



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 04:48 AM EST

PDB ID : 4ZR1  
Title : Hydroxylase domain of scs7p  
Authors : Zhu, G.; Koszelak-Rosenblum, M.; Malkowski, M.G.; Membrane Protein Structural Biology Consortium (MPSBC)  
Deposited on : 2015-05-11  
Resolution : 2.60 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 : 4.02b-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 : 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

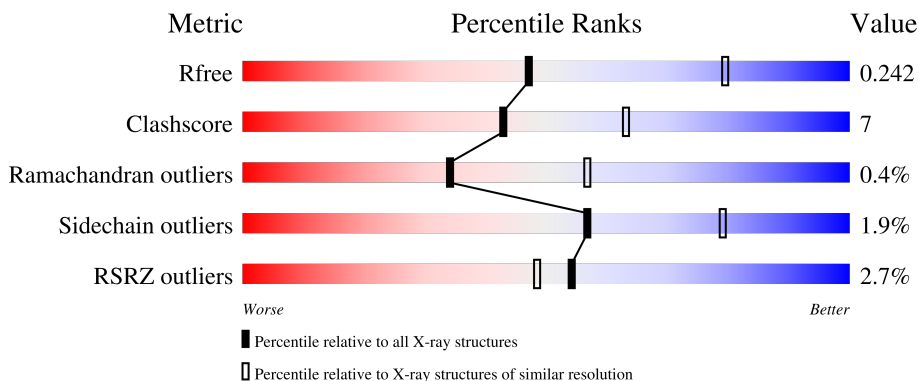
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	298	
1	B	298	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BOG	A	405	-	-	-	X
4	TRD	B	409	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4859 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 Ceramide very long chain fatty acid hydroxylase SCS7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2287	1538	365	371	13	0	0	0
1	B	275	2304	1553	366	372	13	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	MET	-	initiating methionine	UNP Q03529
A	385	SER	-	expression tag	UNP Q03529
A	386	GLY	-	expression tag	UNP Q03529
A	387	LEU	-	expression tag	UNP Q03529
A	388	GLU	-	expression tag	UNP Q03529
A	389	VAL	-	expression tag	UNP Q03529
A	390	LEU	-	expression tag	UNP Q03529
A	391	PHE	-	expression tag	UNP Q03529
A	392	GLN	-	expression tag	UNP Q03529
B	95	MET	-	initiating methionine	UNP Q03529
B	385	SER	-	expression tag	UNP Q03529
B	386	GLY	-	expression tag	UNP Q03529
B	387	LEU	-	expression tag	UNP Q03529
B	388	GLU	-	expression tag	UNP Q03529
B	389	VAL	-	expression tag	UNP Q03529
B	390	LEU	-	expression tag	UNP Q03529
B	391	PHE	-	expression tag	UNP Q03529
B	392	GLN	-	expression tag	UNP Q03529

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

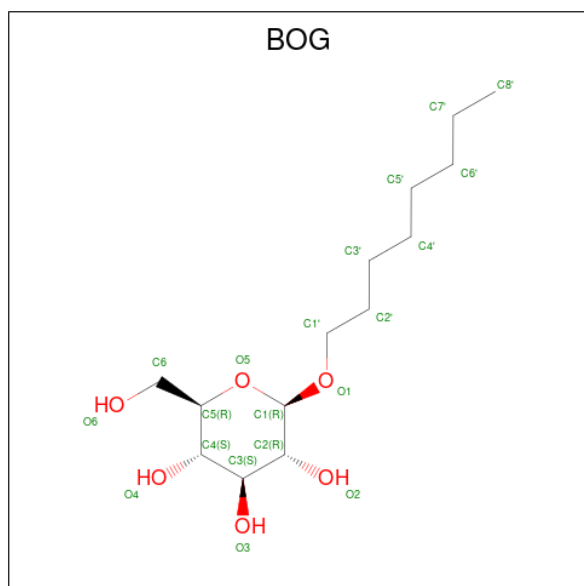
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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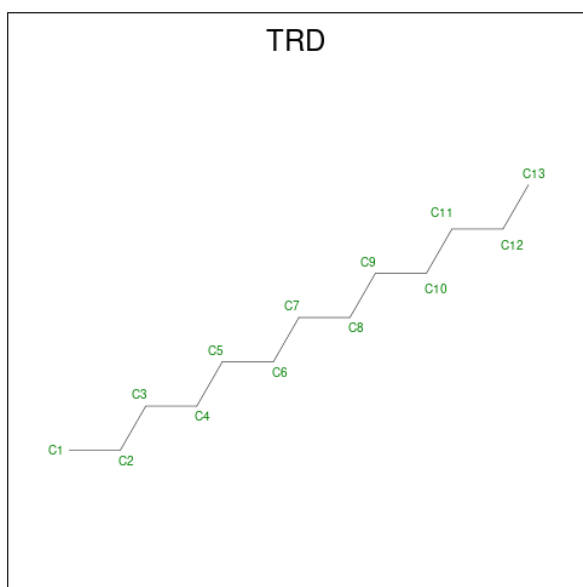
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0
3	B	1	Total C O 20 14 6	0	0
3	B	1	Total C O 20 14 6	0	0

- Molecule 4 is TRIDECANE (three-letter code: TRD) (formula:  $C_{13}H_{28}$ ).

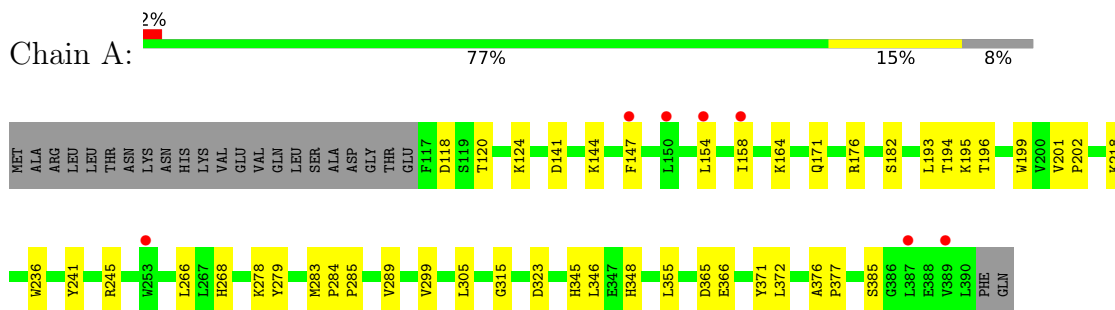


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 13 13	0	0
4	A	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 13 13	0	0

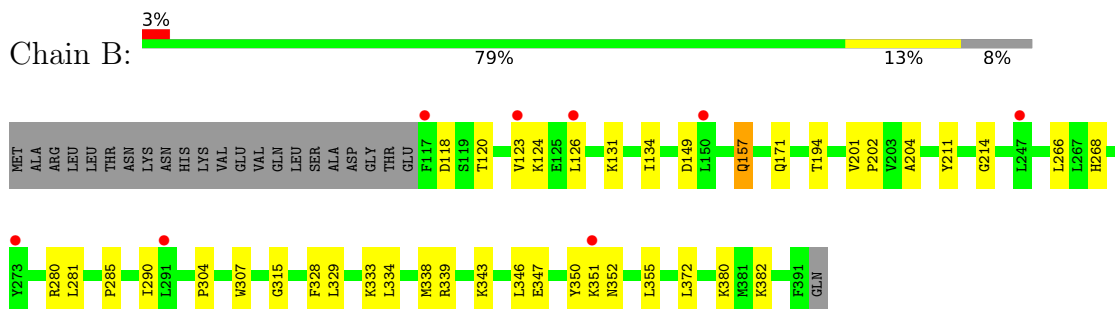
### 3 Residue-property plots [i](#)

