

Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 - 01:10 pm BST

PDB ID	:	8P7Q
Title	:	The impact of molecular variants, crystallization conditions and space group
		on structure-ligand complexes: A case study on Bacterial Phosphotriesterase
		Variants and complexes
Authors	:	Dym, O.; Aggarwal, N.; Ashani, Y.; Albeck, S.; Unger, T.; Hamer Rogotner,
		S.; Silman, I.; Sussman, J.L.
Deposited on		
Resolution	:	1.77 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 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	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report		
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

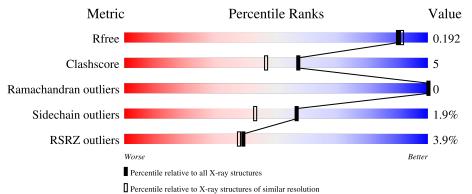


1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	А	332	4% 92%	7% ••

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	А	406	-	Х	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	E8N	А	407	-	-	Х	-



 $\mathbf{2}$

Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2814 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 Parathion hydrolase.

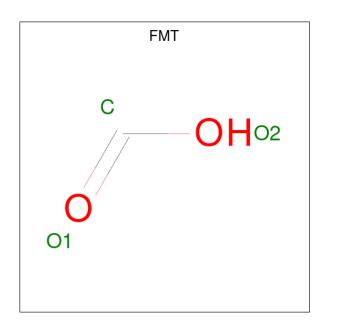
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	330	Total 2501	C 1578	N 448	0 468	${ m S} 7$	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	77	ALA	LYS	conflict	UNP P0A434
А	80	VAL	ALA	conflict	UNP P0A434
А	132	GLU	PHE	conflict	UNP P0A434
А	173	ASN	THR	conflict	UNP P0A434
А	185	ARG	LYS	conflict	UNP P0A434
А	254	GLY	HIS	conflict	UNP P0A434
А	274	ASN	ILE	conflict	UNP P0A434
А	319	SER	ARG	conflict	UNP P0A434
A	342	SER	PRO	conflict	UNP P0A434

• Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂) (labeled as "Ligand of Interest" by depositor).



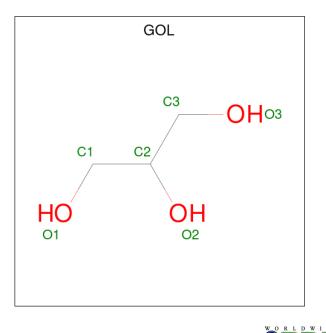


Mol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
2	А	1	Total 3	С 1	O 2	0	0

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

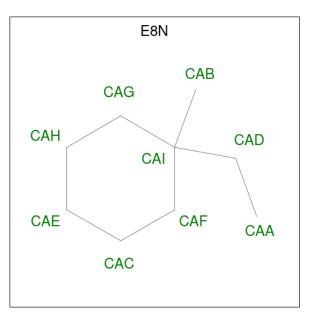
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Zn 2 2	0	0

• 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	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

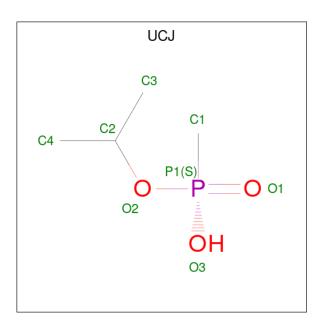
• Molecule 5 is 1-ethyl-1-methyl-cyclohexane (three-letter code: E8N) (formula: C_9H_{18}) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C 9 9	0	0

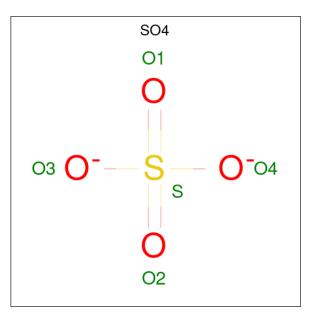
• Molecule 6 is propan-2-yl hydrogen (S)-methylphosphonate (three-letter code: UCJ) (formula: C₄H₁₁O₃P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
6	А	1	Total 8	С 4	$\begin{array}{c} 0\\ 3\end{array}$	Р 1	0	0

• Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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Mol	Chain	Residues	Ato	\mathbf{pms}		ZeroOcc	AltConf
7	А	1	Total 5	0 4	S 1	0	0

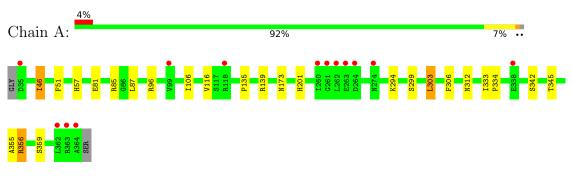
• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	258	Total O 258 258	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: Parathion hydrolase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	69.56Å 69.56Å 186.64Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.80 - 1.77	Depositor
Resolution (A)	34.78 - 1.77	EDS
% Data completeness	99.9 (34.80-1.77)	Depositor
(in resolution range)	100.0 (34.78 - 1.77)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.48 (at 1.77 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
D D.	0.157 , 0.186	Depositor
R, R_{free}	0.169 , 0.192	DCC
R_{free} test set	2285 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	17.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39 , 42.1	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2814	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: E8N, UCJ, FMT, ZN, SO4, 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	Bond lengths I		ond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.79	0/2546	0.97	4/3459~(0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	356	ARG	NE-CZ-NH1	16.38	128.49	120.30
1	А	356	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	А	96	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	А	356	ARG	CG-CD-NE	-5.75	99.72	111.80

