WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 31, 2022 – 07:14 am BST

PDB ID	:	7Q05
Title	:	Crystal structure of TPADO in complex with TPA
Authors	:	Zahn, M.; Kincannon, W.M.; DuBois, J.L.; McGeehan, J.E.
Deposited on	:	2021-10-14
Resolution	:	2.08 Å(reported)

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

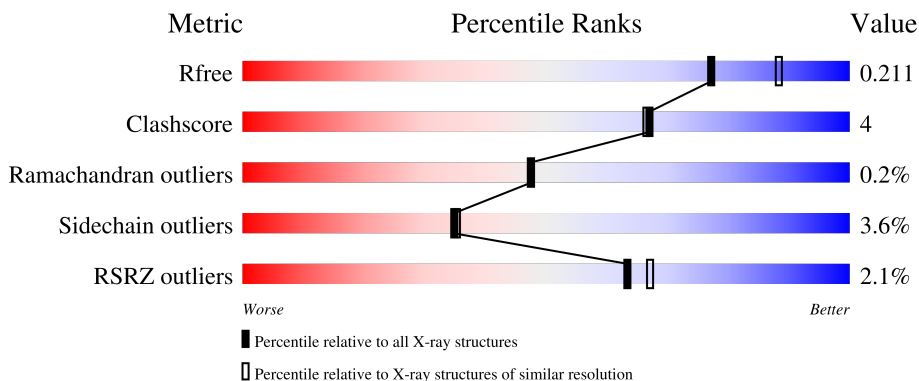|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.08 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	Percentile Ranks	Value
Rfree		0.211
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		3.6%
RSRZ outliers		2.1%

Worse　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

◲ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	154	88% 11% •
1	B	154	.% 86% 12% •
1	C	154	.% 84% 15% •
2	D	428	3% 79% 9% • 11%
2	E	428	2% 84% 10% • •

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	428	4% / 79% / 9% · 10%
3	H	129	87% / 12% ·

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
5	SO4	E	503	-	-	X	-
6	UB7	F	504	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 28454 atoms, of which 13482 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 Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			
1	B	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			
1	C	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			

- Molecule 2 is a protein called Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	382	Total	C	H	N	O	S	84	1	0
			5899	1897	2897	520	572	13			
2	E	409	Total	C	H	N	O	S	100	4	0
			6387	2052	3132	575	615	13			
2	F	384	Total	C	H	N	O	S	87	3	0
			5961	1915	2932	528	572	14			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP Q3C1D5
D	0	GLY	-	expression tag	UNP Q3C1D5
D	414	GLU	-	expression tag	UNP Q3C1D5
D	415	ASN	-	expression tag	UNP Q3C1D5
D	416	LEU	-	expression tag	UNP Q3C1D5
D	417	TYR	-	expression tag	UNP Q3C1D5
D	418	PHE	-	expression tag	UNP Q3C1D5
D	419	GLN	-	expression tag	UNP Q3C1D5
D	420	GLY	-	expression tag	UNP Q3C1D5
D	421	HIS	-	expression tag	UNP Q3C1D5
D	422	HIS	-	expression tag	UNP Q3C1D5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	423	HIS	-	expression tag	UNP Q3C1D5
D	424	HIS	-	expression tag	UNP Q3C1D5
D	425	HIS	-	expression tag	UNP Q3C1D5
D	426	HIS	-	expression tag	UNP Q3C1D5
E	-1	MET	-	initiating methionine	UNP Q3C1D5
E	0	GLY	-	expression tag	UNP Q3C1D5
E	414	GLU	-	expression tag	UNP Q3C1D5
E	415	ASN	-	expression tag	UNP Q3C1D5
E	416	LEU	-	expression tag	UNP Q3C1D5
E	417	TYR	-	expression tag	UNP Q3C1D5
E	418	PHE	-	expression tag	UNP Q3C1D5
E	419	GLN	-	expression tag	UNP Q3C1D5
E	420	GLY	-	expression tag	UNP Q3C1D5
E	421	HIS	-	expression tag	UNP Q3C1D5
E	422	HIS	-	expression tag	UNP Q3C1D5
E	423	HIS	-	expression tag	UNP Q3C1D5
E	424	HIS	-	expression tag	UNP Q3C1D5
E	425	HIS	-	expression tag	UNP Q3C1D5
E	426	HIS	-	expression tag	UNP Q3C1D5
F	-1	MET	-	initiating methionine	UNP Q3C1D5
F	0	GLY	-	expression tag	UNP Q3C1D5
F	414	GLU	-	expression tag	UNP Q3C1D5
F	415	ASN	-	expression tag	UNP Q3C1D5
F	416	LEU	-	expression tag	UNP Q3C1D5
F	417	TYR	-	expression tag	UNP Q3C1D5
F	418	PHE	-	expression tag	UNP Q3C1D5
F	419	GLN	-	expression tag	UNP Q3C1D5
F	420	GLY	-	expression tag	UNP Q3C1D5
F	421	HIS	-	expression tag	UNP Q3C1D5
F	422	HIS	-	expression tag	UNP Q3C1D5
F	423	HIS	-	expression tag	UNP Q3C1D5
F	424	HIS	-	expression tag	UNP Q3C1D5
F	425	HIS	-	expression tag	UNP Q3C1D5
F	426	HIS	-	expression tag	UNP Q3C1D5

- Molecule 3 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	129	1961	613	960	193	185	10	22	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2)

Full wwPDB X-ray Structure Validation Report

(labeled as "Ligand of Interest" by depositor).
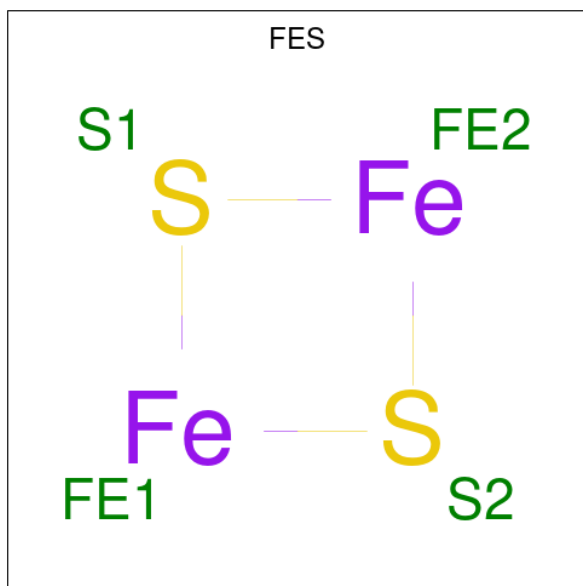
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 4	Fe 2	S 2	0	0
4	E	1	Total 4	Fe 2	S 2	0	0
4	F	1	Total 4	Fe 2	S 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).
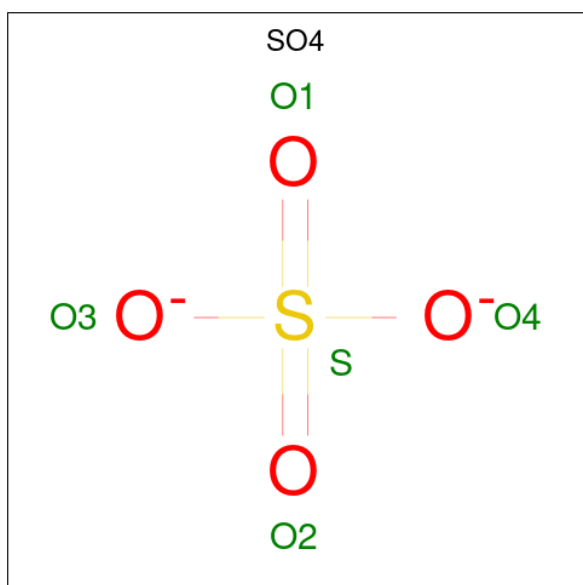
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0