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: Ceramide very long chain fatty acid hydroxylase SCS7



- Molecule 1: Ceramide very long chain fatty acid hydroxylase SCS7



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.76Å 202.76Å 202.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 2.60 47.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.79-2.60) 93.4 (47.79-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.75 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, $R_{free}$	0.197 , 0.239 0.207 , 0.242	Depositor DCC
$R_{free}$ test set	2138 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.104 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRD, ZN, BOG

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	0.36	0/2379	0.50	0/3236
1	B	0.40	0/2398	0.56	0/3261
All	All	0.38	0/4777	0.53	0/6497

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2287	0	2229	27	0
1	B	2304	0	2245	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	120	0	168	7	0
3	B	40	0	56	3	0
4	A	26	0	56	5	0
4	B	78	0	168	8	0
All	All	4859	0	4922	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (66) 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:283:MET:HG2	3:A:403:BOG:H61	1.53	0.87
1:B:355:LEU:HB2	1:B:372:LEU:HD23	1.66	0.75
1:B:343:LYS:O	1:B:347:GLU:HG3	1.93	0.69
1:A:355:LEU:HB2	1:A:372:LEU:HD13	1.76	0.68
1:B:123:VAL:HG12	1:B:351:LYS:HZ2	1.59	0.66
1:B:123:VAL:HG22	1:B:124:LYS:H	1.62	0.64
1:B:380:LYS:HD3	1:B:382:LYS:HE3	1.82	0.61
1:A:199:TRP:CE2	3:A:408:BOG:H4'2	2.36	0.60
1:B:285:PRO:HG2	3:B:403:BOG:H2'1	1.84	0.59
1:A:315:GLY:HA3	4:A:409:TRD:H71	1.85	0.59
1:A:218:LYS:HD2	1:A:218:LYS:O	2.04	0.58
1:A:182:SER:HB2	1:A:195:LYS:HE3	1.87	0.57
1:B:329:LEU:HD23	1:B:334:LEU:HD11	1.87	0.56
1:B:334:LEU:O	1:B:339:ARG:NH2	2.39	0.56
1:B:214:GLY:HA3	4:B:410:TRD:H52	1.88	0.56
1:A:241:TYR:OH	1:A:245:ARG:NH1	2.39	0.55
1:B:123:VAL:O	1:B:351:LYS:HD2	2.07	0.54
1:B:281:LEU:O	4:B:406:TRD:H22	2.07	0.54
1:B:204:ALA:HB1	3:B:403:BOG:H5'1	1.90	0.53
1:B:350:TYR:HB3	1:B:351:LYS:NZ	2.23	0.53
1:B:266:LEU:HD22	4:B:406:TRD:H82	1.91	0.53
1:A:118:ASP:OD2	1:A:120:THR:OG1	2.20	0.52
1:B:304:PRO:HG2	1:B:307:TRP:CD2	2.44	0.52
1:A:193:LEU:HD11	1:B:290:ILE:HD11	1.91	0.52
1:B:380:LYS:HD3	1:B:382:LYS:HG3	1.91	0.52
3:A:408:BOG:H5'2	1:B:211:TYR:CD2	2.45	0.51
1:B:352:ASN:HB3	1:B:372:LEU:HD21	1.95	0.49
1:A:194:THR:HA	3:A:403:BOG:H4'1	1.94	0.49
1:B:304:PRO:HG2	1:B:307:TRP:CG	2.48	0.49
3:B:404:BOG:O2	3:B:404:BOG:H1'1	2.13	0.49
1:A:141:ASP:OD1	1:A:176:ARG:NH2	2.45	0.48
1:B:131:LYS:HA	1:B:134:ILE:HG13	1.94	0.48
1:A:278:LYS:HE3	1:A:279:TYR:CE2	2.49	0.47
1:A:144:LYS:O	1:A:385:SER:HA	2.13	0.47
1:A:283:MET:CG	3:A:403:BOG:H61	2.36	0.47
1:B:315:GLY:HA3	4:B:405:TRD:H52	1.97	0.47
1:B:149:ASP:N	1:B:157:GLN:OE1	2.32	0.47
1:A:147:PHE:CG	1:A:171:GLN:HG2	2.50	0.46
1:B:118:ASP:OD2	1:B:120:THR:OG1	2.17	0.46
4:B:409:TRD:H42	4:B:409:TRD:H12	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD23	1:B:351:LYS:HE2	1.96	0.46
1:B:126:LEU:HD21	1:B:347:GLU:HG2	1.98	0.46
1:A:201:VAL:HB	1:A:202:PRO:HD3	1.97	0.46
1:B:123:VAL:HG12	1:B:351:LYS:NZ	2.29	0.45
1:B:328:PHE:HE1	4:B:408:TRD:H31	1.81	0.45
1:B:131:LYS:HE2	1:B:134:ILE:HD11	1.99	0.44
1:A:196:THR:HG21	1:A:284:PRO:HB3	1.99	0.44
1:B:334:LEU:HD13	1:B:338:MET:HG2	2.00	0.44
4:A:410:TRD:H41	4:B:407:TRD:H11	1.99	0.44
4:A:410:TRD:H62	4:A:410:TRD:H31	1.78	0.44
1:A:283:MET:HE2	1:A:283:MET:HB3	1.45	0.44
1:A:345:HIS:O	1:A:348:HIS:HB3	2.16	0.44
1:B:194:THR:O	1:B:280:ARG:NE	2.42	0.43
1:A:236:TRP:HZ3	4:A:409:TRD:H32	1.83	0.43
1:A:365:ASP:HB3	1:A:371:TYR:HA	2.00	0.43
1:B:328:PHE:CE2	4:B:408:TRD:H102	2.54	0.43
1:A:285:PRO:O	1:A:289:VAL:HG23	2.19	0.42
1:B:333:LYS:HD3	1:B:333:LYS:HA	1.87	0.42
1:A:171:GLN:HG3	1:A:176:ARG:NH1	2.35	0.42
1:B:201:VAL:HB	1:B:202:PRO:HD3	2.01	0.41
1:B:350:TYR:O	1:B:351:LYS:HD3	2.20	0.41
1:A:299:VAL:HG21	4:A:409:TRD:H102	2.01	0.41
1:A:266:LEU:HD22	3:A:403:BOG:H3'1	2.03	0.41
3:A:404:BOG:H8'3	3:A:404:BOG:H5'1	1.87	0.40
1:A:154:LEU:O	1:A:158:ILE:HG13	2.21	0.40
1:A:376:ALA:HA	1:A:377:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/298 (91%)	259 (95%)	12 (4%)	1 (0%)	34	57
1	B	273/298 (92%)	257 (94%)	15 (6%)	1 (0%)	34	57
All	All	545/596 (91%)	516 (95%)	27 (5%)	2 (0%)	34	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	B	268	HIS