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	А	2501	0	2508	24	0
2	А	3	0	0	0	0
3	А	2	0	0	0	0
4	А	18	0	23	3	0
5	А	9	0	0	10	0
6	А	8	0	0	0	0
7	А	15	0	0	0	0

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	3	<i>i</i> previous	1 0			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	А	258	0	0	2	0
All	All	2814	0	2531	25	0

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:345:THR:OG1	5:A:407:E8N:CAE	1.69	1.41
1:A:342:SER:OG	5:A:407:E8N:CAE	2.00	1.08
1:A:345:THR:HG1	5:A:407:E8N:CAE	1.55	1.08
1:A:173:ASN:HD21	1:A:201:HIS:HE2	1.21	0.85
1:A:345:THR:CB	5:A:407:E8N:CAE	2.55	0.84
1:A:356:ARG:HD3	4:A:406:GOL:H12	1.63	0.80
1:A:356:ARG:HD3	4:A:406:GOL:C1	2.12	0.79
1:A:342:SER:H	5:A:407:E8N:CAH	1.95	0.79
5:A:407:E8N:CAC	8:A:698:HOH:O	2.33	0.75
1:A:81:GLU:CG	1:A:85:ARG:NH1	2.60	0.64
1:A:345:THR:OG1	5:A:407:E8N:CAC	2.49	0.59
1:A:294:LYS:O	1:A:356:ARG:NH2	2.36	0.59
1:A:356:ARG:HD3	4:A:406:GOL:H11	1.84	0.59
1:A:46:ILE:HG23	1:A:355:ALA:HB1	1.87	0.56
1:A:342:SER:CB	5:A:407:E8N:CAE	2.83	0.56
1:A:173:ASN:ND2	1:A:201:HIS:HE2	1.98	0.53
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.91	0.51
1:A:345:THR:HG1	5:A:407:E8N:CAC	2.20	0.51
1:A:57:HIS:O	1:A:303:LEU:HA	2.11	0.50
1:A:135:PRO:O	1:A:139[A]:ARG:HG3	2.14	0.48
1:A:312:ASN:HA	8:A:699:HOH:O	2.15	0.46
1:A:46:ILE:HG13	1:A:359:SER:OG	2.16	0.45
1:A:87:LEU:HD12	1:A:116:VAL:HG12	2.00	0.44
1:A:342:SER:OG	5:A:407:E8N:CAC	2.67	0.41
1:A:106:ILE:HG22	1:A:106:ILE:O	2.21	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	329/332~(99%)	318~(97%)	11 (3%)	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.

N	Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
	1	А	260/265~(98%)	255~(98%)	5(2%)	57 43

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	46	ILE
1	А	51	PHE
1	А	299	SER
1	А	303	LEU
1	А	306	PHE

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

Mol	Chain	Res	Type
1	А	173	ASN
1	А	312	ASN



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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	Tuno	Chain	Res	Link	B	ond leng	gths	B	ond ang	gles
	Type	Ullaili	Jiani Res Lin		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	FMT	А	401	3,1	2,2,2	0.53	0	$1,\!1,\!1$	0.50	0
4	GOL	А	404	-	$5,\!5,\!5$	1.13	0	$5,\!5,\!5$	1.29	1 (20%)
7	SO4	А	411	-	4,4,4	0.31	0	$6,\!6,\!6$	0.24	0
6	UCJ	А	408	3	7,7,7	2.56	4 (57%)	6,10,10	0.99	0
5	E8N	А	407	-	8,9,9	3.06	4 (50%)	8,12,12	2.43	3 (37%)
4	GOL	А	406	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	2.75	4 (80%)
7	SO4	А	410	-	4,4,4	0.39	0	$6,\!6,\!6$	0.32	0
7	SO4	А	409	-	4,4,4	0.41	0	$6,\!6,\!6$	0.13	0
4	GOL	А	405	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	1.41	1 (20%)

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
4	GOL	А	404	-	-	3/4/4/4	-
6	UCJ	А	408	3	-	3/4/5/5	-
5	E8N	А	407	-	-	0/3/13/13	0/1/1/1
4	GOL	А	406	-	-	2/4/4/4	-
4	GOL	А	405	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	407	E8N	CAG-CAH	-5.73	1.38	1.52
6	А	408	UCJ	O2-C2	-4.50	1.31	1.46
5	А	407	E8N	CAH-CAE	-3.76	1.36	1.51
6	А	408	UCJ	P1-C1	3.53	1.86	1.77
5	А	407	E8N	CAG-CAI	-3.40	1.45	1.53
5	А	407	E8N	CAF-CAC	-3.19	1.44	1.52
6	А	408	UCJ	P1-O2	-2.87	1.53	1.57
6	А	408	UCJ	P1-O3	2.17	1.58	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	407	E8N	CAF-CAC-CAE	-4.84	103.88	111.37
4	А	406	GOL	O2-C2-C1	4.10	127.17	109.12
5	А	407	E8N	CAA-CAD-CAI	-3.78	103.44	115.39
4	А	406	GOL	C3-C2-C1	3.04	123.52	111.70
4	А	406	GOL	O3-C3-C2	-2.68	97.34	110.20
5	А	407	E8N	CAB-CAI-CAF	2.55	113.30	109.48
4	А	404	GOL	O2-C2-C1	2.31	119.32	109.12
4	А	405	GOL	O3-C3-C2	-2.30	99.16	110.20
4	А	406	GOL	O1-C1-C2	2.14	120.45	110.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	404	GOL	C1-C2-C3-O3
4	А	405	GOL	O1-C1-C2-C3
4	А	405	GOL	C1-C2-C3-O3
4	А	406	GOL	O1-C1-C2-O2
4	А	406	GOL	C1-C2-C3-O3
6	А	408	UCJ	C2-O2-P1-O1