- Molecule 6 is terephthalic acid (three-letter code: UB7) (formula: $C_8H_6O_4$) (labeled as "Ligand of Interest" by depositor).
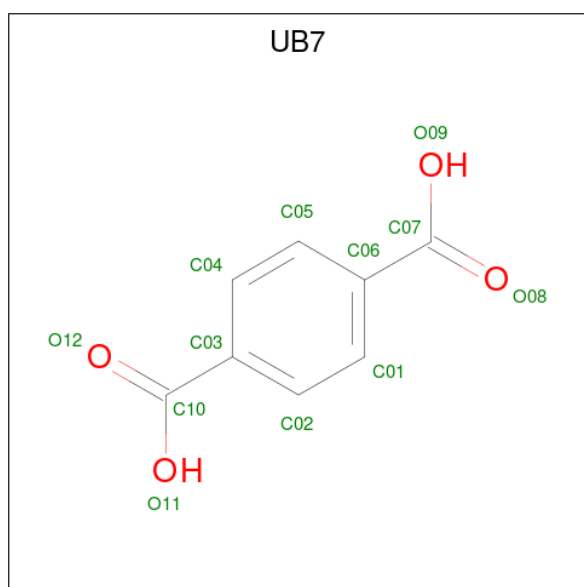
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total 18	C 8	H 6	O 4	1	0
6	E	1	Total 18	C 8	H 6	O 4	1	0
6	F	1	Total 18	C 8	H 6	O 4	1	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Fe 1	0	0
7	F	1	Total 1	Fe 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	122	Total 122	O 122	0	0
8	B	98	Total 98	O 98	0	0
8	C	97	Total 97	O 97	0	0
8	D	136	Total 136	O 136	0	0
8	E	254	Total 254	O 254	0	0
8	F	193	Total 193	O 193	0	0
8	H	53	Total 53	O 53	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: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain A:

- Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain B:
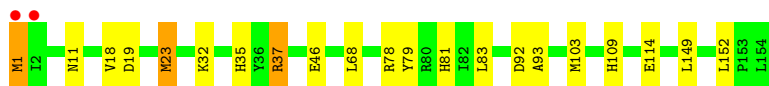
- Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain C:

- Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2
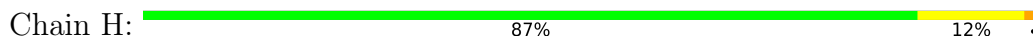
Chain D:
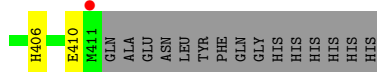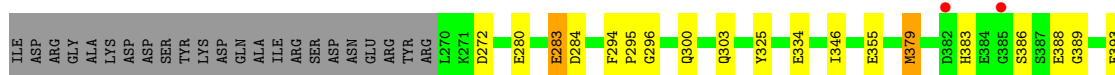
- Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2
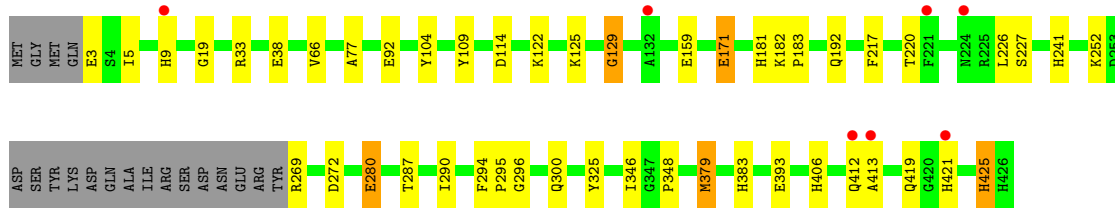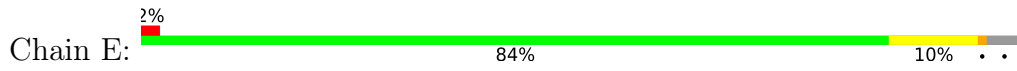
Chain E:

• Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

Chain F:
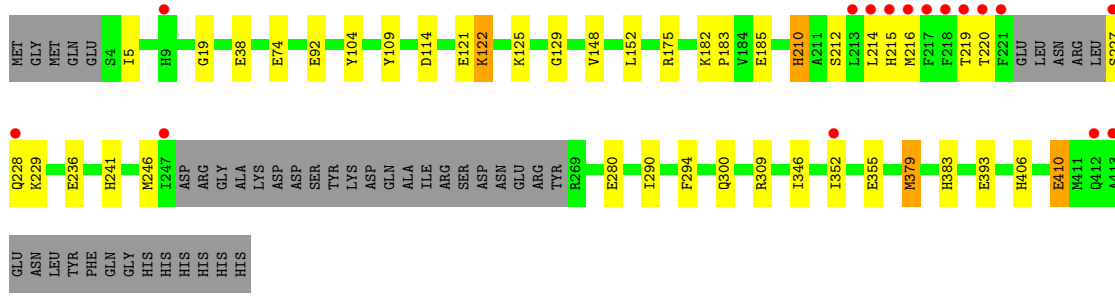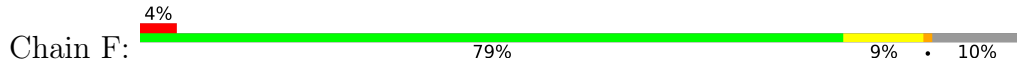
• Molecule 3: Lysozyme

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	219.71Å 219.71Å 82.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	190.28 – 2.08 190.28 – 2.08	Depositor EDS
% Data completeness (in resolution range)	81.0 (190.28-2.08) 74.3 (190.28-2.08)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.214 0.173 , 0.211	Depositor DCC
R_{free} test set	5502 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28454	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: FES, UB7, SO4, FE