### 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	242/264 (92%)	236 (98%)	6 (2%)	47	73
1	B	244/264 (92%)	241 (99%)	3 (1%)	71	87
All	All	486/528 (92%)	477 (98%)	9 (2%)	57	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	A	164	LYS
1	A	305	LEU
1	A	323	ASP
1	A	346	LEU
1	A	366	GLU
1	B	157	GLN
1	B	171	GLN
1	B	346	LEU

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

Mol	Chain	Res	Type
1	A	171	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	BOG	A	408	-	20,20,20	0.52	0	25,25,25	0.99	1 (4%)
3	BOG	B	404	-	20,20,20	0.48	0	25,25,25	0.88	0
4	TRD	B	407	-	12,12,12	0.14	0	11,11,11	0.79	0
4	TRD	B	405	-	12,12,12	0.17	0	11,11,11	0.75	0
3	BOG	A	407	-	20,20,20	0.47	0	25,25,25	0.81	1 (4%)
3	BOG	A	403	-	20,20,20	0.54	0	25,25,25	1.11	3 (12%)
4	TRD	A	409	-	12,12,12	0.21	0	11,11,11	0.62	0
4	TRD	B	408	-	12,12,12	0.13	0	11,11,11	0.77	0
4	TRD	A	410	-	12,12,12	0.12	0	11,11,11	0.84	0
3	BOG	A	406	-	20,20,20	0.46	0	25,25,25	0.92	1 (4%)
3	BOG	B	403	-	20,20,20	0.54	0	25,25,25	1.15	2 (8%)
4	TRD	B	406	-	12,12,12	0.14	0	11,11,11	0.80	0
4	TRD	B	409	-	12,12,12	0.12	0	11,11,11	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TRD	B	410	-	12,12,12	0.16	0	11,11,11	0.68	0
3	BOG	A	405	-	20,20,20	0.50	0	25,25,25	0.96	1 (4%)
3	BOG	A	404	-	20,20,20	0.44	0	25,25,25	0.89	1 (4%)

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	BOG	A	408	-	-	8/11/31/31	0/1/1/1
3	BOG	B	404	-	-	8/11/31/31	0/1/1/1
4	TRD	B	407	-	-	4/10/10/10	-
4	TRD	B	405	-	-	3/10/10/10	-
3	BOG	A	407	-	-	8/11/31/31	0/1/1/1
3	BOG	A	403	-	-	7/11/31/31	0/1/1/1
4	TRD	A	409	-	-	2/10/10/10	-
4	TRD	B	408	-	-	5/10/10/10	-
4	TRD	A	410	-	-	2/10/10/10	-
3	BOG	A	406	-	-	6/11/31/31	0/1/1/1
3	BOG	B	403	-	-	6/11/31/31	0/1/1/1
4	TRD	B	406	-	-	6/10/10/10	-
4	TRD	B	409	-	-	5/10/10/10	-
4	TRD	B	410	-	-	3/10/10/10	-
3	BOG	A	405	-	-	7/11/31/31	0/1/1/1
3	BOG	A	404	-	-	3/11/31/31	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	BOG	C1-O5-C5	-3.54	106.74	113.69
3	A	405	BOG	C1-O5-C5	-3.38	107.05	113.69
3	A	406	BOG	C1-O5-C5	-3.14	107.52	113.69
3	B	403	BOG	C1-O5-C5	-3.14	107.53	113.69
3	A	403	BOG	O5-C5-C6	2.60	112.90	106.44
3	A	403	BOG	C1-O5-C5	-2.60	108.59	113.69
3	A	403	BOG	C6-C5-C4	-2.46	107.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	BOG	O3-C3-C2	-2.43	104.73	110.35
3	A	404	BOG	C1-O5-C5	-2.21	109.35	113.69
3	A	407	BOG	C1-O5-C5	-2.08	109.60	113.69

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	BOG	C2-C1-O1-C1'
3	A	405	BOG	O5-C1-O1-C1'
3	A	406	BOG	C2'-C1'-O1-C1
3	A	408	BOG	O5-C1-O1-C1'
3	B	404	BOG	O5-C1-O1-C1'
3	A	404	BOG	O5-C5-C6-O6
3	A	408	BOG	O5-C5-C6-O6
3	A	407	BOG	O5-C5-C6-O6
3	A	406	BOG	O5-C5-C6-O6
3	B	403	BOG	O5-C5-C6-O6
3	A	406	BOG	C4-C5-C6-O6
3	A	408	BOG	C2-C1-O1-C1'
3	B	404	BOG	C2-C1-O1-C1'
3	A	404	BOG	C4-C5-C6-O6
3	B	403	BOG	C4-C5-C6-O6
3	A	403	BOG	O5-C5-C6-O6
3	B	404	BOG	O5-C5-C6-O6
4	B	408	TRD	C3-C4-C5-C6
4	B	409	TRD	C2-C3-C4-C5
3	A	407	BOG	C4-C5-C6-O6
3	A	407	BOG	O1-C1'-C2'-C3'
4	B	405	TRD	C11-C10-C9-C8
4	B	406	TRD	C6-C7-C8-C9
3	A	408	BOG	C4-C5-C6-O6
3	B	404	BOG	C2'-C3'-C4'-C5'
4	A	410	TRD	C2-C3-C4-C5
3	A	408	BOG	C1'-C2'-C3'-C4'
4	B	409	TRD	C9-C10-C11-C12
4	B	409	TRD	C3-C4-C5-C6
3	A	408	BOG	C2'-C1'-O1-C1
3	B	403	BOG	C2'-C1'-O1-C1
3	B	403	BOG	C4'-C5'-C6'-C7'
4	B	405	TRD	C6-C7-C8-C9
4	A	409	TRD	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	B	408	TRD	C7-C8-C9-C10
3	A	403	BOG	C1'-C2'-C3'-C4'
4	B	408	TRD	C6-C7-C8-C9
4	B	406	TRD	C3-C4-C5-C6
4	B	407	TRD	C3-C4-C5-C6
4	B	408	TRD	C2-C3-C4-C5
4	B	406	TRD	C2-C3-C4-C5
3	A	405	BOG	C3'-C4'-C5'-C6'
4	B	410	TRD	C5-C6-C7-C8
3	A	408	BOG	C2'-C3'-C4'-C5'
3	B	403	BOG	C2'-C3'-C4'-C5'
3	A	403	BOG	C2-C1-O1-C1'
3	A	405	BOG	C4-C5-C6-O6
4	B	406	TRD	C7-C8-C9-C10
4	B	409	TRD	C1-C2-C3-C4
3	A	403	BOG	C4-C5-C6-O6
4	B	405	TRD	C5-C6-C7-C8
3	A	406	BOG	C4'-C5'-C6'-C7'
4	B	408	TRD	C1-C2-C3-C4
4	B	409	TRD	C11-C10-C9-C8
3	B	403	BOG	C3'-C4'-C5'-C6'
3	B	404	BOG	C2'-C1'-O1-C1
4	B	410	TRD	C2-C3-C4-C5
4	B	407	TRD	C4-C5-C6-C7
3	A	407	BOG	C2'-C3'-C4'-C5'
3	B	404	BOG	C3'-C4'-C5'-C6'
3	A	403	BOG	O5-C1-O1-C1'
3	A	403	BOG	C2'-C3'-C4'-C5'
4	B	406	TRD	C11-C10-C9-C8
3	A	406	BOG	C3'-C4'-C5'-C6'
3	A	407	BOG	C4'-C5'-C6'-C7'
3	A	405	BOG	C4'-C5'-C6'-C7'
3	A	406	BOG	C2'-C3'-C4'-C5'
3	A	407	BOG	C1'-C2'-C3'-C4'
3	A	405	BOG	O5-C5-C6-O6
3	B	404	BOG	C4-C5-C6-O6
3	A	403	BOG	O1-C1'-C2'-C3'
4	B	407	TRD	C2-C3-C4-C5
3	A	407	BOG	O5-C1-O1-C1'
3	B	404	BOG	C4'-C5'-C6'-C7'
4	B	406	TRD	C1-C2-C3-C4
4	A	409	TRD	C6-C7-C8-C9