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Mol	Chain	Res	Type	Atoms
4	А	404	GOL	O2-C2-C3-O3
4	А	404	GOL	O1-C1-C2-C3
4	А	405	GOL	O2-C2-C3-O3
4	А	405	GOL	O1-C1-C2-O2
6	А	408	UCJ	C3-C2-O2-P1
6	А	408	UCJ	C4-C2-O2-P1

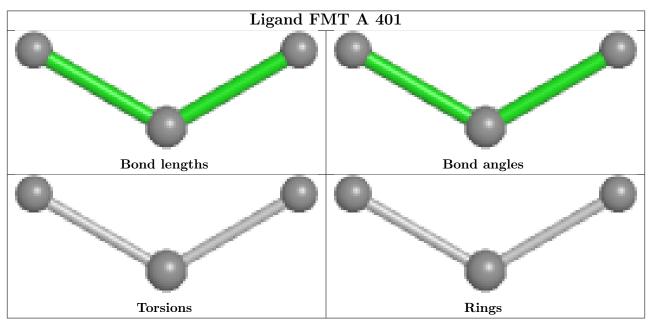
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There are no ring outliers.

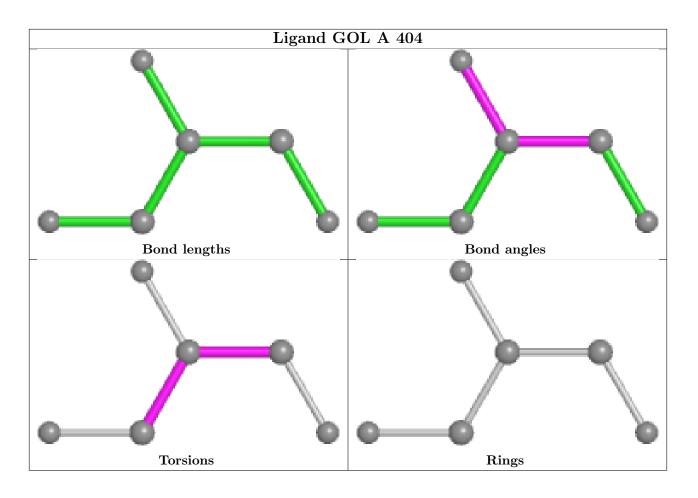
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	407	E8N	10	0
4	А	406	GOL	3	0

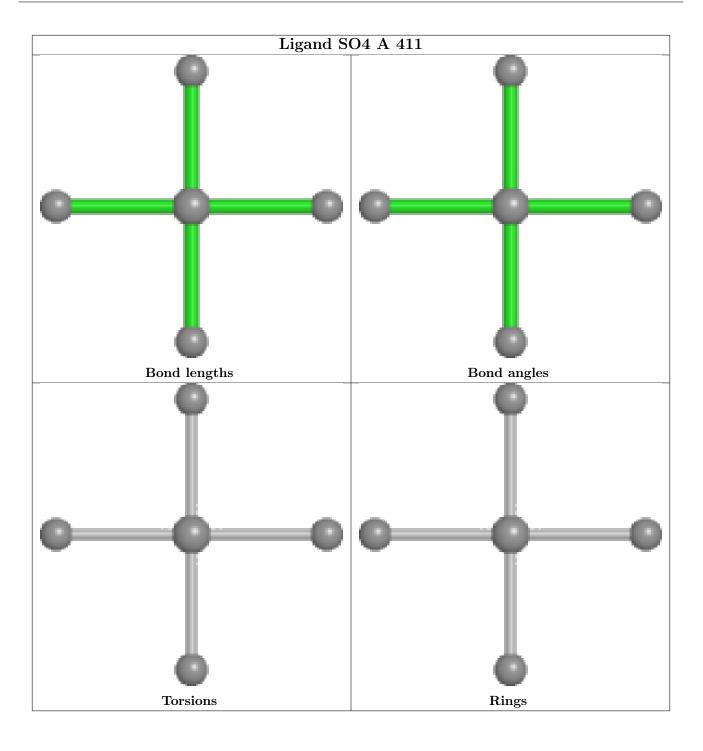
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