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	0.87	1/1232 (0.1%)	0.97	2/1671 (0.1%)
1	B	0.91	2/1232 (0.2%)	0.98	2/1671 (0.1%)
1	C	0.83	2/1232 (0.2%)	1.02	5/1671 (0.3%)
2	D	0.84	2/3073 (0.1%)	0.93	4/4148 (0.1%)
2	E	0.88	6/3345 (0.2%)	0.97	3/4514 (0.1%)
2	F	0.85	5/3107 (0.2%)	0.95	2/4194 (0.0%)
3	H	0.92	3/1021 (0.3%)	1.12	3/1379 (0.2%)
All	All	0.86	21/14242 (0.1%)	0.98	21/19248 (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
2	D	0	2
2	E	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	GLU	CD-OE2	13.18	1.40	1.25
1	A	114	GLU	CD-OE2	6.91	1.33	1.25
2	D	334	GLU	CD-OE2	6.67	1.32	1.25
2	F	92	GLU	CD-OE2	6.54	1.32	1.25
2	D	272	ASP	CB-CG	6.54	1.65	1.51
2	E	129	GLY	CA-C	6.54	1.62	1.51
1	B	46	GLU	CD-OE2	6.33	1.32	1.25
2	E	129	GLY	C-O	5.96	1.33	1.23
2	F	74	GLU	CD-OE2	-5.73	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	413	ALA	C-O	5.68	1.34	1.23
2	E	92	GLU	CD-OE1	5.44	1.31	1.25
1	C	46	GLU	CD-OE1	5.43	1.31	1.25
2	E	272	ASP	CB-CG	5.42	1.63	1.51
3	H	23	TYR	CE1-CZ	5.37	1.45	1.38
2	F	185	GLU	CD-OE1	-5.31	1.19	1.25
2	F	410	GLU	CD-OE1	5.29	1.31	1.25
3	H	20	TYR	C-O	5.20	1.33	1.23
1	C	136	GLU	CD-OE1	-5.09	1.20	1.25
3	H	118	THR	C-O	5.07	1.32	1.23
2	F	121	GLU	CD-OE2	-5.03	1.20	1.25
2	E	171	GLU	CD-OE2	5.02	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	133	ARG	CG-CD-NE	-8.57	93.81	111.80
1	C	133	ARG	NE-CZ-NH1	-8.54	116.03	120.30
3	H	73	ARG	NE-CZ-NH2	-7.39	116.61	120.30
2	D	379	MET	CG-SD-CE	-6.70	89.49	100.20
2	E	379	MET	CG-SD-CE	-6.67	89.52	100.20
2	F	309	ARG	NE-CZ-NH1	-6.33	117.14	120.30
2	D	182	LYS	CB-CA-C	-6.19	98.01	110.40
2	E	325	TYR	CB-CG-CD1	5.97	124.58	121.00
2	F	379	MET	CG-SD-CE	-5.84	90.86	100.20
2	D	325	TYR	CB-CG-CD1	5.83	124.50	121.00
1	A	37	ARG	NE-CZ-NH1	-5.63	117.48	120.30
3	H	20	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	C	76	ARG	CG-CD-NE	-5.43	100.39	111.80
1	A	78	ARG	NE-CZ-NH2	-5.33	117.63	120.30
3	H	119	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	76	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	106	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	E	9	HIS	CB-CA-C	5.13	120.66	110.40
2	D	189	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	23	MET	CG-SD-CE	-5.11	92.02	100.20
1	B	37	ARG	NE-CZ-NH2	5.09	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	126	GLY	Peptide
2	D	3	GLU	Peptide
2	E	412	GLN	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	1209	1181	1176	9	0
1	B	1209	1181	1176	15	0
1	C	1209	1181	1176	15	0
2	D	3002	2897	2882	22	0
2	E	3255	3132	3114	25	0
2	F	3029	2932	2918	21	0
3	H	1001	960	959	9	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	D	10	0	0	0	0
5	E	25	0	0	3	0
5	F	10	0	0	0	0
5	H	10	0	0	0	0
6	D	12	6	0	0	0
6	E	12	6	0	2	0
6	F	12	6	0	1	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	122	0	0	1	0
8	B	98	0	0	2	0
8	C	97	0	0	2	0
8	D	136	0	0	3	0
8	E	254	0	0	8	0
8	F	193	0	0	1	0
8	H	53	0	0	0	0
All	All	14972	13482	13401	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (108) 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)
5:E:503:SO4:O3	8:E:601:HOH:O	1.75	1.04
1:C:21:ASP:HA	1:C:23:MET:HE2	1.62	0.81
1:A:46:GLU:OE2	8:A:201:HOH:O	2.03	0.76
2:D:379:MET:HE3	2:E:129:GLY:HA2	1.68	0.74
2:D:21:TYR:CE1	2:D:200:LEU:HD13	2.24	0.72
1:C:21:ASP:HA	1:C:23:MET:CE	2.19	0.72
1:C:26:TRP:CE3	1:C:65:ILE:HD11	2.29	0.69
1:B:92:ASP:OD2	8:B:201:HOH:O	2.10	0.67
1:B:18:VAL:O	1:B:23:MET:HE1	1.95	0.67
3:H:75:LEU:O	3:H:97:LYS:HE3	1.98	0.63
1:B:103:MET:HE1	1:C:103:MET:CE	2.33	0.58
1:C:78:ARG:NH1	8:C:201:HOH:O	2.35	0.58
2:D:29:GLN:OE1	2:D:33:ARG:NH2	2.36	0.57
1:A:73:ILE:HB	2:D:355:GLU:HG2	1.84	0.57
2:E:287:THR:HA	5:E:504:SO4:O1	2.05	0.57
2:F:210:HIS:HD2	2:F:214:LEU:HB3	1.68	0.57
2:E:33:ARG:HD3	8:E:642:HOH:O	2.06	0.56
2:F:228:GLN:HB2	2:F:246:MET:O	2.06	0.55
1:A:21:ASP:HA	1:A:23:MET:HE2	1.87	0.55
2:E:425:HIS:CD2	2:E:425:HIS:O	2.60	0.55
2:F:210:HIS:HD2	2:F:214:LEU:CB	2.20	0.55
2:E:379:MET:HE3	2:F:129:GLY:HA2	1.89	0.55
2:F:210:HIS:CD2	2:F:214:LEU:HD23	2.43	0.54
2:D:33:ARG:NE	8:D:606:HOH:O	2.42	0.53
2:D:379:MET:CE	2:E:129:GLY:HA2	2.38	0.53
