WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2023 – 05:17 AM EDT

PDB ID	:	8SWS
Title	:	Structure of K. lactis PNP S42E-H98R variant bound to transition state analog DADMe-IMMUCILLIN G and sulfate
Authors	:	Fedorov, E.; Ghosh, A.
Deposited on	:	2023-05-19
Resolution	:	1.99 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.35.1
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)	:	2.35.1

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 1.99 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.
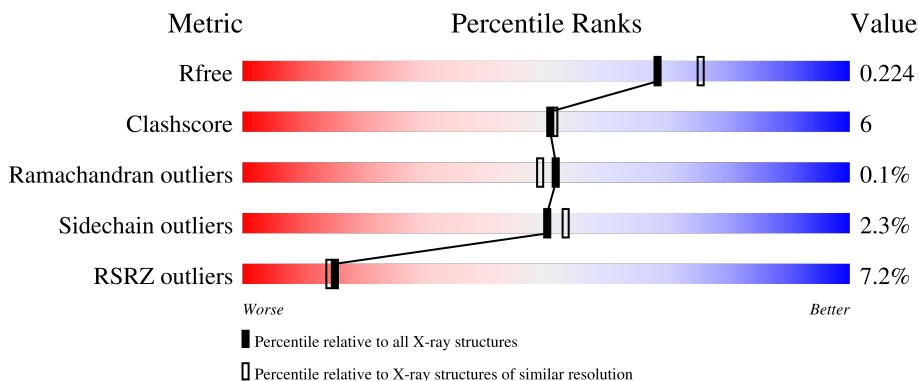
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	307	
1	B	307	
1	C	307	
1	D	307	
1	E	307	

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Mol	Chain	Length	Quality of chain
1	F	307	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13481 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	2	0
			2319	1477	401	432	9			
1	B	277	Total	C	N	O	S	0	0	0
			2124	1352	364	399	9			
1	C	265	Total	C	N	O	S	0	2	0
			2040	1306	348	377	9			
1	D	288	Total	C	N	O	S	0	0	0
			2195	1396	376	414	9			
1	E	295	Total	C	N	O	S	0	1	0
			2270	1446	394	421	9			
1	F	271	Total	C	N	O	S	0	3	0
			2085	1330	359	387	9			

There are 18 discrepancies between the modelled and reference sequences:

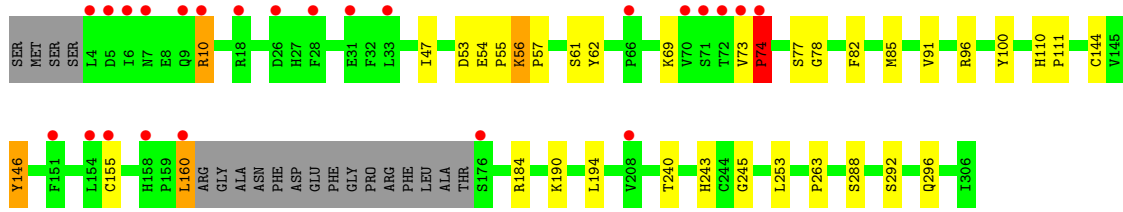| Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6CSZ6
A	42	GLU	SER	engineered mutation	UNP Q6CSZ6
A	98	ARG	HIS	engineered mutation	UNP Q6CSZ6
B	0	SER	-	expression tag	UNP Q6CSZ6
B	42	GLU	SER	engineered mutation	UNP Q6CSZ6
B	98	ARG	HIS	engineered mutation	UNP Q6CSZ6
C	0	SER	-	expression tag	UNP Q6CSZ6
C	42	GLU	SER	engineered mutation	UNP Q6CSZ6
C	98	ARG	HIS	engineered mutation	UNP Q6CSZ6
D	0	SER	-	expression tag	UNP Q6CSZ6
D	42	GLU	SER	engineered mutation	UNP Q6CSZ6
D	98	ARG	HIS	engineered mutation	UNP Q6CSZ6
E	0	SER	-	expression tag	UNP Q6CSZ6
E	42	GLU	SER	engineered mutation	UNP Q6CSZ6
E	98	ARG	HIS	engineered mutation	UNP Q6CSZ6
F	0	SER	-	expression tag	UNP Q6CSZ6
F	42	GLU	SER	engineered mutation	UNP Q6CSZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	98	ARG	HIS	engineered mutation	UNP Q6CSZ6

- Molecule 2 is 2-amino-7-{[(3R,4R)-3-hydroxy-4-(hydroxymethyl)pyrrolidin-1-yl]methyl}-3,5 -dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: IM5) (formula: $C_{12}H_{17}N_5O_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 20	C 12	N 5	O 3	0	0
2	B	1	Total 20	C 12	N 5	O 3	0	0
2	D	1	Total 20	C 12	N 5	O 3	0	0
2	E	1	Total 20	C 12	N 5	O 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).

SO4

O1

O⁻ O3

S

S

O⁻ O4

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total 75	O 75	0	1
4	B	59	Total 60	O 60	0	1

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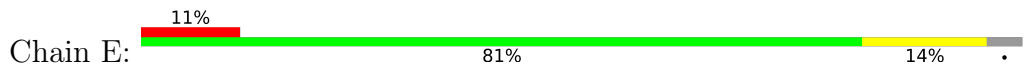| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	27	Total 28	O 28	0	1
4	D	47	Total 47	O 47	0	0
4	E	50	Total 52	O 52	0	2
4	F	56	Total 56	O 56	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Purine nucleoside phosphorylase

Chain A:

• Molecule 1: Purine nucleoside phosphorylase

Chain B:

• Molecule 1: Purine nucleoside phosphorylase

Chain C:

• Molecule 1: Purine nucleoside phosphorylase

Chain D:

8%

82% 10% • 6%

SER MET SER SER L4 D5 I6 N7 E8 Q9 R10 R18 D26 H27 F28 E31 F32 L33 I47 D53 E54 P55 K56 P57 S61 Y62 P66 K69 V70 S71 T72 V73 P74 S77 G78 F82 M85 V91 R96 Y100 H110 P111 C144 V145

Y146 F151 L154 C155 H158 P159 L160 ARG GLY ALA ASN PHE ASP GLU PHE GLY PRO ARG PHE LEU ALA THR S176 R184 K190 L194 V208 T240 H243 C244 G245 L253 P263 S288 S292 Q296 I306

• Molecule 1: Purine nucleoside phosphorylase

Chain E:

11%

81% 14% •

SER MET SER SER LEU D5 I6 N7 R10 A11 L12 S15 A16 H17 R18 Y19 I20 S21 E22 K23 L24 E25 D26 H27 F28 L33 P34 K35 V38 G46 I47 S48 T49 K50 I51 A52 D53 E54 P55 K56 P57 L58 I59 L60 I65 F68 K69 V70 SER THR VAL PRO GLY

HIS SER G78 E79 L80 I81 N86 L92 L97 Y100 H103 L118 G119 S120 T127 I133 V145 Y146 F172 K190 N195 V208 H209 R223 V230 A250 L253 P263 E269 S288 S292 K293 Q296 E297 L298 I299 F300