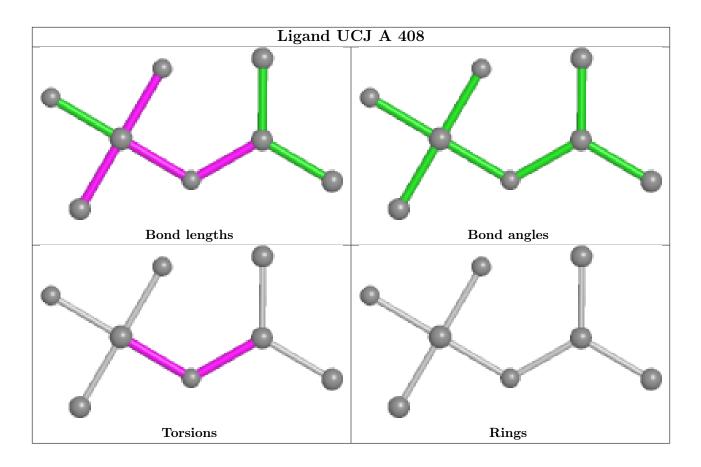






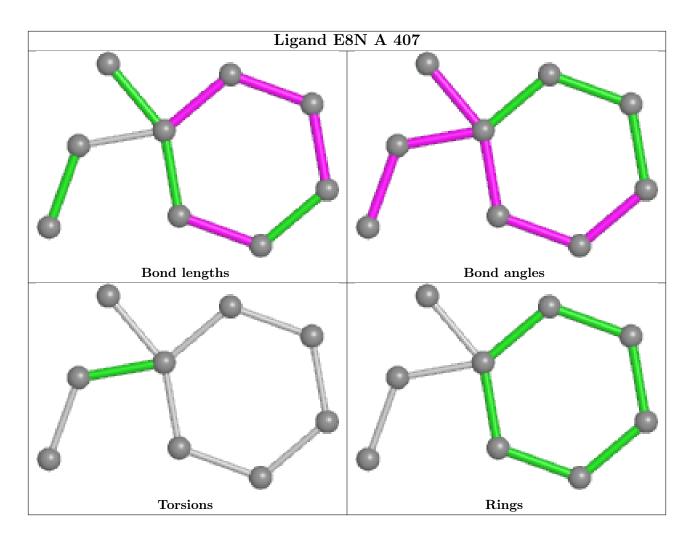




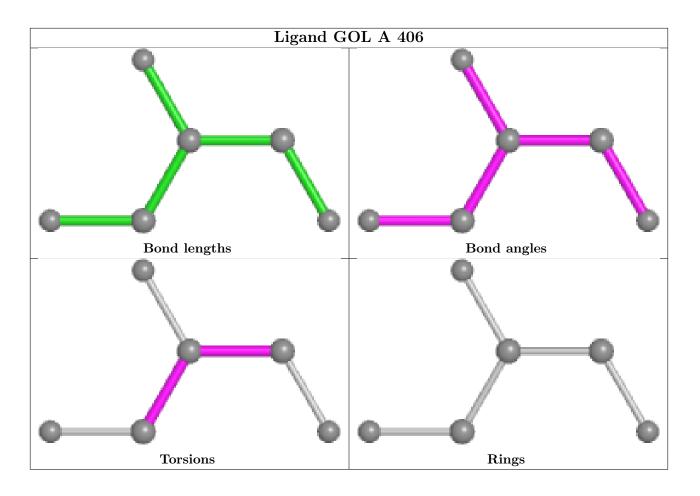




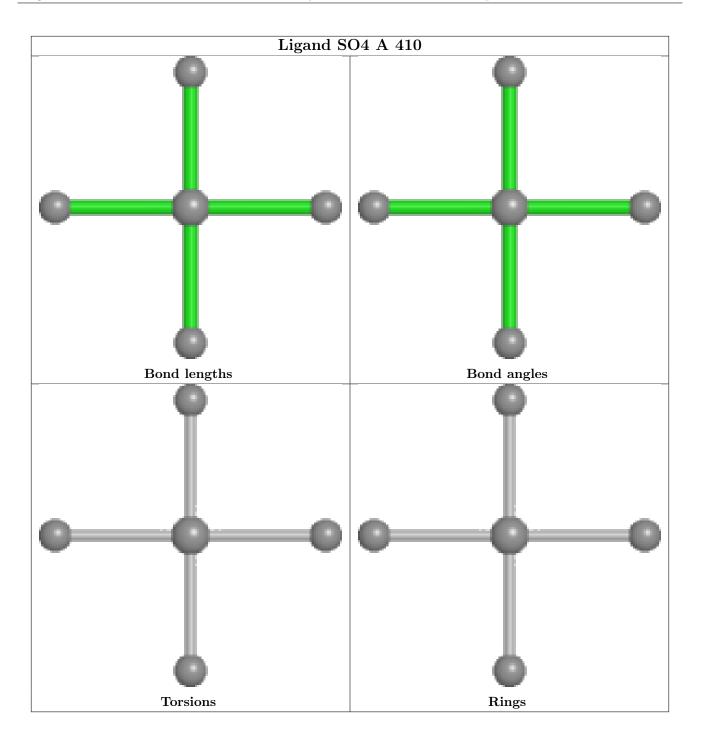




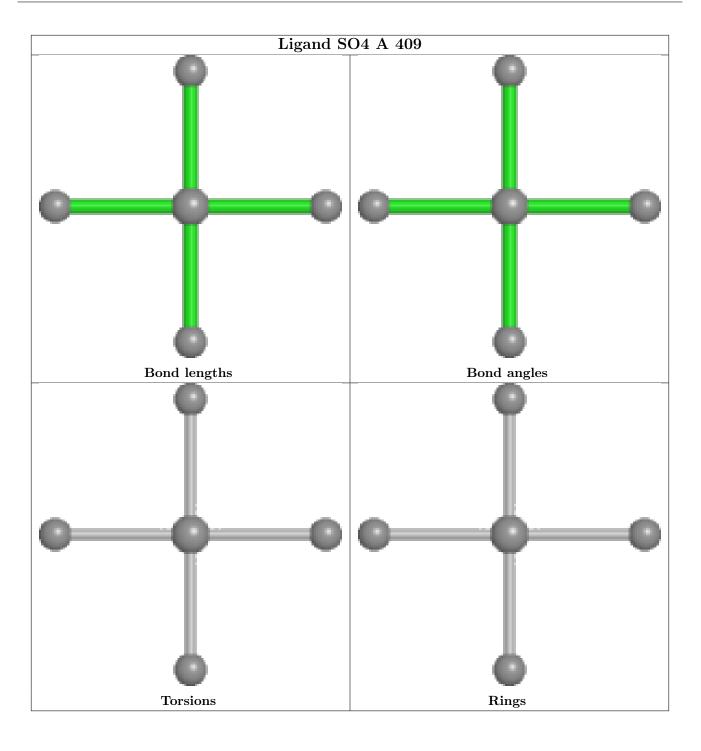




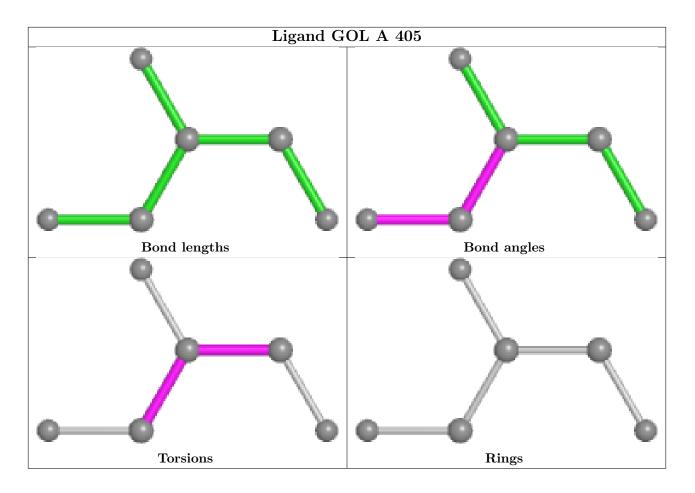












5.7 Other polymers (i)

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>2		$OWAB(Å^2)$	Q<0.9	
1	А	330/332~(99%)	0.07	13 (3%)	39	38	11, 16, 30, 58	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	362	LEU	4.9