2:F:122:LYS:HA	2:F:122:LYS:HE3	1.91	0.53
1:C:65:ILE:HD12	1:C:65:ILE:N	2.24	0.52
2:F:175:ARG:NH2	8:F:606:HOH:O	2.42	0.52
1:A:79:TYR:CE2	1:A:152:LEU:HB2	2.45	0.52
2:D:218:PHE:O	2:D:222:GLU:HB2	2.10	0.51
2:D:410:GLU:HB2	8:D:666:HOH:O	2.10	0.51
2:F:300:GLN:HE22	2:F:346:ILE:HG21	1.76	0.51
2:D:386:SER:N	8:D:601:HOH:O	2.33	0.51
2:E:181:HIS:HD2	8:E:817:HOH:O	1.94	0.51
1:C:19:ASP:OD1	1:C:81:HIS:ND1	2.41	0.51
1:B:79:TYR:CE2	1:B:152:LEU:HB2	2.45	0.50
1:C:11:ASN:HB3	1:C:83:LEU:HD13	1.92	0.50
1:A:35:HIS:NE2	1:A:37:ARG:HD3	2.26	0.50
3:H:21:ARG:HH11	3:H:21:ARG:HG2	1.74	0.50
1:C:79:TYR:CE2	1:C:152:LEU:HB2	2.47	0.49
1:A:52:ILE:HD11	1:A:150:MET:SD	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:210:HIS:CD2	2:F:214:LEU:CD2	2.94	0.49
1:B:35:HIS:NE2	1:B:37:ARG:HD3	2.27	0.49
2:D:294:PHE:CE1	2:D:406:HIS:CD2	3.02	0.48
2:E:280:GLU:HG2	8:E:796:HOH:O	2.13	0.48
2:E:290:ILE:HG13	6:E:506:UB7:C01	2.43	0.48
2:D:171:GLU:HG2	2:D:233:ILE:HG21	1.95	0.48
2:D:181:HIS:CD2	2:D:182:LYS:HG3	2.49	0.48
2:F:290:ILE:HG13	6:F:504:UB7:C02	2.43	0.48
1:C:26:TRP:CZ3	1:C:65:ILE:HD11	2.48	0.48
3:H:23:TYR:CD2	3:H:105:MET:HG3	2.49	0.48
1:B:1:MET:HA	1:B:93:ALA:HA	1.96	0.48
1:B:103:MET:HE1	1:C:103:MET:HE1	1.96	0.47
1:C:35:HIS:NE2	1:C:37:ARG:HD3	2.28	0.47
2:E:182:LYS:HB2	2:E:183:PRO:CD	2.44	0.47
2:E:406:HIS:HE1	8:E:801:HOH:O	1.97	0.47
2:D:182:LYS:HB3	2:D:183:PRO:CD	2.43	0.47
2:E:300:GLN:HE22	2:E:346:ILE:HG21	1.79	0.47
3:H:26:GLY:C	3:H:120:VAL:HG13	2.34	0.47
2:D:379:MET:HB2	2:D:393:GLU:OE1	2.15	0.47
2:D:283:GLU:HG3	2:D:284:ASP:N	2.30	0.47
3:H:23:TYR:CZ	3:H:105:MET:HG3	2.50	0.46
2:E:171:GLU:HB2	8:E:802:HOH:O	2.15	0.46
2:D:129:GLY:HA2	2:F:379:MET:HE3	1.97	0.46
2:E:109:TYR:HA	2:E:114:ASP:O	2.16	0.46
1:A:149:LEU:C	1:A:149:LEU:HD12	2.36	0.46
2:D:109:TYR:HA	2:D:114:ASP:O	2.16	0.46
1:B:11:ASN:HB3	1:B:83:LEU:HD13	1.99	0.45
2:F:148:VAL:HA	2:F:152:LEU:O	2.17	0.45
1:B:78:ARG:HD2	8:C:247:HOH:O	2.15	0.45
3:H:23:TYR:CE2	3:H:105:MET:HG3	2.52	0.45
1:A:103:MET:HE1	1:B:103:MET:CE	2.47	0.45
2:E:406:HIS:HD2	8:E:632:HOH:O	2.00	0.45
2:F:109:TYR:HA	2:F:114:ASP:O	2.17	0.45
1:A:52:ILE:HD11	1:A:150:MET:CE	2.47	0.45
1:C:149:LEU:C	1:C:149:LEU:HD12	2.38	0.45
2:F:294:PHE:CE1	2:F:406:HIS:CD2	3.04	0.44
2:E:379:MET:HB2	2:E:393:GLU:OE1	2.18	0.44
2:E:5:ILE:O	2:E:19:GLY:HA3	2.18	0.44
3:H:19:ASN:N	3:H:23:TYR:O	2.50	0.43
2:E:217:PHE:O	2:E:220:THR:HB	2.18	0.43
2:E:159:GLU:OE1	5:E:503:SO4:O2	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HB	1:C:103:MET:HE3	2.00	0.43
1:B:18:VAL:O	1:B:23:MET:CE	2.66	0.43
2:F:182:LYS:HB2	2:F:183:PRO:CD	2.49	0.43
1:B:149:LEU:HD12	1:B:149:LEU:C	2.39	0.43
2:E:421:HIS:ND1	2:E:421:HIS:O	2.51	0.43
2:F:215:HIS:CE1	2:F:352:ILE:O	2.72	0.43
3:H:83:LEU:HD22	3:H:91:SER:HA	2.00	0.43
2:D:389:GLY:HA3	8:E:815:HOH:O	2.19	0.42
2:E:192:GLN:HG3	2:E:348:PRO:HG3	2.01	0.42
2:F:5:ILE:O	2:F:19:GLY:HA3	2.18	0.42
2:D:210:HIS:HD2	2:D:214:LEU:CB	2.32	0.42
2:F:379:MET:HB2	2:F:393:GLU:OE1	2.19	0.42
2:D:210:HIS:HD2	2:D:214:LEU:HB3	1.84	0.42
2:E:425:HIS:O	2:E:425:HIS:HD2	2.01	0.42
2:D:294:PHE:HA	2:D:295:PRO:HA	1.81	0.42
2:E:290:ILE:HG13	6:E:506:UB7:C06	2.50	0.42
2:D:300:GLN:HE22	2:D:346:ILE:HG21	1.84	0.42
2:E:294:PHE:HA	2:E:295:PRO:HA	1.83	0.41
1:B:78:ARG:NH2	8:B:207:HOH:O	2.53	0.41
1:B:68:LEU:HD21	1:B:152:LEU:HD23	2.02	0.41
2:F:210:HIS:CD2	2:F:214:LEU:HB3	2.52	0.41
2:F:216:MET:O	2:F:220:THR:HG23	2.20	0.41
3:H:63:TRP:CE2	3:H:98:ILE:HG12	2.56	0.41
1:B:19:ASP:OD1	1:B:81:HIS:ND1	2.47	0.41
1:C:72:ASN:HA	2:F:355:GLU:OE2	2.21	0.40
2:E:66:VAL:O	2:E:77:ALA:HA	2.22	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	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
1	B	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	C	152/154 (99%)	147 (97%)	5 (3%)	0	100	100
2	D	377/428 (88%)	362 (96%)	14 (4%)	1 (0%)	41	39
2	E	409/428 (96%)	389 (95%)	18 (4%)	2 (0%)	29	25
2	F	381/428 (89%)	366 (96%)	14 (4%)	1 (0%)	41	39
3	H	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
All	All	1750/1875 (93%)	1677 (96%)	69 (4%)	4 (0%)	47	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	425	HIS
2	F	212	SER
2	E	296	GLY
2	D	296	GLY