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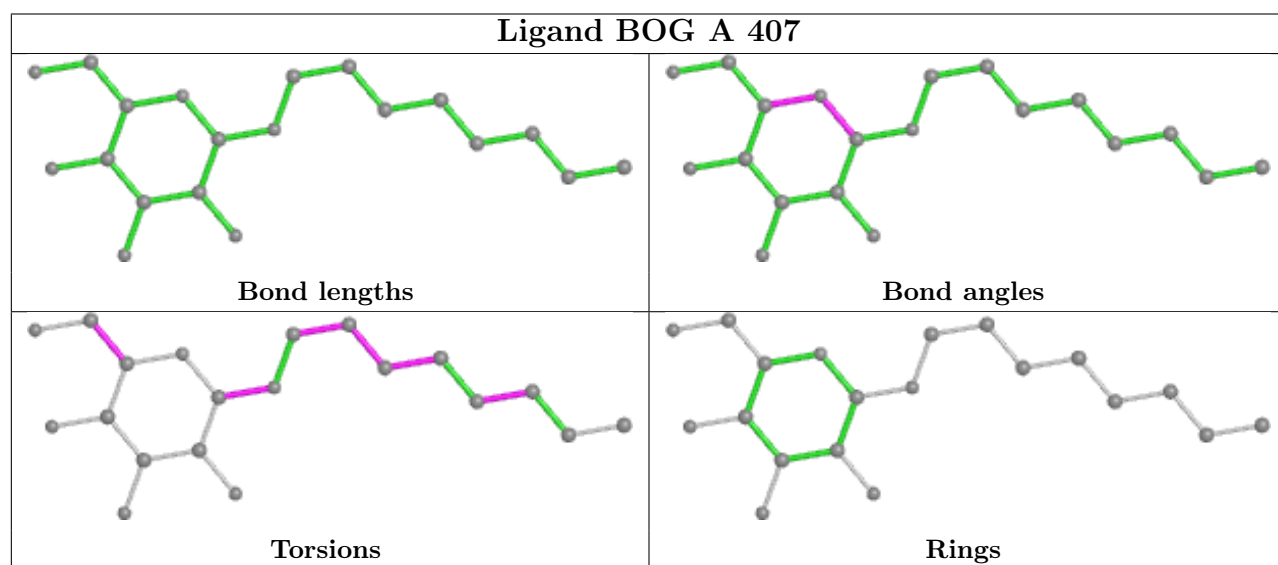
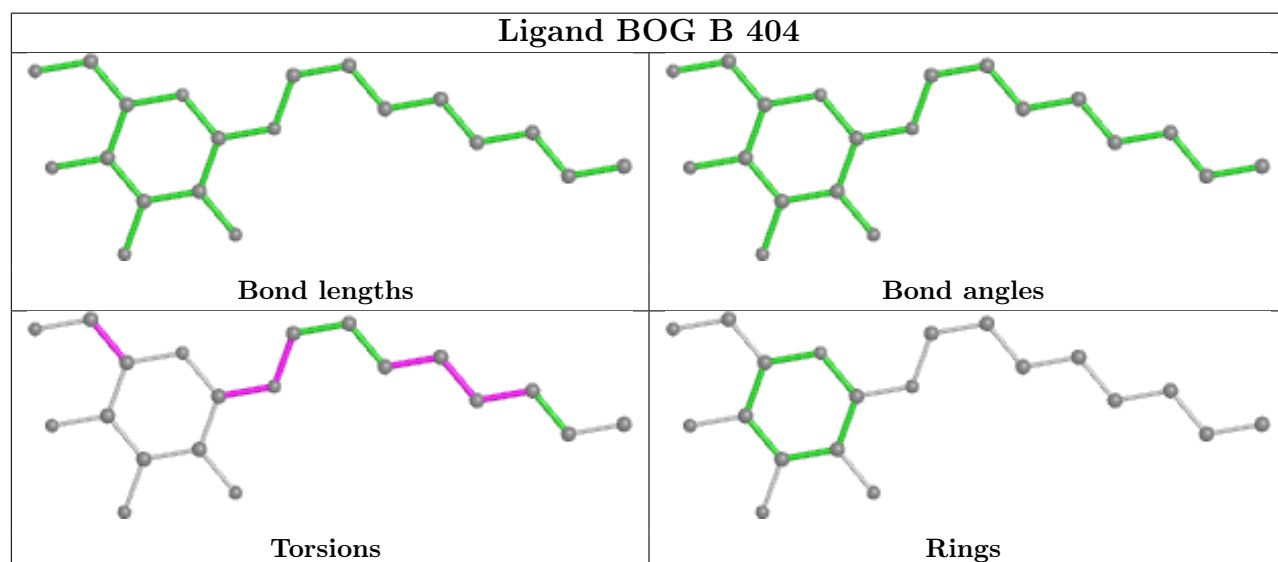
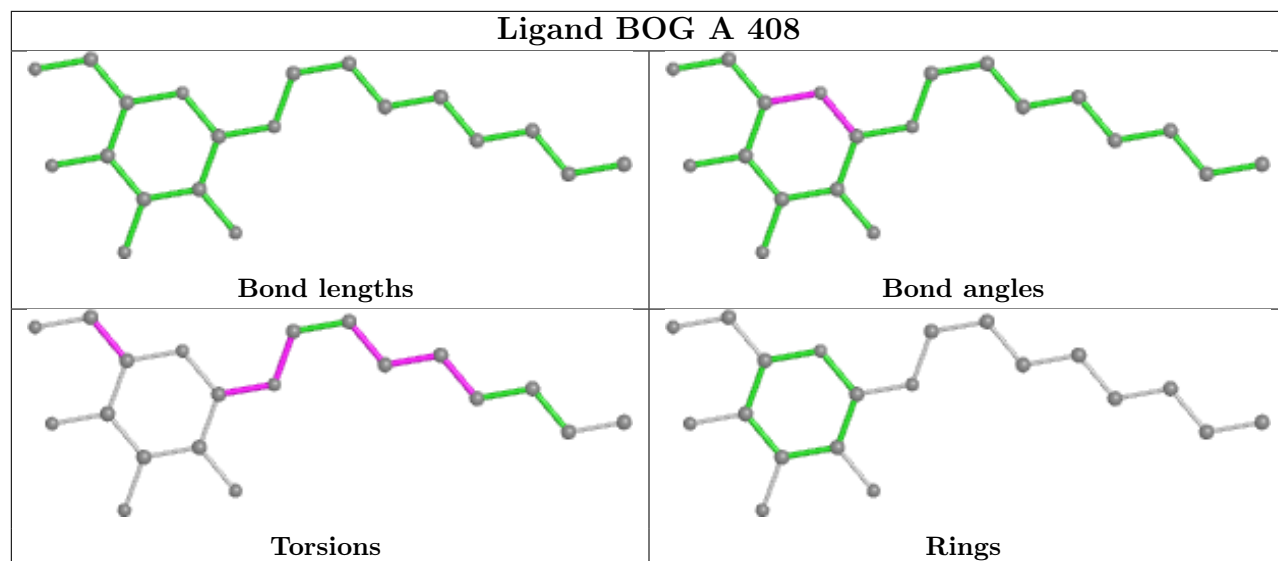
Mol	Chain	Res	Type	Atoms
3	A	404	BOG	C4'-C5'-C6'-C7'
4	A	410	TRD	C9-C10-C11-C12
3	A	405	BOG	C1'-C2'-C3'-C4'
3	A	407	BOG	C2-C1-O1-C1'
4	B	407	TRD	C7-C8-C9-C10
3	A	408	BOG	C3'-C4'-C5'-C6'
4	B	410	TRD	C4-C5-C6-C7