1	А	363	ARG	4.7
1	А	261	GLY	4.2
1	А	264	ASP	3.4
1	А	260	ILE	3.3
1	А	35	ASP	3.0
1	А	263	GLU	3.0
1	А	99	VAL	2.8
1	А	364	ALA	2.6
1	А	118	ARG	2.3
1	А	274	ASN	2.3
1	А	338	GLU	2.2
1	А	262	LEU	2.2

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.



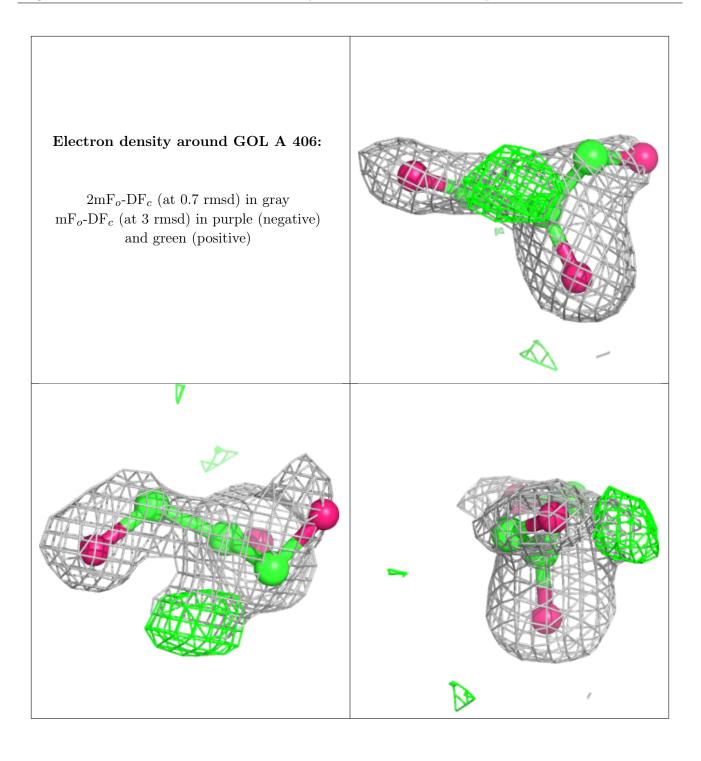
6.4 Ligands (i)

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^{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.