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	129/129 (100%)	125 (97%)	4 (3%)	40	41
1	B	129/129 (100%)	126 (98%)	3 (2%)	50	53
1	C	129/129 (100%)	124 (96%)	5 (4%)	32	32
2	D	316/355 (89%)	303 (96%)	13 (4%)	30	30
2	E	342/355 (96%)	329 (96%)	13 (4%)	33	33
2	F	319/355 (90%)	306 (96%)	13 (4%)	30	30
3	H	105/105 (100%)	103 (98%)	2 (2%)	57	61
All	All	1469/1557 (94%)	1416 (96%)	53 (4%)	35	35

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLU
1	A	87	SER
1	A	109	HIS
1	A	135	GLN
1	B	1	MET
1	B	32	LYS
1	B	109	HIS
1	C	32	LYS
1	C	76	ARG
1	C	109	HIS
1	C	129	ASP
1	C	133	ARG
2	D	104	TYR
2	D	122	LYS
2	D	125	LYS
2	D	179	VAL
2	D	200	LEU
2	D	210	HIS
2	D	218	PHE
2	D	241	HIS
2	D	280	GLU
2	D	283	GLU
2	D	303	GLN
2	D	383	HIS
2	D	388	GLU
2	E	3	GLU
2	E	38	GLU
2	E	104	TYR
2	E	122	LYS
2	E	125	LYS
2	E	226	LEU
2	E	227	SER
2	E	241	HIS
2	E	252	LYS
2	E	269	ARG
2	E	280	GLU
2	E	383	HIS
2	E	419	GLN
2	F	38	GLU
2	F	104	TYR
2	F	122	LYS
2	F	125	LYS
2	F	210	HIS

Continued from previous page...

Mol	Chain	Res	Type
2	F	219	THR
2	F	227	SER
2	F	229	LYS
2	F	236	GLU
2	F	241	HIS
2	F	280	GLU
2	F	383	HIS
2	F	410	GLU
3	H	68	ARG
3	H	120	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	C	72	ASN
2	D	406	HIS
2	E	127	GLN
2	E	303	GLN
2	E	425	HIS
2	F	210	HIS
2	F	303	GLN
2	F	406	HIS
3	H	46	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	#$|Z| > 2$
5	SO4	E	504	-	4,4,4	0.34	0	6,6,6	0.32	0
4	FES	F	501	2	0,4,4	-	-	-		
5	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	E	503	-	4,4,4	0.16	0	6,6,6	0.25	0
6	UB7	E	506	-	12,12,12	1.82	2 (16%)	16,16,16	0.95	2 (12%)
6	UB7	D	504	-	12,12,12	0.92	0	16,16,16	0.32	0
5	SO4	E	502	-	4,4,4	0.39	0	6,6,6	0.34	0
5	SO4	D	502	-	4,4,4	0.55	0	6,6,6	0.25	0
5	SO4	F	503	-	4,4,4	0.63	0	6,6,6	0.33	0
4	FES	E	501	2	0,4,4	-	-	-		
5	SO4	H	201	-	4,4,4	0.31	0	6,6,6	0.27	0
4	FES	D	501	2	0,4,4	-	-	-		
5	SO4	E	507	-	4,4,4	0.27	0	6,6,6	0.09	0
5	SO4	H	202	-	4,4,4	0.25	0	6,6,6	0.22	0
5	SO4	E	505	-	4,4,4	0.30	0	6,6,6	0.12	0
5	SO4	F	502	-	4,4,4	0.29	0	6,6,6	0.19	0
6	UB7	F	504	-	12,12,12	1.20	1 (8%)	16,16,16	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	F	501	2	-	-	0/1/1/1
6	UB7	E	506	-	-	0/8/8/8	0/1/1/1
6	UB7	D	504	-	-	0/8/8/8	0/1/1/1
4	FES	E	501	2	-	-	0/1/1/1
4	FES	D	501	2	-	-	0/1/1/1
6	UB7	F	504	-	-	0/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	506	UB7	O11-C10	4.70	1.44	1.30
6	F	504	UB7	O08-C07	2.65	1.30	1.22
6	E	506	UB7	O12-C10	2.28	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	506	UB7	O12-C10-C03	-2.22	115.53	121.45
6	E	506	UB7	O11-C10-C03	2.18	120.49	114.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	504	SO4	1	0
5	E	503	SO4	2	0
6	E	506	UB7	2	0
6	F	504	UB7	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 E 504

Bond lengths

Bond angles

Torsions

Rings

Ligand FES F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 E 503

Bond lengths

Bond angles

Torsions

Rings

Ligand UB7 E 506

Bond lengths

Bond angles

Torsions

Rings

Ligand UB7 D 504

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 F 503

Bond lengths

Bond angles

Torsions

Rings

Ligand FES E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FES D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 E 507