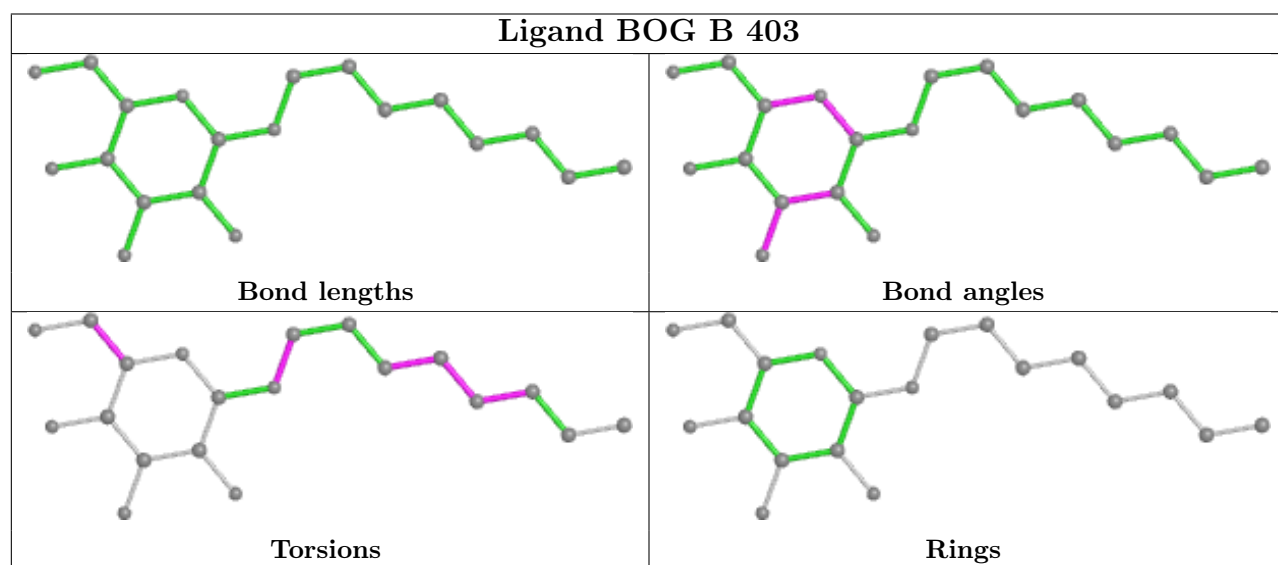
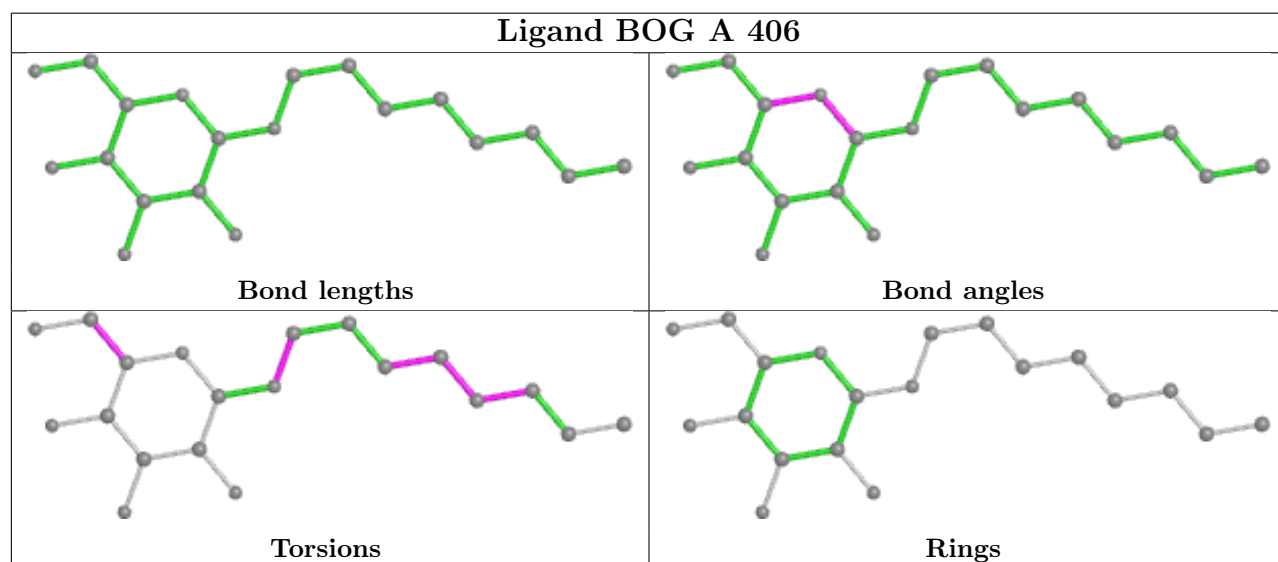
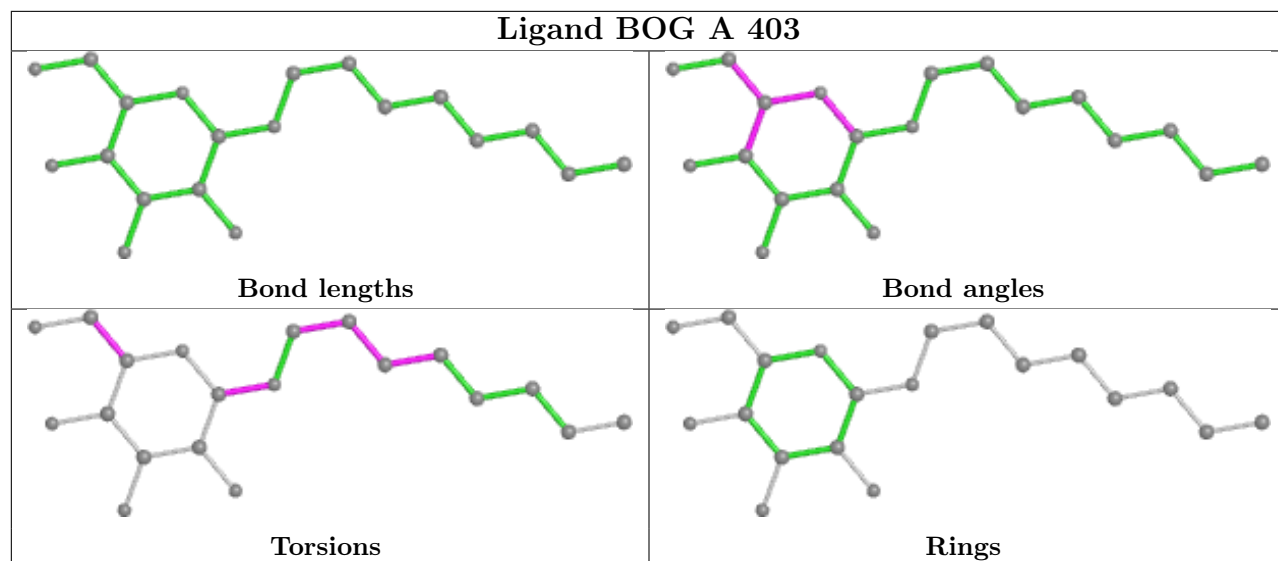
There are no ring outliers.

