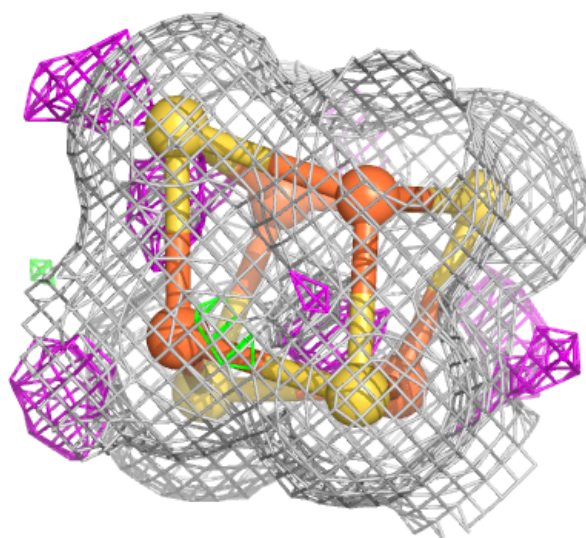
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SF4 C 504:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.