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 H 202

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 E 505

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 F 502

Bond lengths

Bond angles

Torsions

Rings

Ligand UB7 F 504

Bond lengths
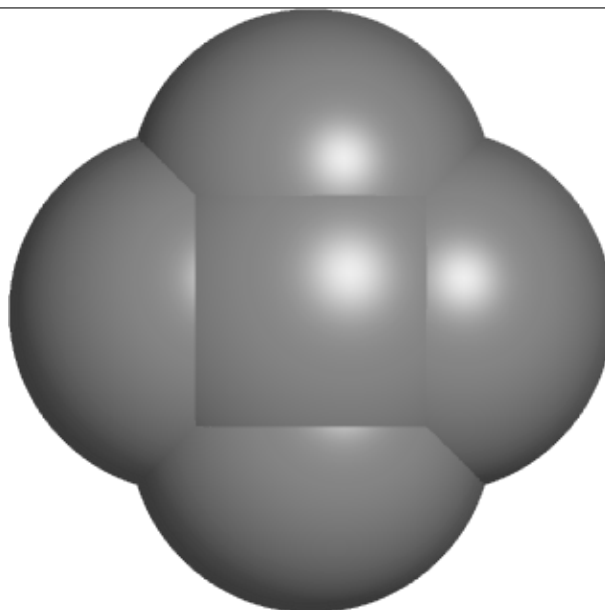
Bond angles
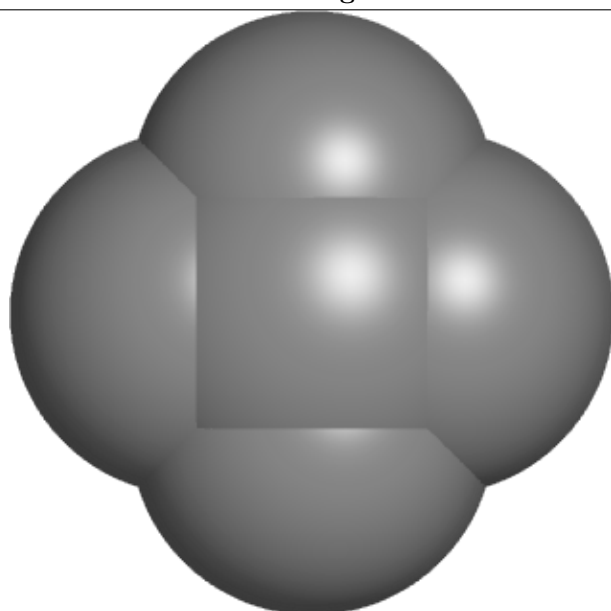
Torsions
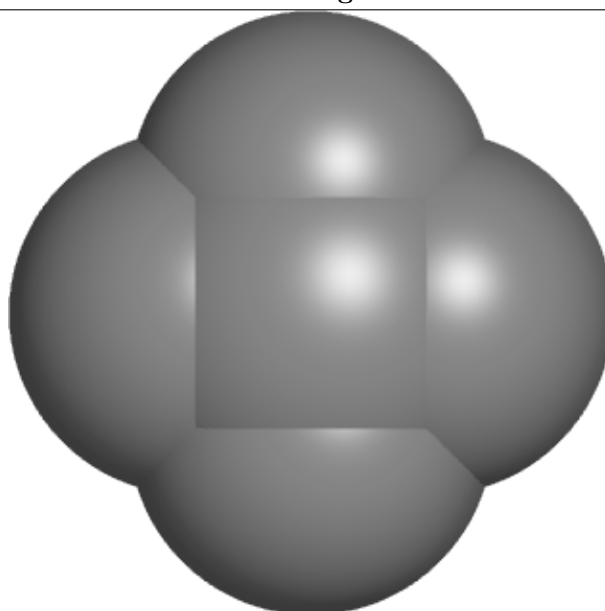
Rings
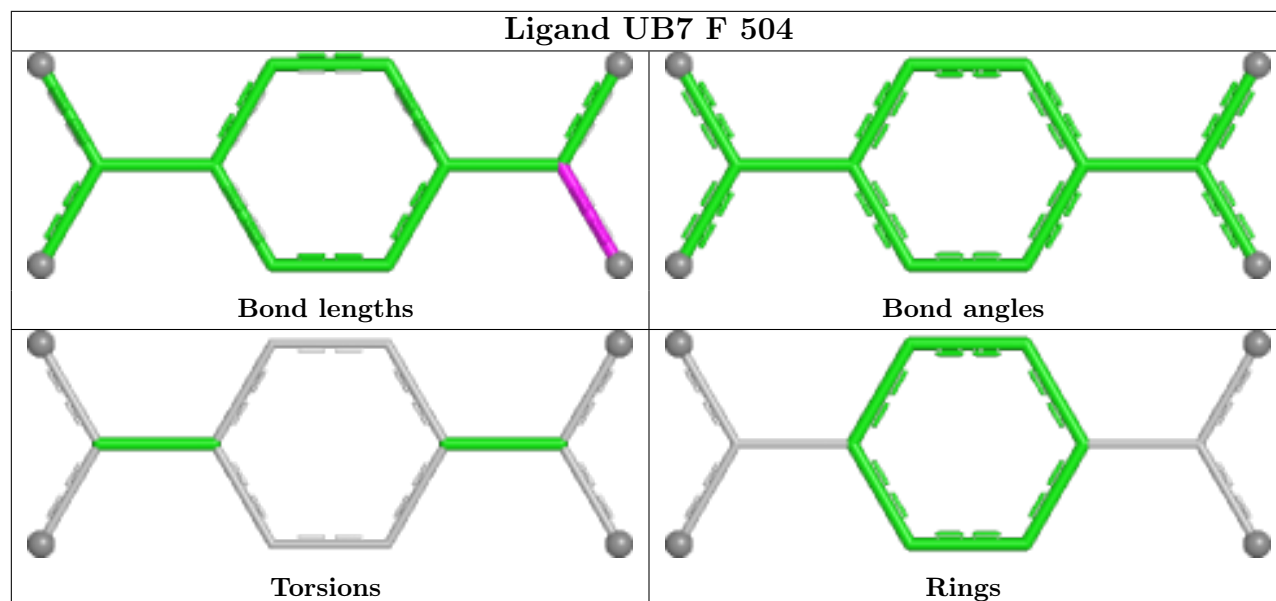
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	154/154 (100%)	0.02	0	100	100	31, 40, 66, 86	0
1	B	154/154 (100%)	0.05	2 (1%)	77	79	32, 42, 66, 97	0
1	C	154/154 (100%)	0.03	1 (0%)	89	91	31, 44, 63, 82	0
2	D	382/428 (89%)	0.13	11 (2%)	51	56	36, 52, 86, 117	0
2	E	409/428 (95%)	0.06	7 (1%)	70	73	30, 42, 81, 120	0
2	F	384/428 (89%)	0.16	16 (4%)	36	41	32, 45, 82, 124	0
3	H	129/129 (100%)	0.01	0	100	100	34, 46, 74, 83	0
All	All	1766/1875 (94%)	0.09	37 (2%)	63	67	30, 45, 80, 124	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	214	LEU	10.7
2	F	217	PHE	7.7
2	F	215	HIS	6.9
2	D	219	THR	5.5
2	D	218	PHE	5.4
2	F	216	MET	5.2
2	F	213	LEU	5.0
2	F	247	ILE	5.0
2	F	412	GLN	5.0
2	F	220	THR	4.8
2	E	132	ALA	4.8
2	F	413	ALA	4.7
2	D	214	LEU	3.8
2	D	221	PHE	3.6
2	E	224	ASN	3.5
2	D	382	ASP	3.3
2	E	412	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	218	PHE	3.0
1	C	73	ILE	2.9
2	E	221	PHE	2.9
2	F	228	GLN	2.8
2	F	9[A]	HIS	2.8
2	E	421	HIS	2.8
2	D	213	LEU	2.7
1	B	1	MET	2.7
2	F	221	PHE	2.7
2	D	385	GLY	2.6
2	F	352	ILE	2.6
2	D	411	MET	2.6
2	D	233	ILE	2.6
2	E	9	HIS	2.5
1	B	2	ILE	2.3
2	F	219	THR	2.3
2	D	222	GLU	2.2
2	E	413	ALA	2.2
2	F	227	SER	2.1
2	D	9	HIS	2.1