I306

• Molecule 1: Purine nucleoside phosphorylase

Chain F:

5%

77% 11% 12%

SER MET SER SER LEU D5 Y19 S29 S30 L37 S45 S48 K56 S61 Y62 S63 T64 K69 VAL SER THR VAL PRO GLY HIS S77 F82 V91 L92 M93 N94 G95 R96 LEU ARG SER TYR GLU GLY HIS S104 L105 T108 R113 V145 Y146 D147

C155 G156 F157 F168 R184 E202 V208 H209 G210 P211 T212 R220 M232 A250 C258 D268 E269 ASN PRO VAL PRO ILE GLN GLU GLY LYS ALA THR HIS GLU VAL LEU GLU N287 S288 A289 K290 A291 S292 Q296 I306

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.88Å 111.12Å 97.96Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	47.68 – 1.99 47.68 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.68-1.99) 99.9 (47.68-1.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.194 , 0.227 0.191 , 0.224	Depositor DCC
R_{free} test set	6255 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	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	0.96	EDS
Total number of atoms	13481	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IM5, SO4

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	0.60	0/2377	0.72	2/3223 (0.1%)
1	B	0.62	1/2167 (0.0%)	0.74	1/2933 (0.0%)
1	C	0.51	0/2088	0.78	7/2826 (0.2%)
1	D	0.52	0/2240	0.69	1/3036 (0.0%)
1	E	0.53	0/2322	0.70	1/3146 (0.0%)
1	F	0.59	1/2136 (0.0%)	0.76	1/2890 (0.0%)
All	All	0.56	2/13330 (0.0%)	0.73	13/18054 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	5
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	258	CYS	CB-SG	5.51	1.91	1.82
1	B	91	VAL	CB-CG2	-5.02	1.42	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	224	LEU	CB-CG-CD2	8.03	124.64	111.00
1	C	53	ASP	C-N-CA	7.87	141.37	121.70
1	C	56	LYS	CA-CB-CG	7.59	130.09	113.40
1	F	146	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	E	146	TYR	CB-CG-CD2	-7.43	116.54	121.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	B	10	ARG	Sidechain
1	C	52	ALA	Peptide
1	C	53	ASP	Peptide
1	C	56	LYS	Peptide

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	2319	0	2305	26	0
1	B	2124	0	2125	23	0
1	C	2040	0	2038	44	0
1	D	2195	0	2188	21	0
1	E	2270	0	2260	29	0
1	F	2085	0	2074	25	0
2	A	20	0	17	0	0
2	B	20	0	17	0	0
2	D	20	0	17	0	0
2	E	20	0	17	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	D	10	0	0	1	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0
4	A	75	0	0	0	0
4	B	60	0	0	1	0
4	C	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	47	0	0	0	0
4	E	52	0	0	0	0
4	F	56	0	0	1	0
All	All	13481	0	13058	150	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 6.

The worst 5 of 150 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:B:69:LYS:HE3	1:B:107:GLU:HG2	1.55	0.88
1:B:113:ARG:HH21	1:B:160:LEU:HD23	1.39	0.87
1:B:10:ARG:HH12	1:F:69:LYS:HD3	1.44	0.83
1:F:208:VAL:HG23	1:F:211:PRO:HD3	1.66	0.77
1:C:157[B]:PHE:CE2	1:C:209:HIS:HE1	2.03	0.76

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	302/307 (98%)	296 (98%)	6 (2%)	0	100	100
1	B	271/307 (88%)	267 (98%)	4 (2%)	0	100	100
1	C	259/307 (84%)	249 (96%)	9 (4%)	1 (0%)	34	30
1	D	284/307 (92%)	278 (98%)	5 (2%)	1 (0%)	34	30
1	E	292/307 (95%)	282 (97%)	10 (3%)	0	100	100
1	F	266/307 (87%)	261 (98%)	5 (2%)	0	100	100
All	All	1674/1842 (91%)	1633 (98%)	39 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	PRO
1	C	211	PRO

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	250/258 (97%)	246 (98%)	4 (2%)	62	67
1	B	231/258 (90%)	228 (99%)	3 (1%)	69	74
1	C	220/258 (85%)	215 (98%)	5 (2%)	50	53
1	D	238/258 (92%)	229 (96%)	9 (4%)	33	31
1	E	244/258 (95%)	236 (97%)	8 (3%)	38	37
1	F	224/258 (87%)	221 (99%)	3 (1%)	69	74
All	All	1407/1548 (91%)	1375 (98%)	32 (2%)	50	53

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	293	LYS
1	F	45	SER
1	D	10	ARG
1	C	224	LEU
1	F	146	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	270	ASN
1	E	287	ASN
1	F	94	ASN
1	F	9	GLN
1	C	296	GLN

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

14 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	$\#|Z| > 2$
3	SO4	B	402	-	4,4,4	0.35	0	6,6,6	0.41	0
3	SO4	E	402	-	4,4,4	0.14	0	6,6,6	0.37	0
2	IM5	D	401	-	18,22,22	0.85	1 (5%)	18,32,32	1.26	1 (5%)
2	IM5	A	401	-	18,22,22	0.89	1 (5%)	18,32,32	0.86	0
2	IM5	B	401	-	18,22,22	0.76	1 (5%)	18,32,32	1.15	1 (5%)
3	SO4	D	403	-	4,4,4	0.17	0	6,6,6	0.47	0
3	SO4	A	403	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	F	401	-	4,4,4	0.22	0	6,6,6	0.26	0
3	SO4	D	402	-	4,4,4	0.10	0	6,6,6	0.27	0
3	SO4	F	402	-	4,4,4	0.31	0	6,6,6	0.68	0
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.35	0
3	SO4	E	403	-	4,4,4	0.18	0	6,6,6	0.33	0
3	SO4	A	402	-	4,4,4	0.09	0	6,6,6	0.31	0
2	IM5	E	401	-	18,22,22	0.80	1 (5%)	18,32,32	0.83	1 (5%)

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
2	IM5	E	401	-	-	0/5/18/18	0/3/3/3
2	IM5	A	401	-	-	0/5/18/18	0/3/3/3
2	IM5	B	401	-	-	0/5/18/18	0/3/3/3
2	IM5	D	401	-	-	0/5/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IM5	C5-C6	-2.66	1.42	1.47
2	B	401	IM5	C5-C6	-2.36	1.42	1.47
2	E	401	IM5	C5-C6	-2.33	1.42	1.47
2	D	401	IM5	C5-C6	-2.08	1.43	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	IM5	C9-C10-N1'	3.84	119.47	112.75
2	B	401	IM5	C9-C10-N1'	3.52	118.90	112.75
2	E	401	IM5	C9-C10-N1'	2.01	116.27	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	SO4	1	0
3	F	402	SO4	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.