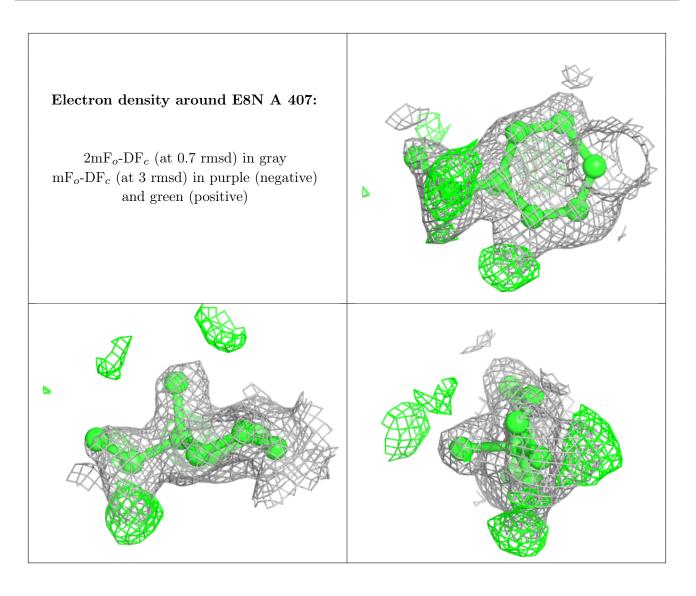
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
4	GOL	А	406	6/6	0.78	0.23	33,42,47,49	0
5	E8N	А	407	9/9	0.80	0.21	16,24,28,32	0
7	SO4	А	411	5/5	0.82	0.44	$63,\!70,\!81,\!88$	0
4	GOL	А	405	6/6	0.84	0.16	33,45,49,49	0
4	GOL	А	404	6/6	0.91	0.12	22,31,35,38	0
7	SO4	А	410	5/5	0.94	0.22	$42,\!46,\!53,\!58$	0
6	UCJ	А	408	8/8	0.94	0.22	12,22,30,30	8
7	SO4	А	409	5/5	0.97	0.23	$27,\!29,\!38,\!39$	0
2	FMT	А	401	3/3	0.98	0.07	12,12,12,12	0
3	ZN	А	402	1/1	1.00	0.03	$13,\!13,\!13,\!13$	0
3	ZN	А	403	1/1	1.00	0.03	$13,\!13,\!13,\!13$	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.