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 ⓘ

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
5	SO4	F	502	5/5	0.65	0.21	85,90,114,118	0
6	UB7	E	506	12/12	0.74	0.39	0,83,89,93	1
6	UB7	F	504	12/12	0.75	0.48	0,87,92,95	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	D	503	5/5	0.80	0.34	107,114,119,124	0
5	SO4	E	505	5/5	0.83	0.10	116,118,118,120	0
5	SO4	H	202	5/5	0.83	0.26	94,102,124,132	0
7	FE	F	505	1/1	0.84	0.36	114,114,114,114	0
7	FE	D	505	1/1	0.87	0.09	101,101,101,101	0
5	SO4	E	504	5/5	0.87	0.15	87,91,95,99	0
6	UB7	D	504	12/12	0.88	0.26	0,63,68,70	1
5	SO4	E	503	5/5	0.90	0.15	86,89,95,107	0
5	SO4	E	507	5/5	0.94	0.10	75,89,97,97	0
5	SO4	D	502	5/5	0.95	0.16	56,62,73,84	0
5	SO4	F	503	5/5	0.95	0.11	53,58,72,77	0
5	SO4	E	502	5/5	0.96	0.22	57,60,70,74	0
5	SO4	H	201	5/5	0.98	0.17	55,55,60,75	0
4	FES	D	501	4/4	0.99	0.14	43,45,46,46	0
4	FES	E	501	4/4	0.99	0.14	39,41,43,43	0
4	FES	F	501	4/4	1.00	0.18	35,35,35,36	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 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