Ligand SO4 B 402

Bond lengths   Bond angles

Torsions   Rings

Ligand SO4 E 402

Bond lengths

Bond angles

Torsions

Rings

Ligand IM5 D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand IM5 A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand IM5 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 402

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 E 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand IM5 E 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	A	302/307 (98%)	0.27	14 (4%)	32	31	23, 38, 69, 136	0
1	B	277/307 (90%)	0.18	11 (3%)	38	37	21, 35, 63, 91	0
1	C	265/307 (86%)	0.56	24 (9%)	9	8	30, 49, 87, 137	0
1	D	288/307 (93%)	0.48	24 (8%)	11	10	26, 44, 88, 128	0
1	E	295/307 (96%)	0.67	33 (11%)	5	4	25, 47, 93, 123	0
1	F	271/307 (88%)	0.20	16 (5%)	22	21	23, 37, 70, 110	0
All	All	1698/1842 (92%)	0.39	122 (7%)	15	14	21, 42, 85, 137	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	13.3
1	D	74	PRO	6.6
1	D	6	ILE	5.4
1	F	212	THR	5.3
1	D	4	LEU	5.0

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3　Carbohydrates ⓘ

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, 95th 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
3	SO4	F	402	5/5	0.90	0.33	51,54,64,74	0
2	IM5	E	401	20/20	0.94	0.15	24,29,37,37	0
2	IM5	A	401	20/20	0.95	0.15	26,29,36,37	0
3	SO4	A	403	5/5	0.95	0.20	47,49,57,58	0
2	IM5	D	401	20/20	0.95	0.14	28,33,40,40	0
3	SO4	F	401	5/5	0.96	0.20	43,44,52,54	0
2	IM5	B	401	20/20	0.96	0.12	20,24,29,31	0
3	SO4	B	403	5/5	0.97	0.14	41,45,53,59	0
3	SO4	D	403	5/5	0.97	0.14	45,47,53,54	0
3	SO4	E	403	5/5	0.98	0.13	47,48,53,54	0
3	SO4	D	402	5/5	0.98	0.12	43,46,50,52	0
3	SO4	E	402	5/5	0.98	0.08	45,49,53,56	0
3	SO4	B	402	5/5	0.99	0.13	36,36,38,39	0
3	SO4	A	402	5/5	0.99	0.12	38,39,42,43	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 SO4 F 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
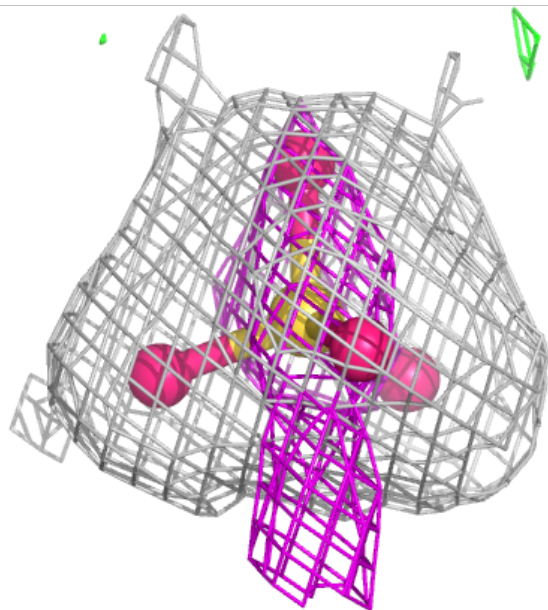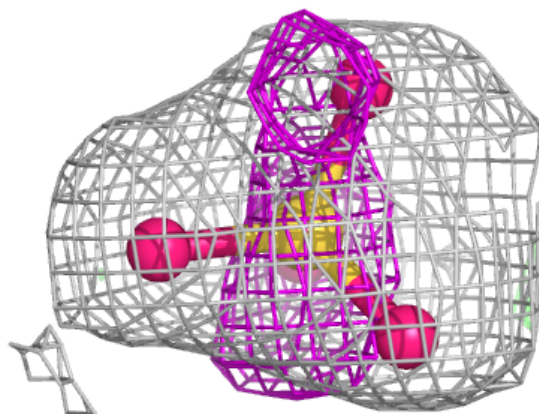$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
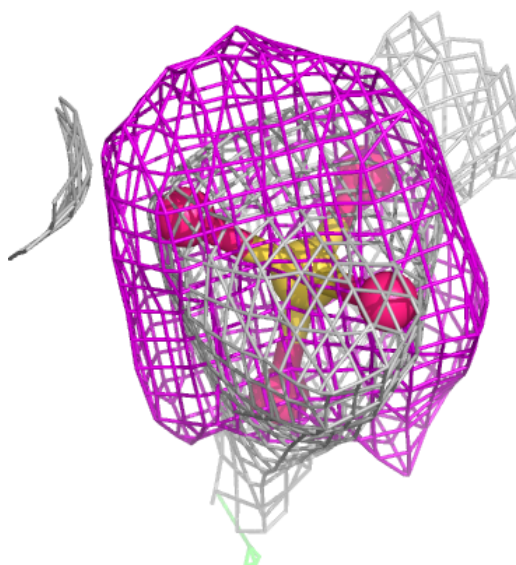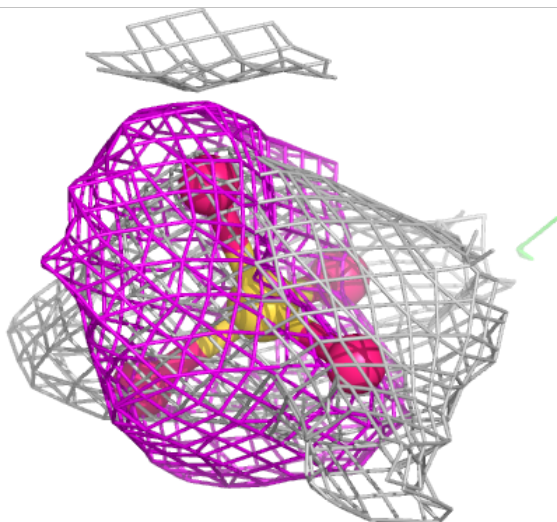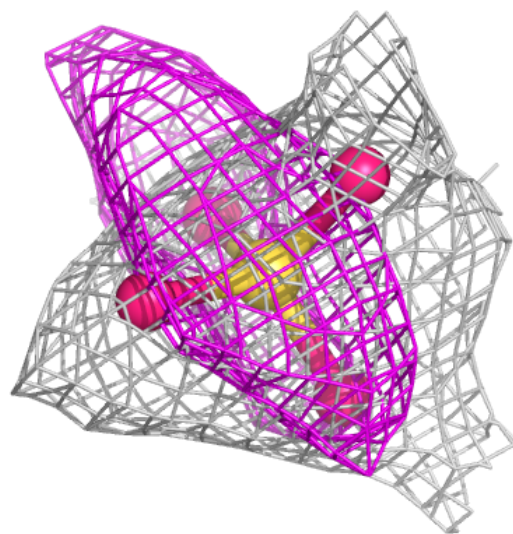