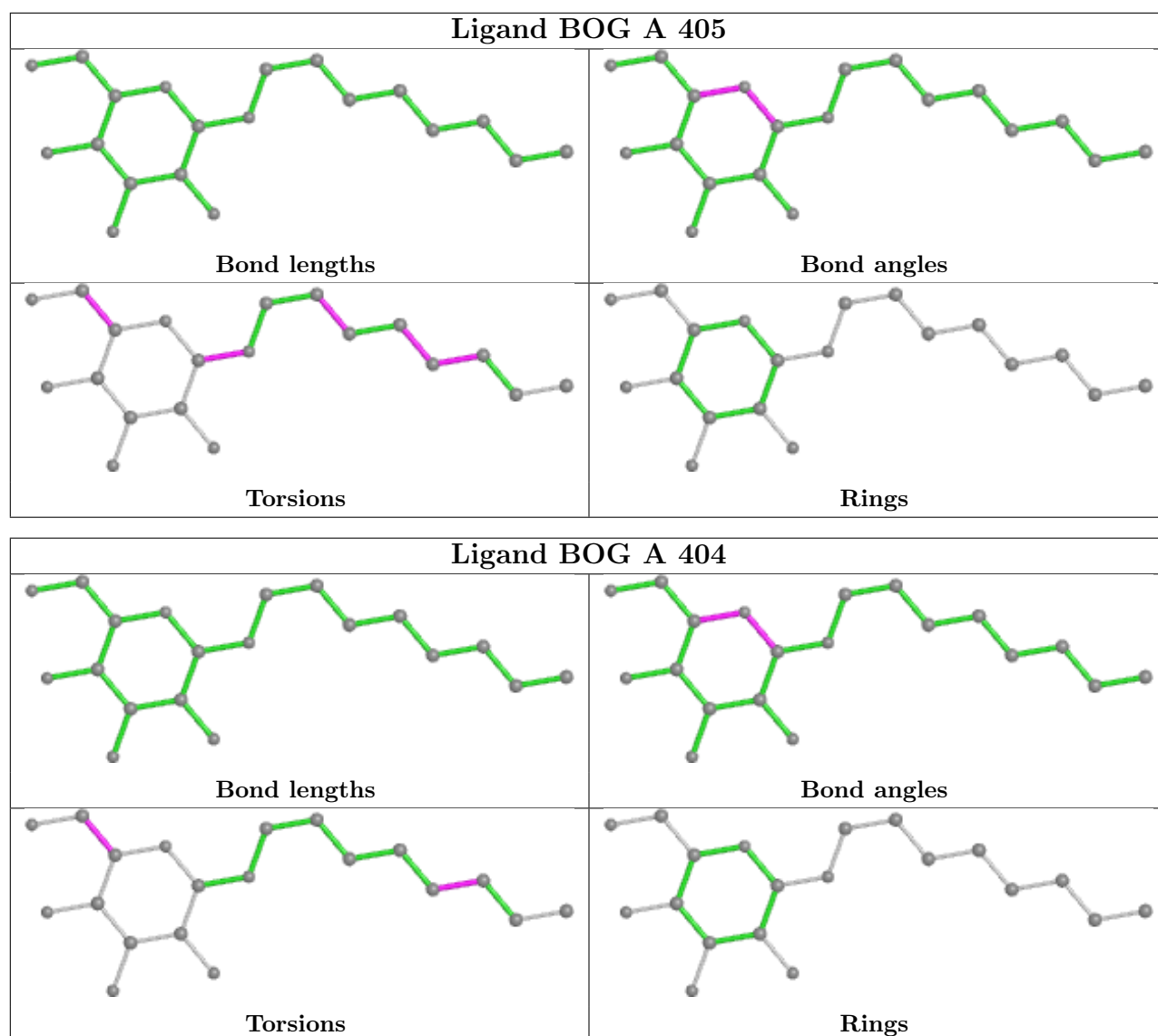
13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	BOG	2	0
3	B	404	BOG	1	0
4	B	407	TRD	1	0
4	B	405	TRD	1	0
3	A	403	BOG	4	0
4	A	409	TRD	3	0
4	B	408	TRD	2	0
4	A	410	TRD	2	0
3	B	403	BOG	2	0
4	B	406	TRD	2	0
4	B	409	TRD	1	0
4	B	410	TRD	1	0
3	A	404	BOG	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.







## 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	274/298 (91%)	0.20	7 (2%) 56 50	59, 79, 120, 160	0
1	B	275/298 (92%)	0.27	8 (2%) 51 45	55, 77, 125, 159	0
All	All	549/596 (92%)	0.23	15 (2%) 54 48	55, 78, 122, 160	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	3.9
1	B	351	LYS	3.8
1	A	147	PHE	3.6
1	B	117	PHE	3.3
1	A	154	LEU	3.1
1	A	253	TRP	2.4
1	B	291	LEU	2.4
1	A	389	VAL	2.3
1	B	123	VAL	2.3
1	B	150	LEU	2.3
1	B	273	TYR	2.1
1	B	247	LEU	2.1
1	A	150	LEU	2.0
1	B	126	LEU	2.0
1	A	158	ILE	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 monosaccharides in this entry.