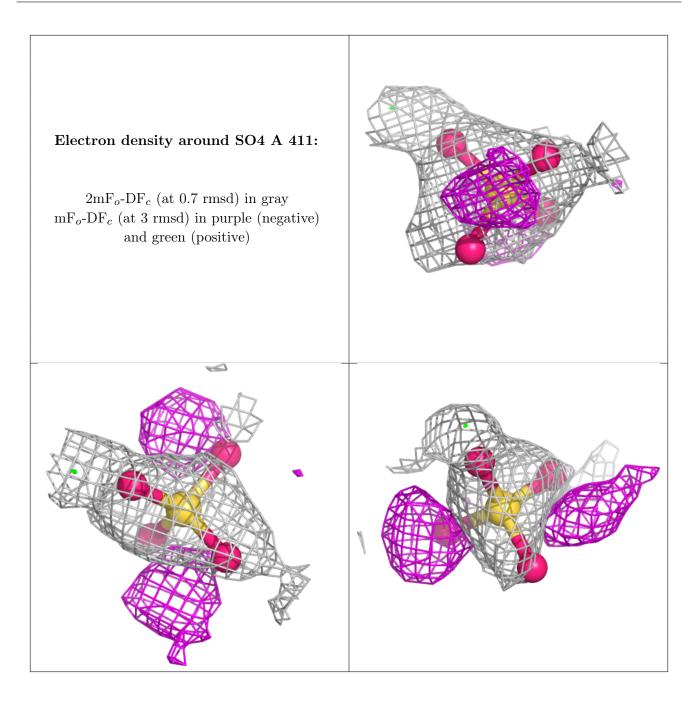




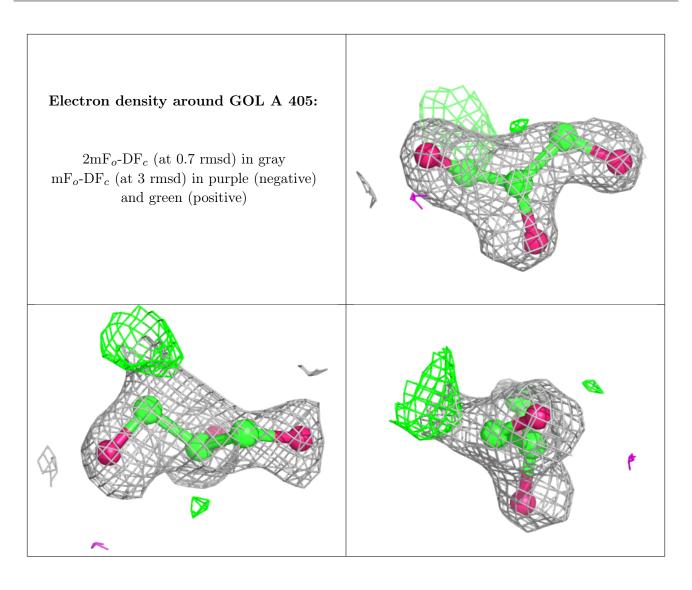




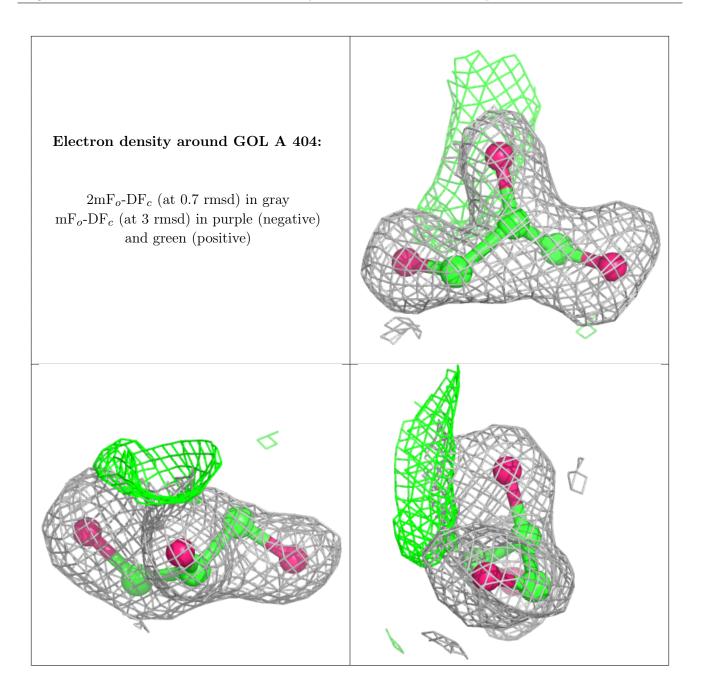




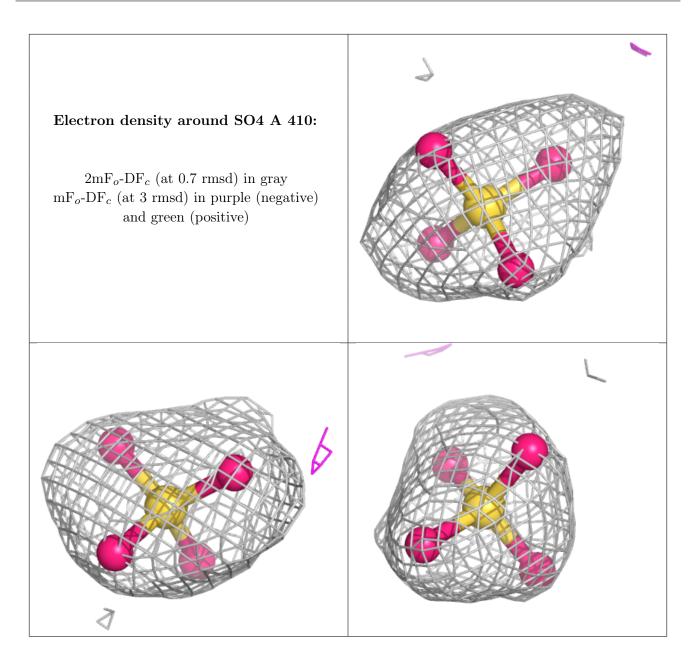




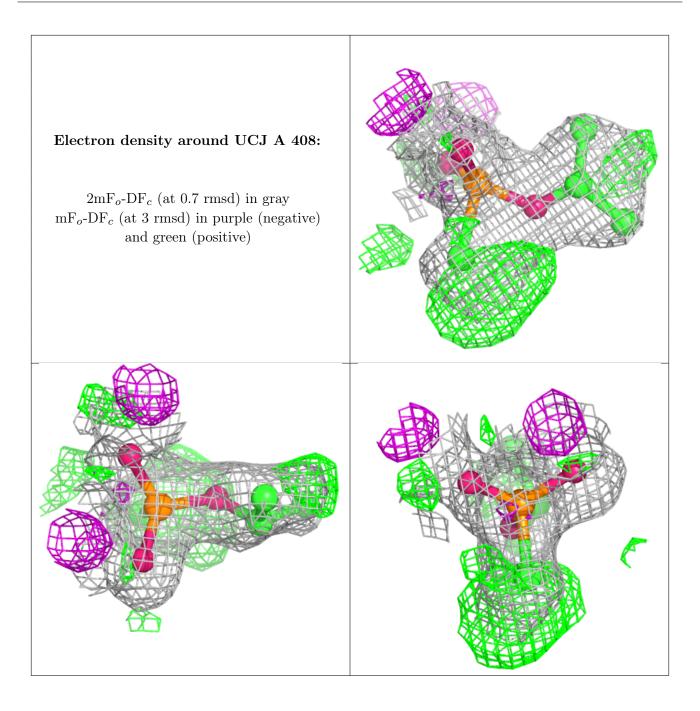