Electron density around IM5 E 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
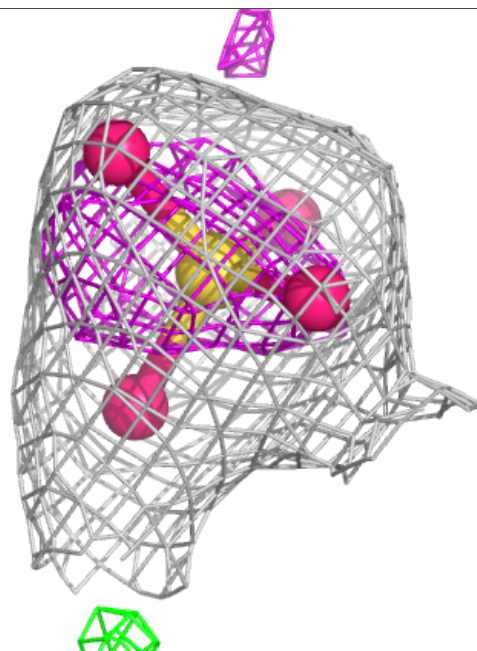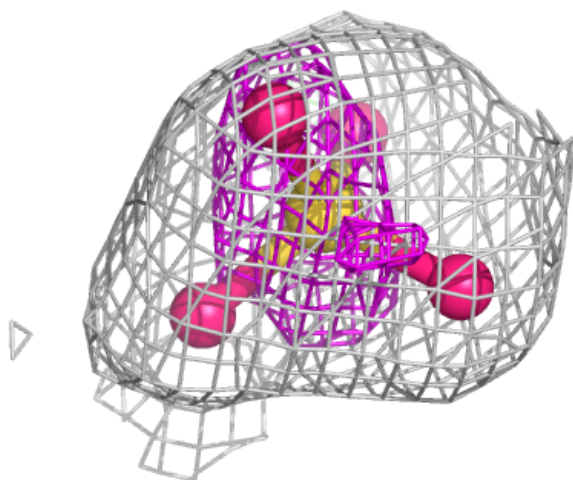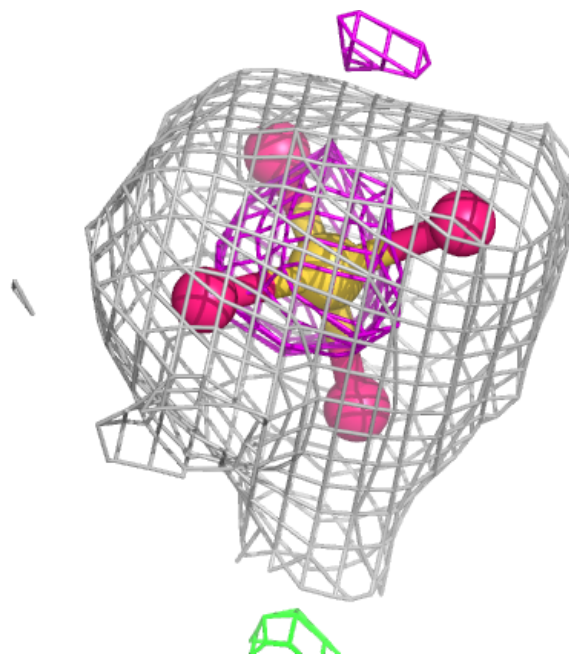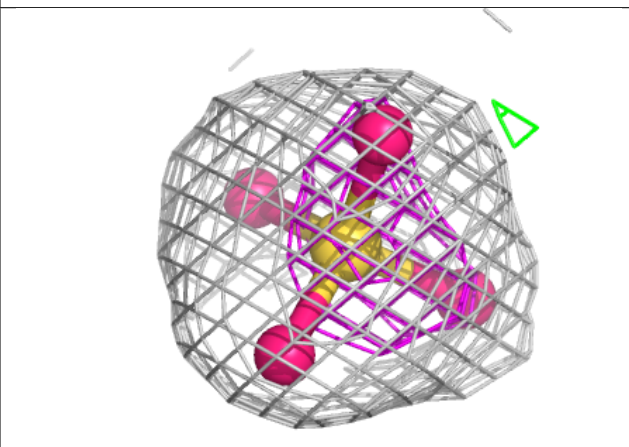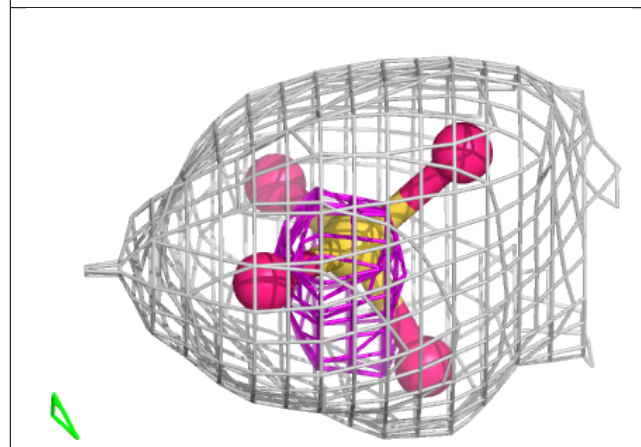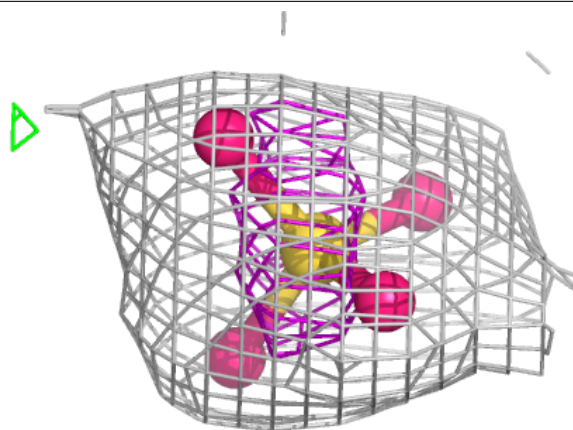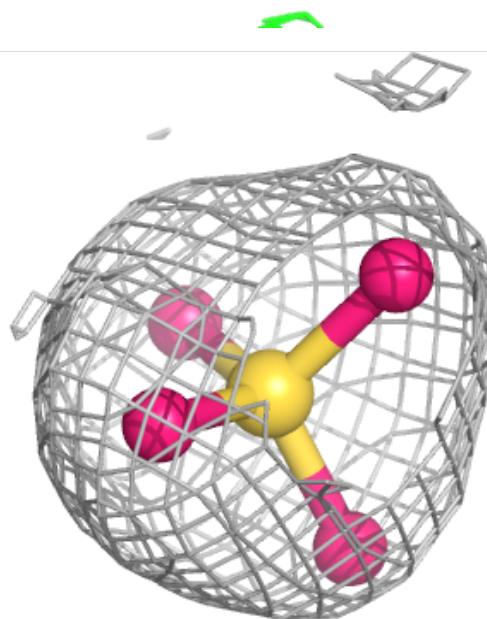$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
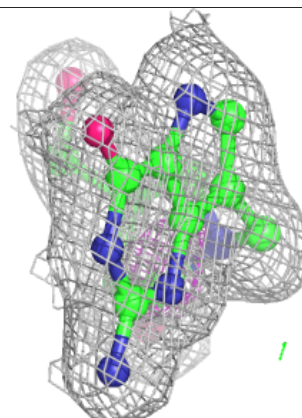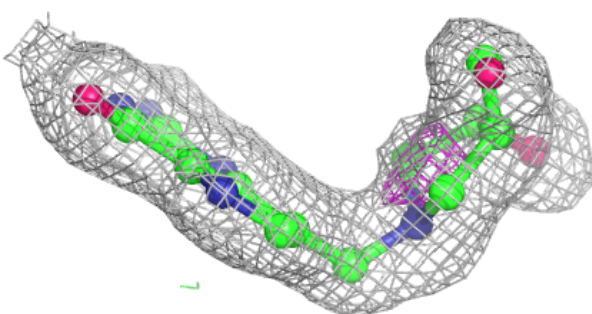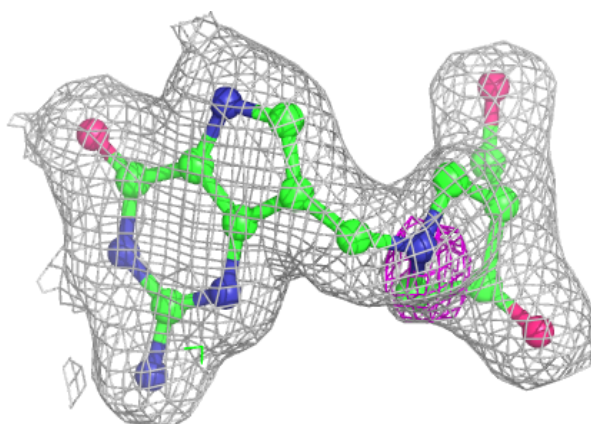
Electron density around IM5 A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
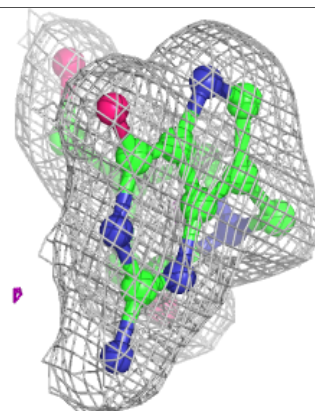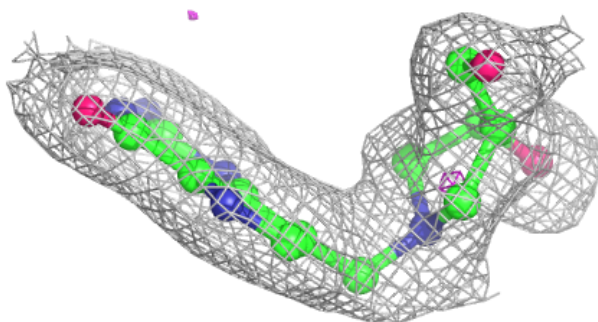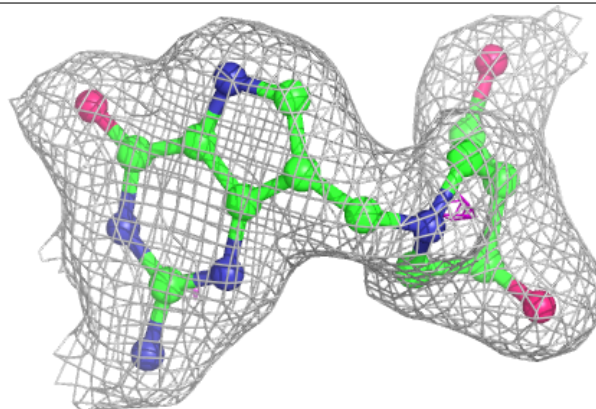
Electron density around SO4 A 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
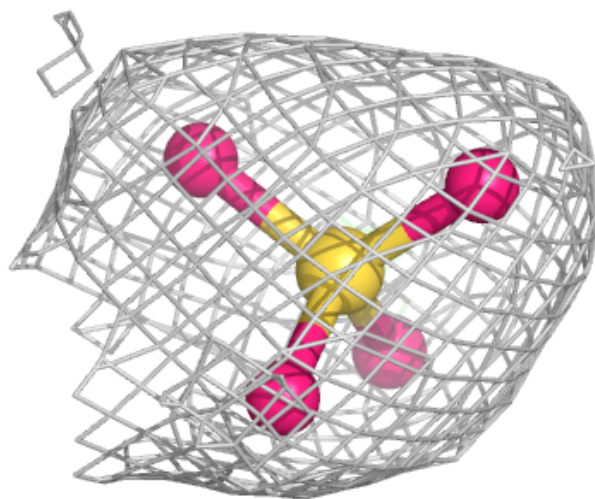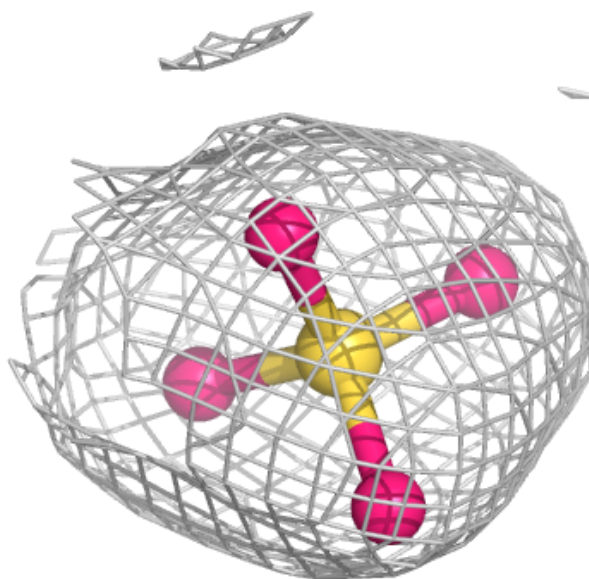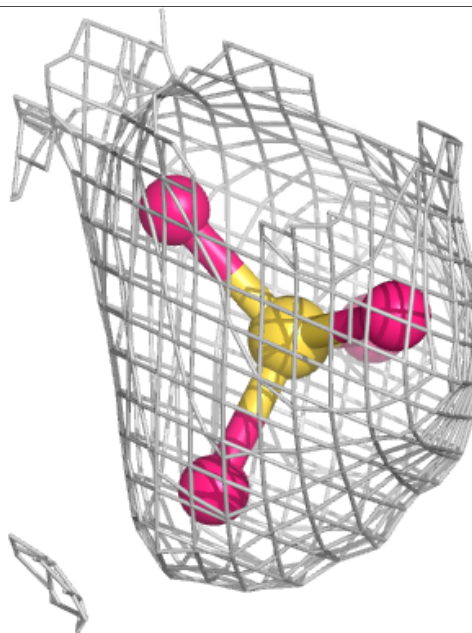and green (positive)