## 6.4 Ligands

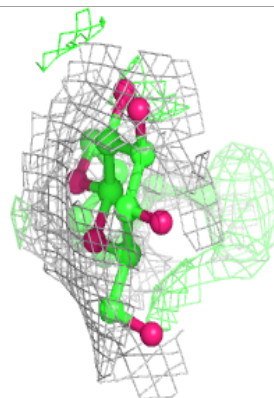
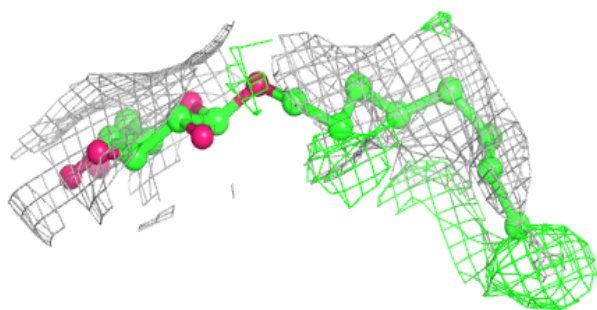
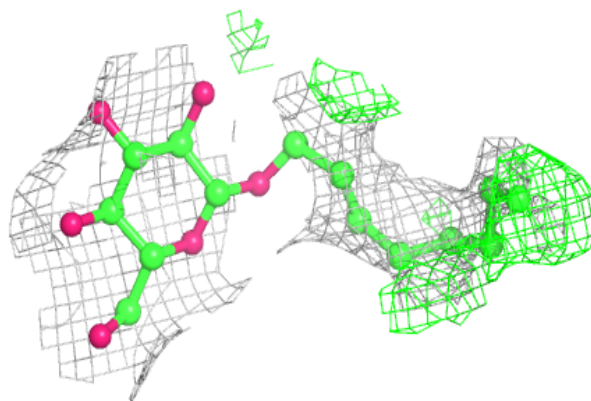
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	TRD	B	410	13/13	0.53	0.28	72,98,113,113	0
3	BOG	B	404	20/20	0.72	0.15	120,136,146,148	0
3	BOG	A	407	20/20	0.72	0.26	85,139,154,157	0
3	BOG	A	406	20/20	0.75	0.28	86,120,145,146	0
3	BOG	A	405	20/20	0.75	0.42	88,148,160,161	0
4	TRD	B	408	13/13	0.76	0.21	86,99,109,111	0
4	TRD	B	409	13/13	0.77	0.44	75,88,104,105	0
3	BOG	A	408	20/20	0.82	0.17	62,134,149,151	0
3	BOG	B	403	20/20	0.84	0.30	78,110,122,127	0
4	TRD	B	407	13/13	0.85	0.29	60,81,108,110	0
4	TRD	B	405	13/13	0.88	0.48	64,79,87,92	0
4	TRD	A	409	13/13	0.89	0.28	62,73,84,84	0
3	BOG	A	404	20/20	0.90	0.30	75,96,125,125	0
3	BOG	A	403	20/20	0.91	0.35	71,92,103,111	0
4	TRD	B	406	13/13	0.91	0.17	61,75,89,93	0
4	TRD	A	410	13/13	0.93	0.18	77,104,114,115	0
2	ZN	A	401	1/1	0.99	0.23	81,81,81,81	0
2	ZN	A	402	1/1	0.99	0.24	84,84,84,84	0
2	ZN	B	401	1/1	0.99	0.22	81,81,81,81	0
2	ZN	B	402	1/1	0.99	0.22	82,82,82,82	0

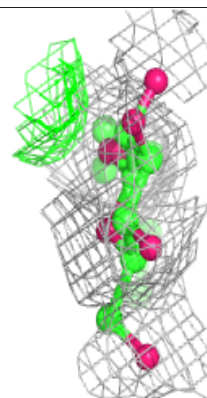
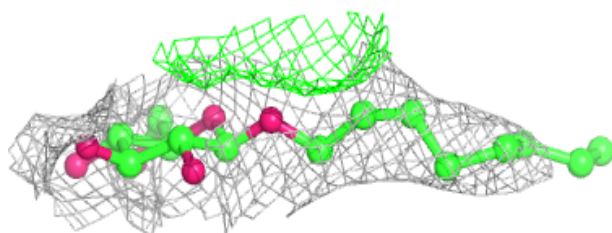
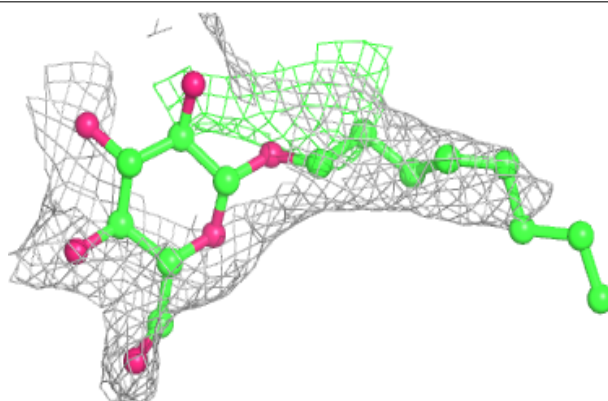
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BOG B 404:**

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

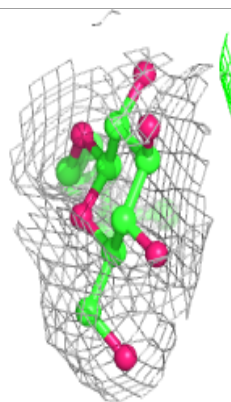
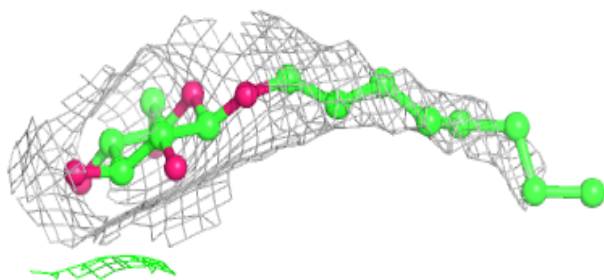
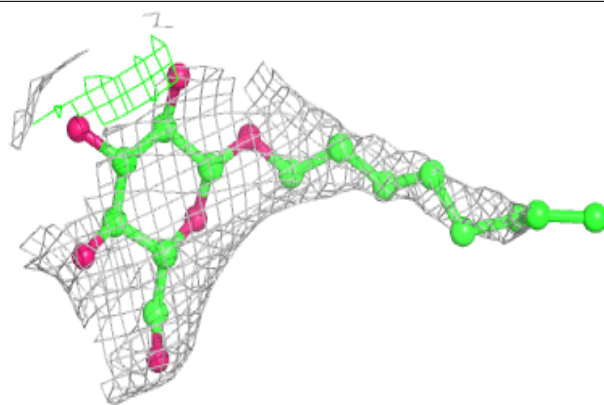
**Electron density around BOG A 407:**

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

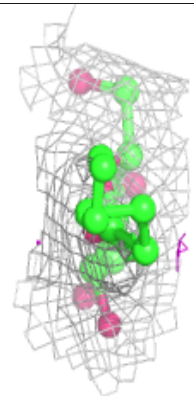
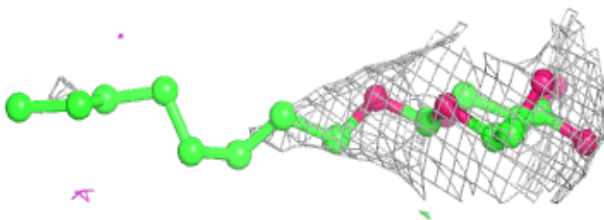
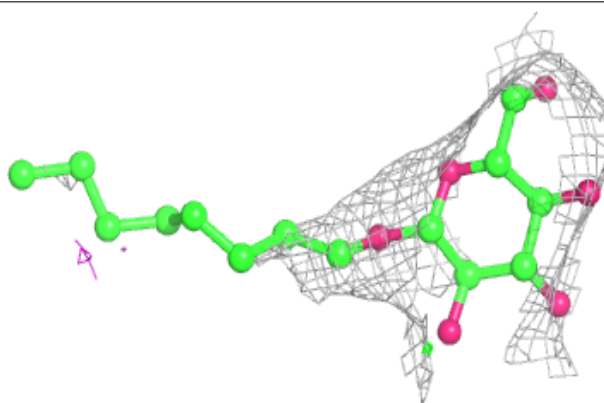