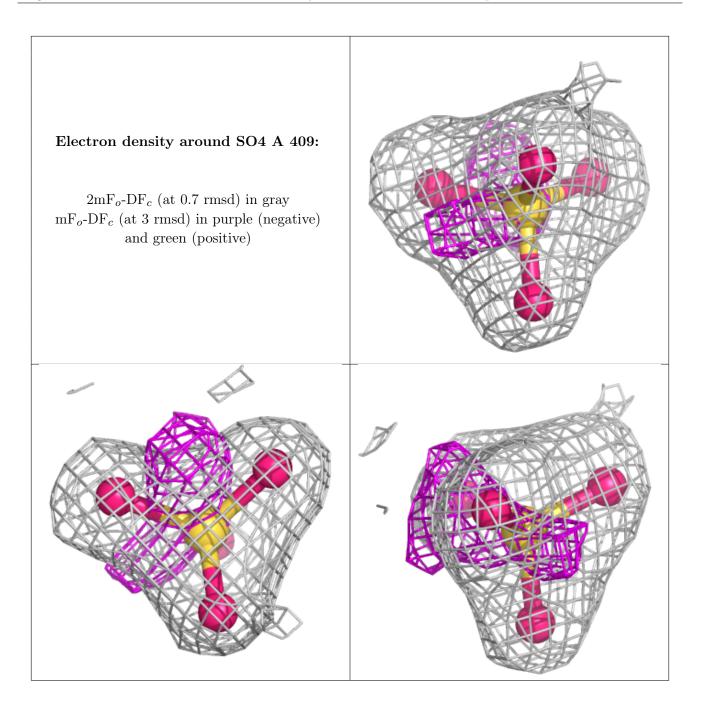




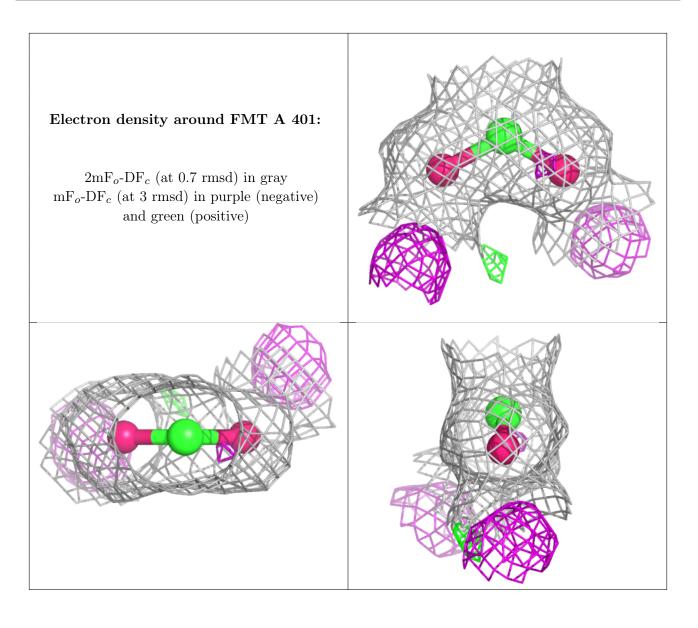




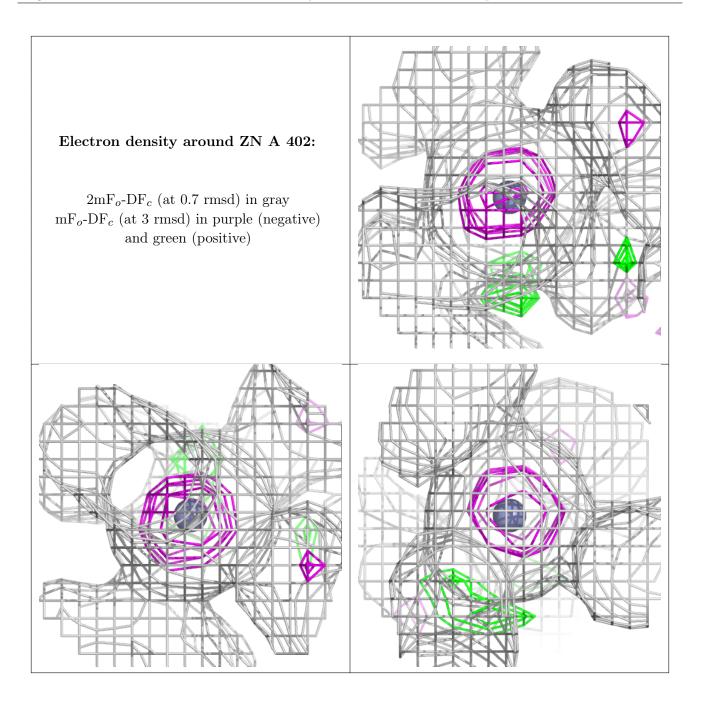




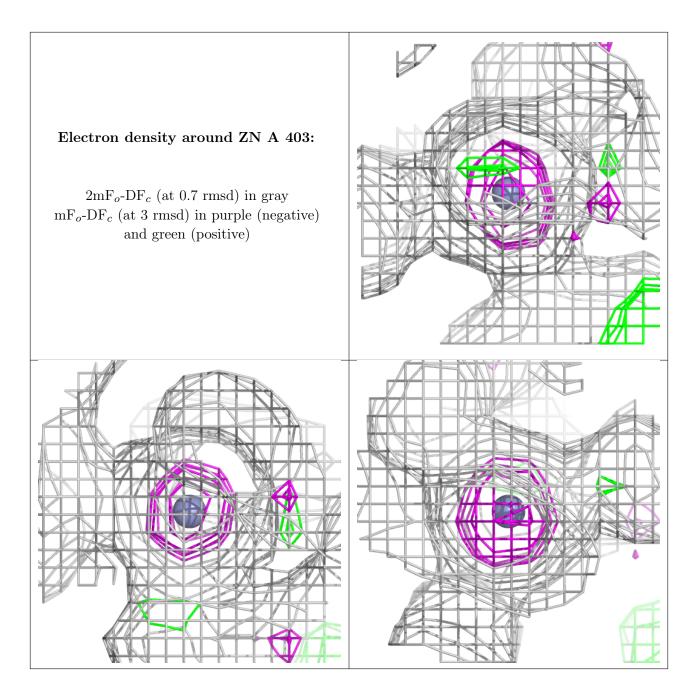












6.5 Other polymers (i)

There are no such residues in this entry.