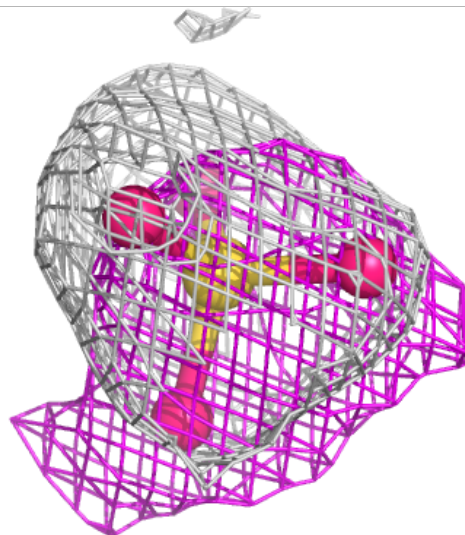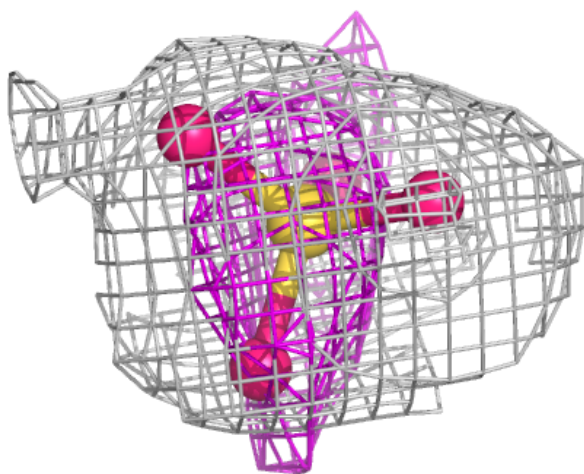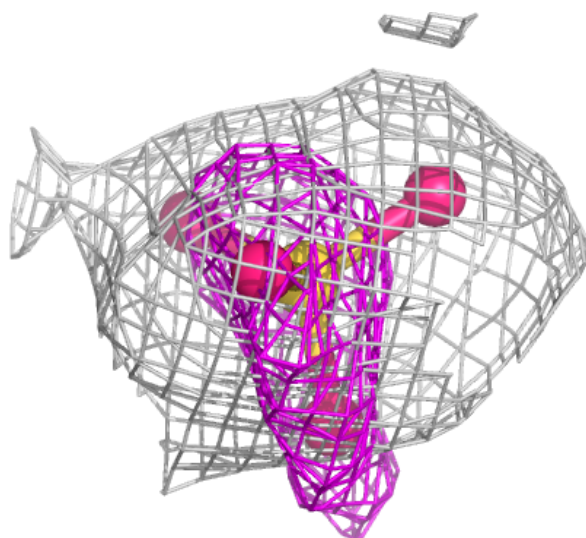
Electron density around IM5 D 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
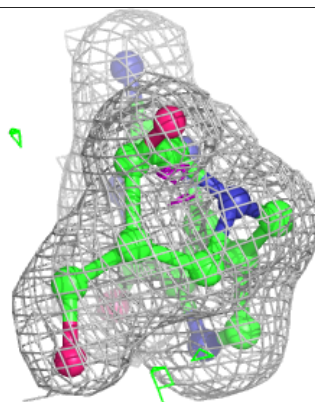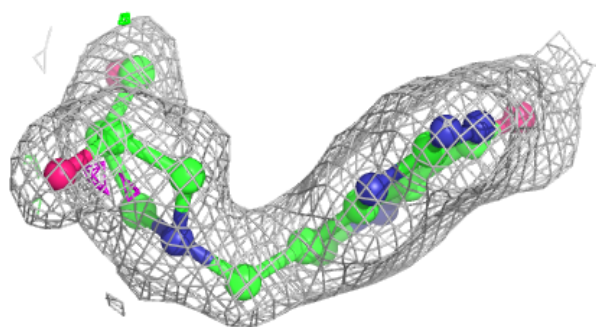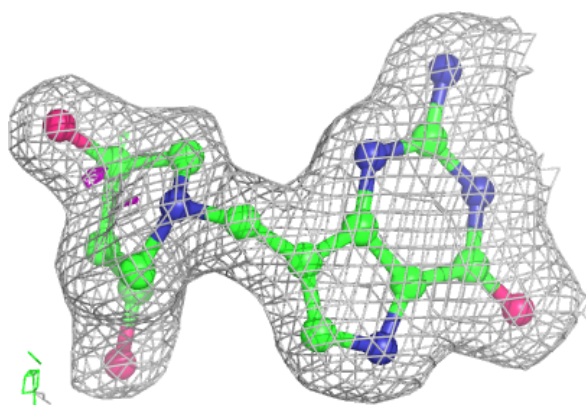
Electron density around SO4 F 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
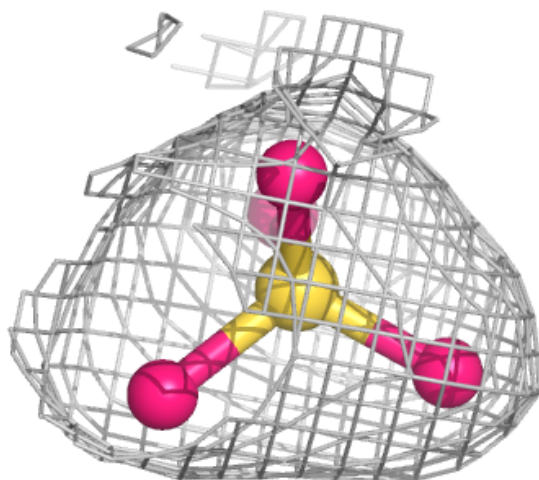$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
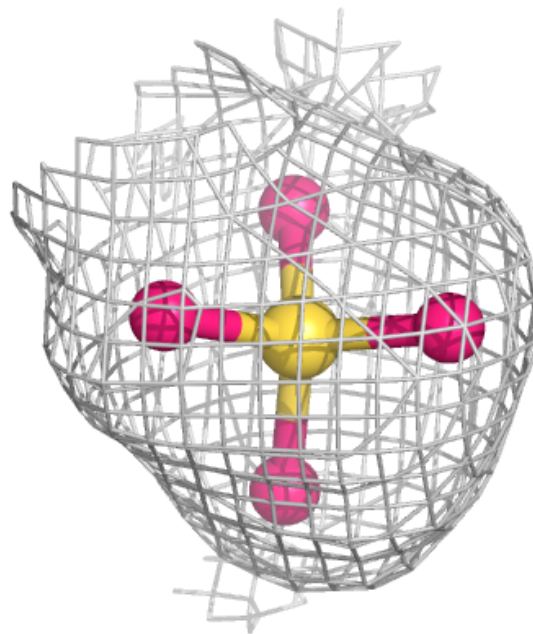and green (positive)
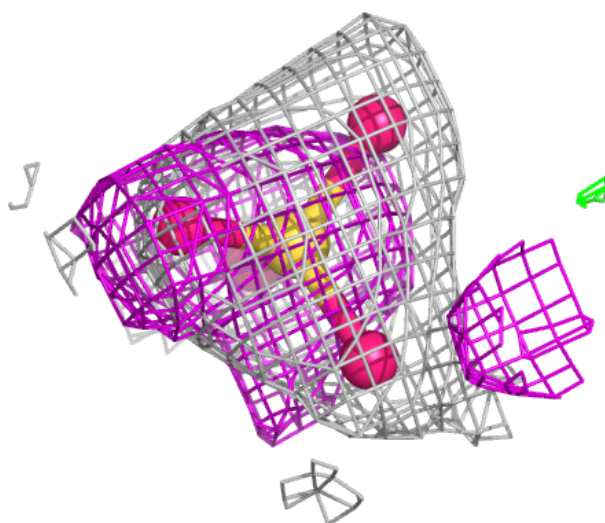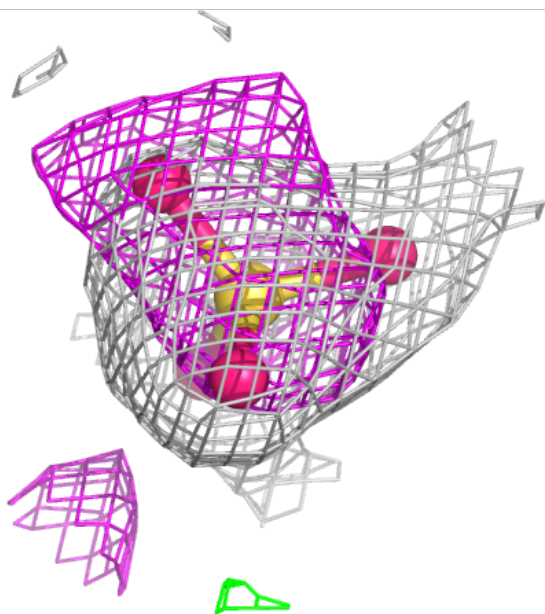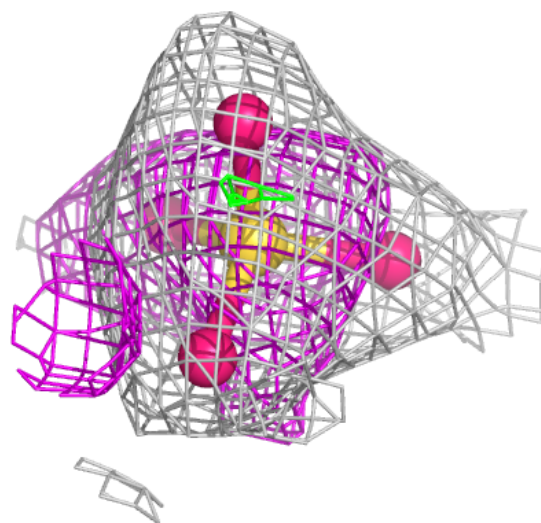
Electron density around IM5 B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
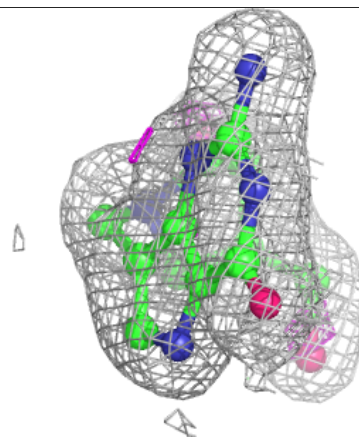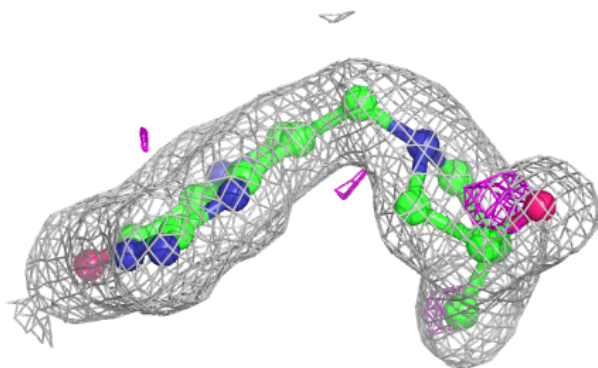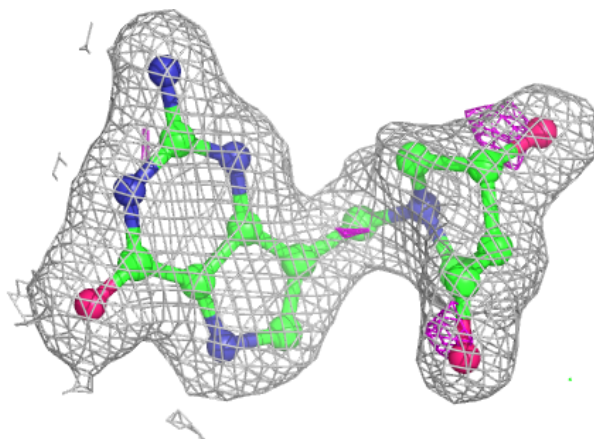
Electron density around SO4 B 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
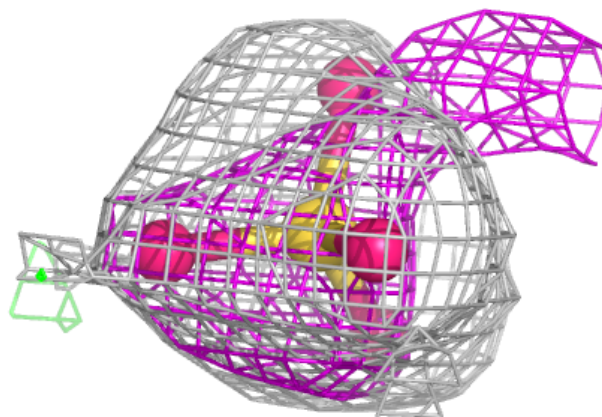
Electron density around SO4 D 403:

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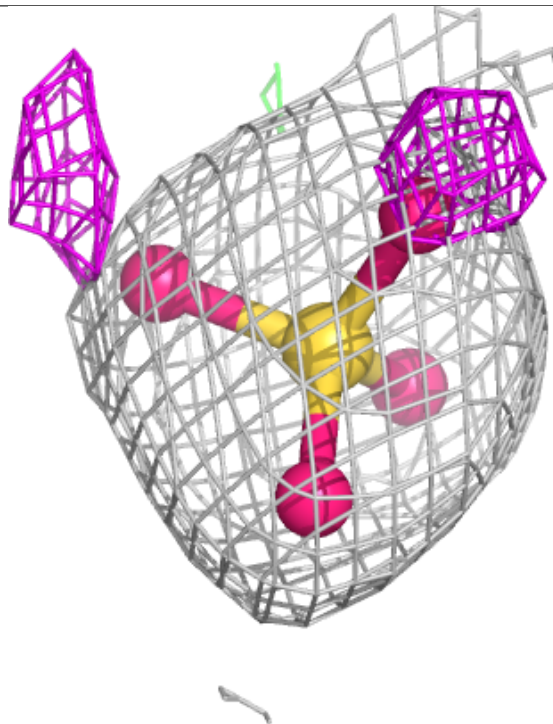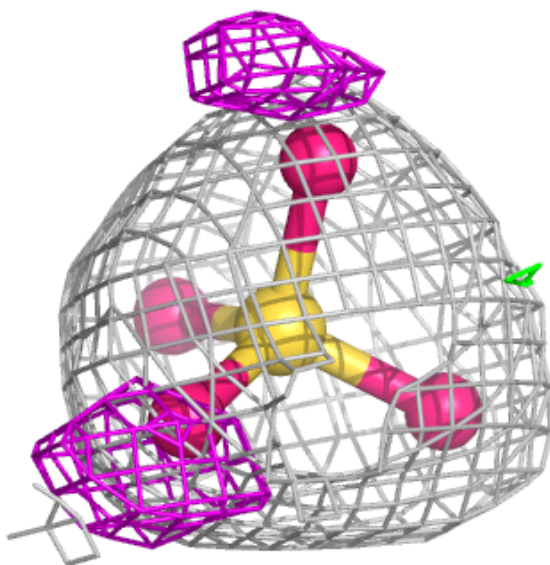mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 E 403:

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

Electron density around SO4 D 402:

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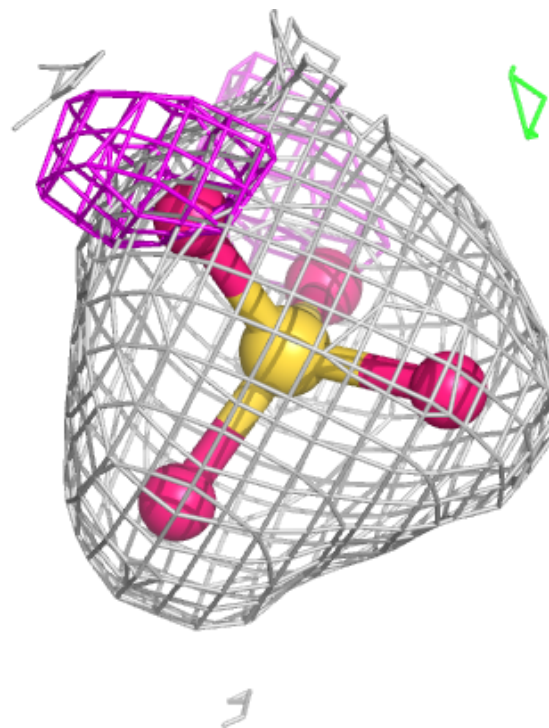and green (positive)

Electron density around SO4 E 402:

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

Electron density around SO4 B 402:
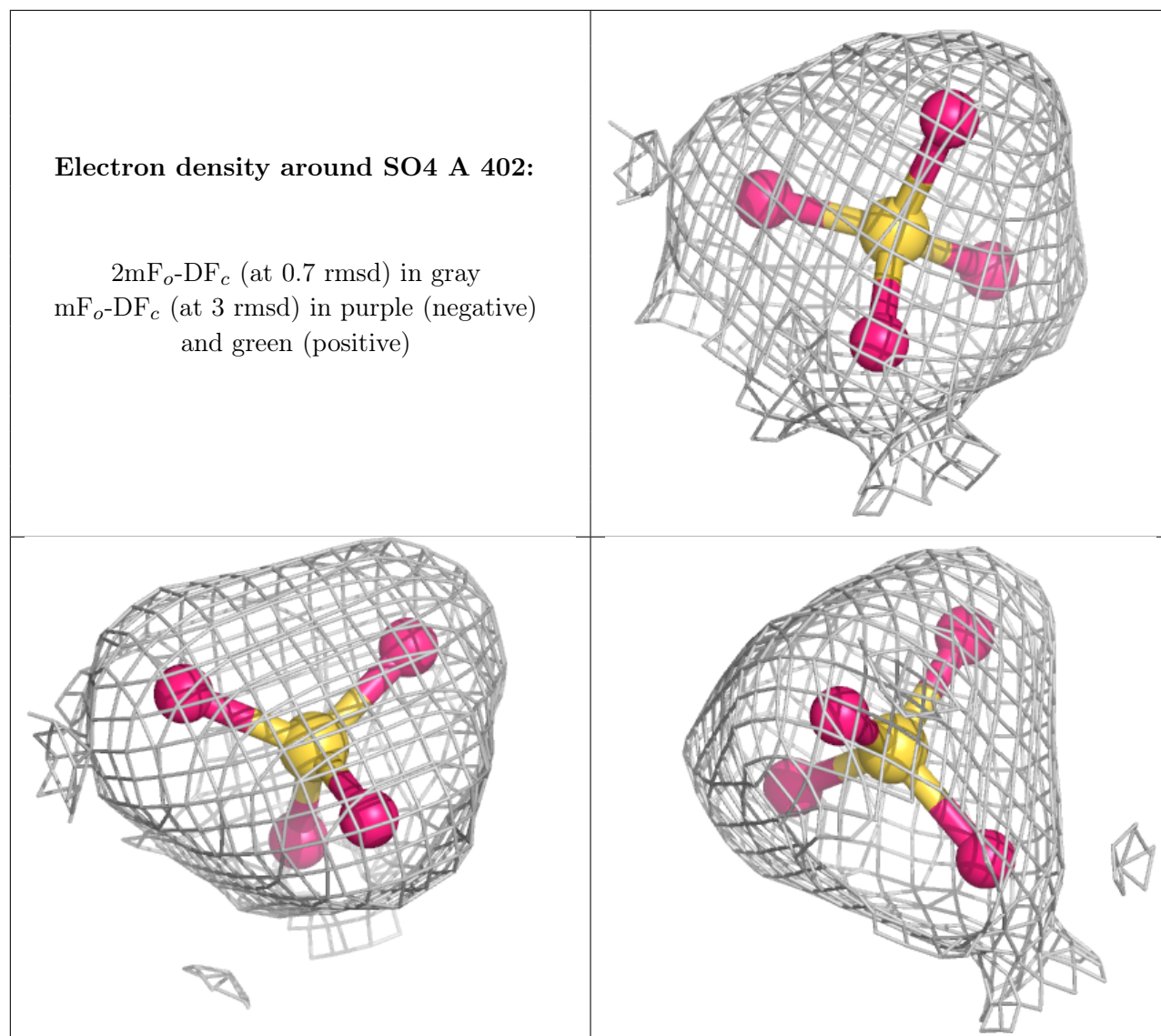
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 A 402:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.