**Electron density around BOG A 406:**

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

**Electron density around BOG A 405:**

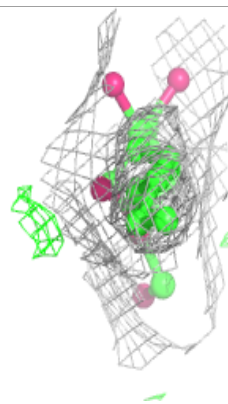
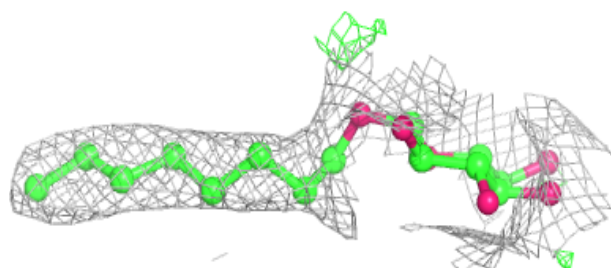
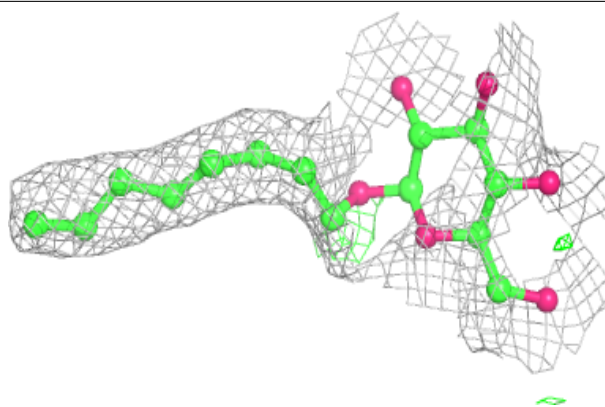
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



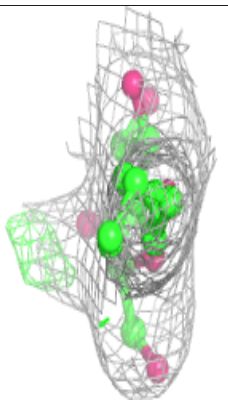
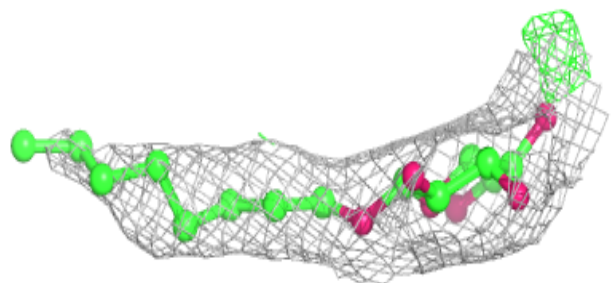
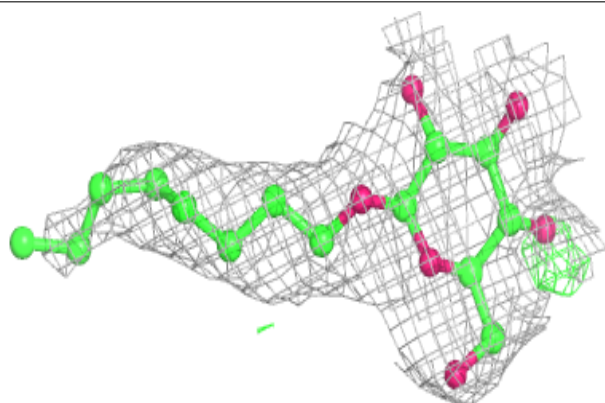


**Electron density around BOG A 408:**

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

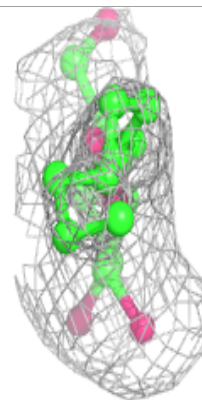
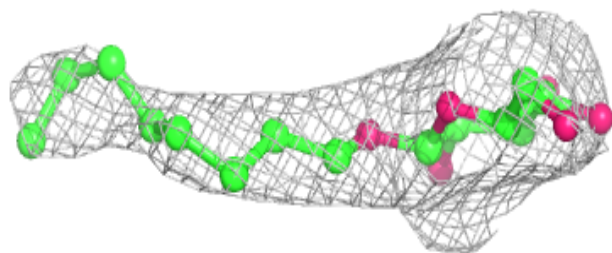
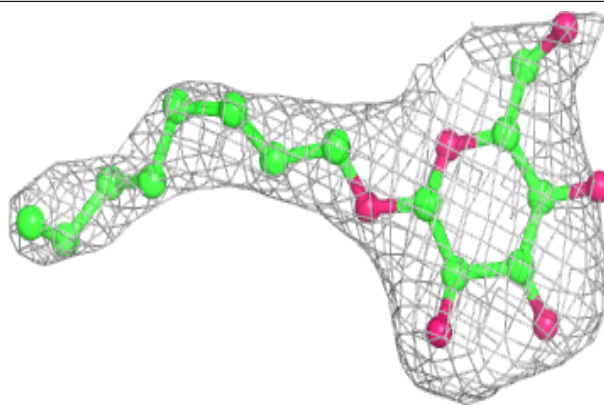
**Electron density around BOG B 403:**

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

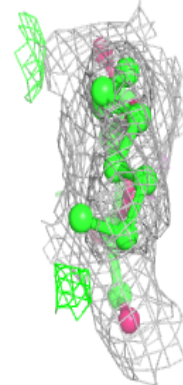
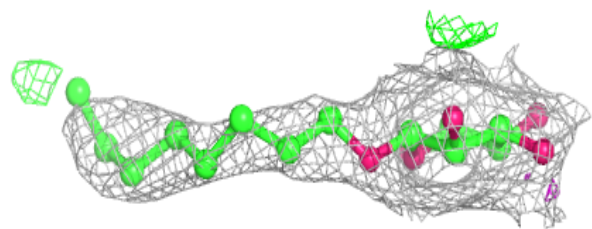
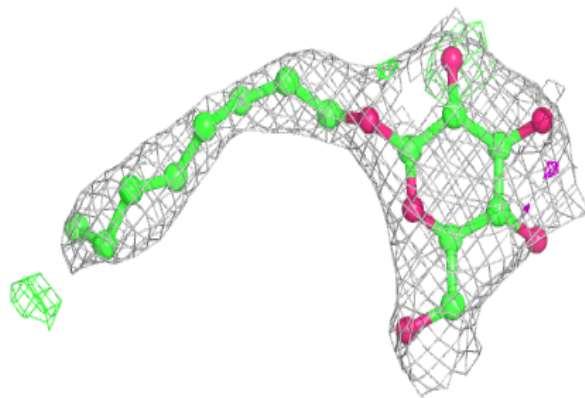


**Electron density around BOG A 404:**

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

**Electron density around BOG A 403:**

$2mF_o-DF_c$  (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.