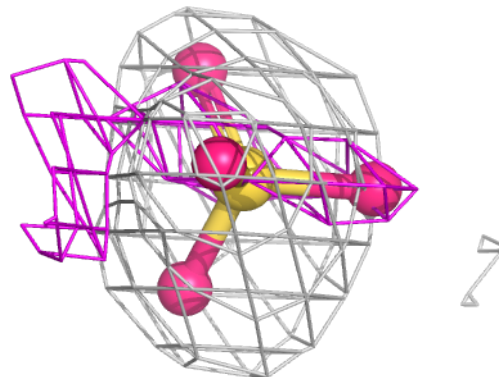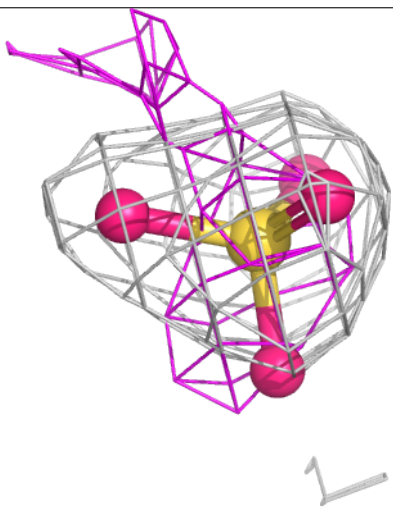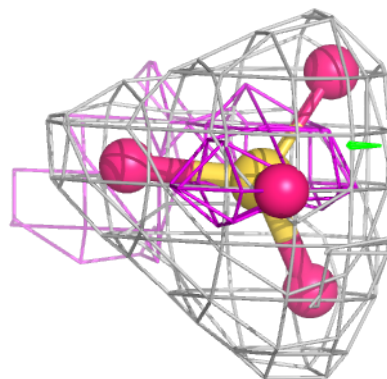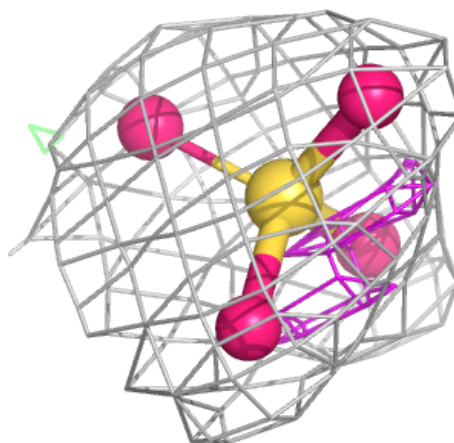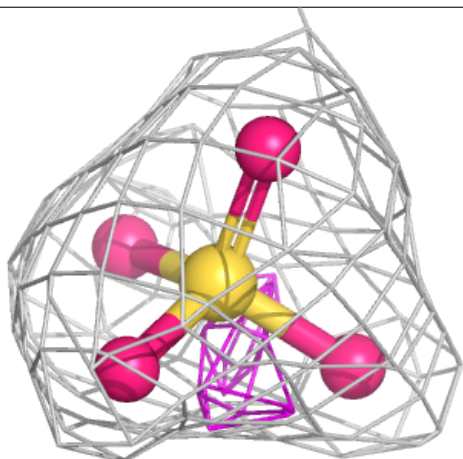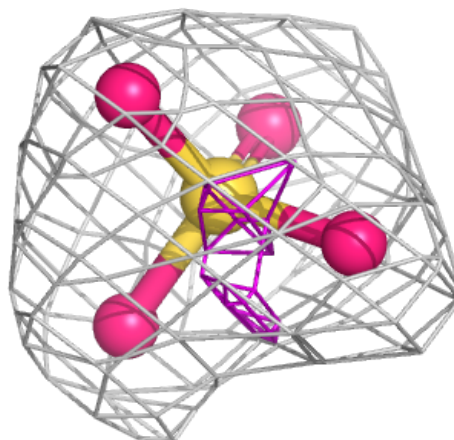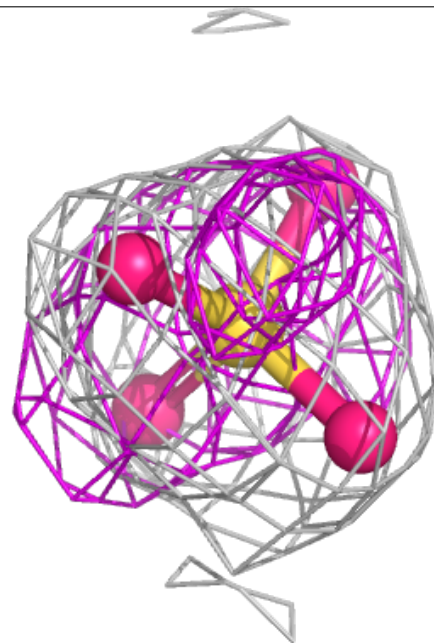and green (positive)
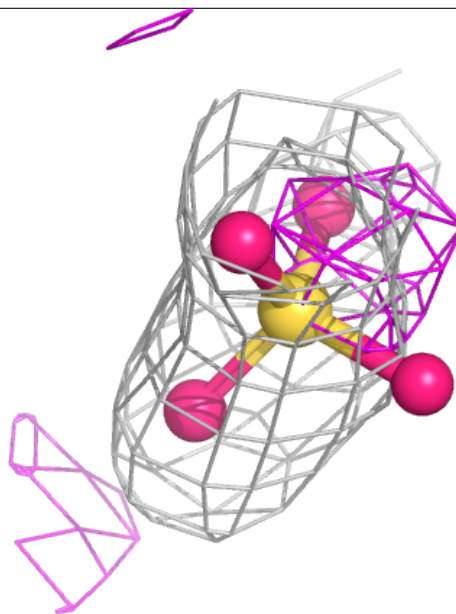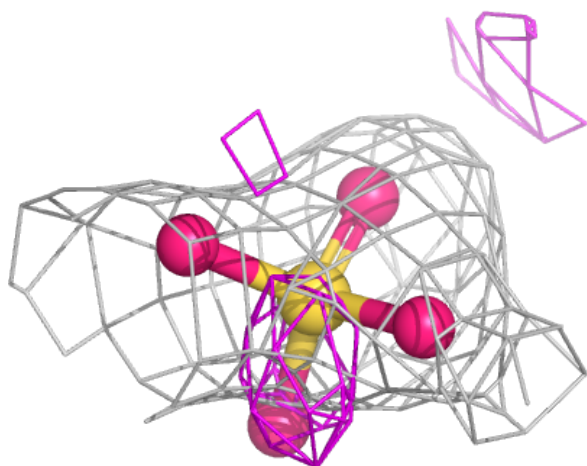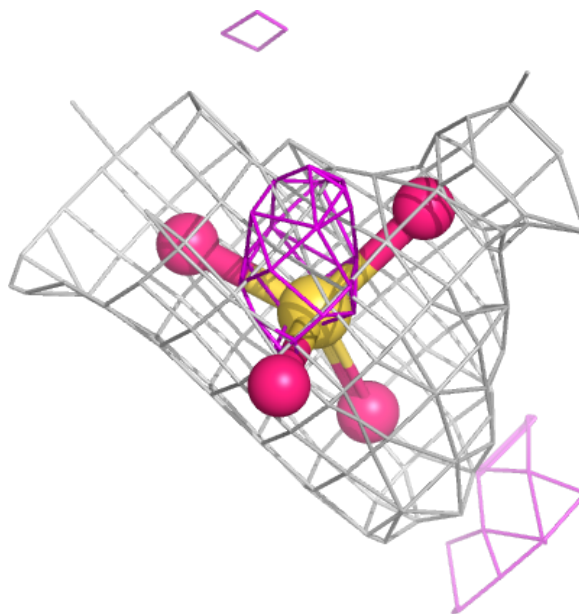
Electron density around UB7 E 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
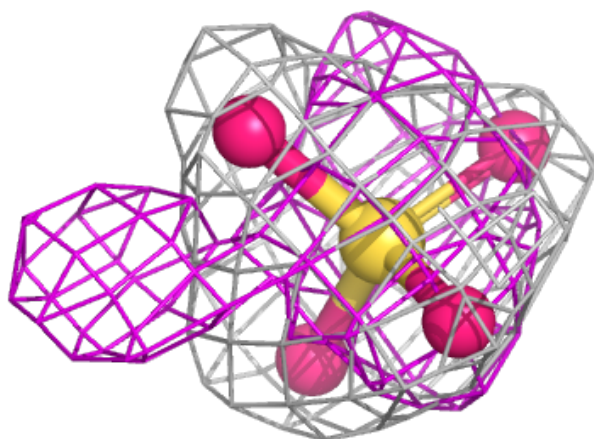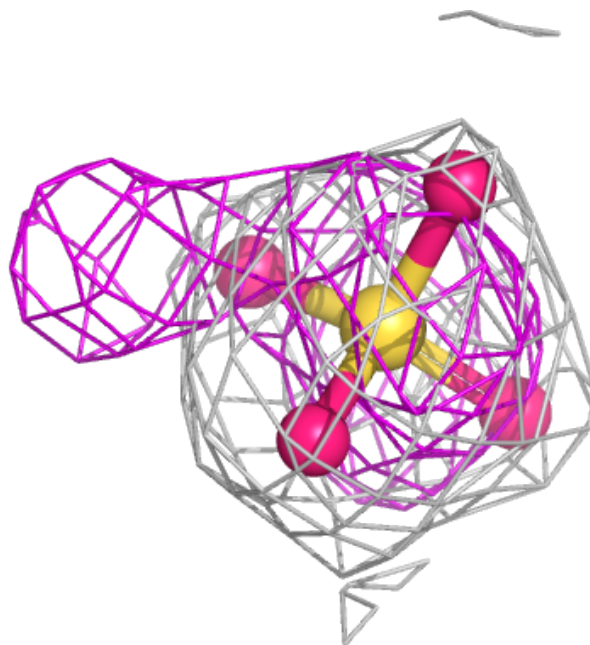and green (positive)
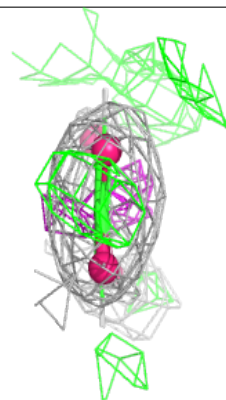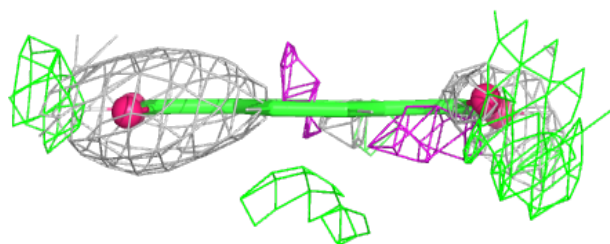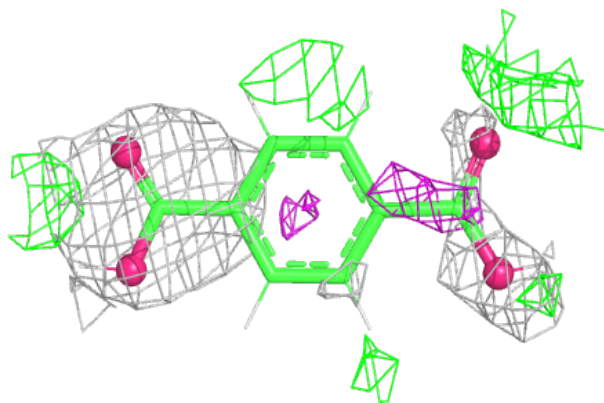
Electron density around UB7 F 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
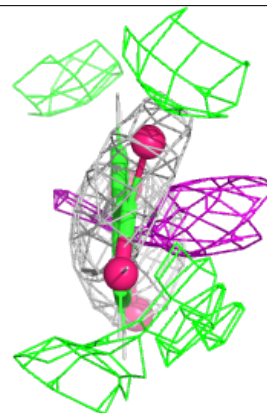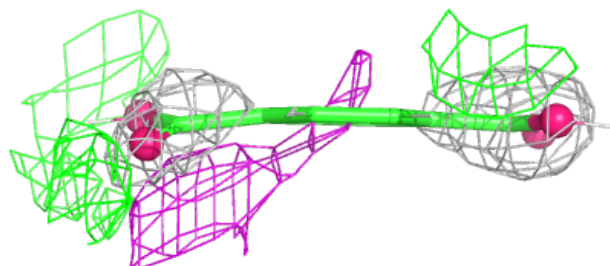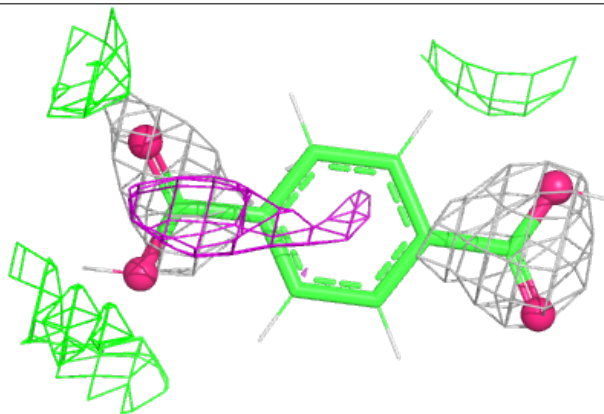
Electron density around SO4 D 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
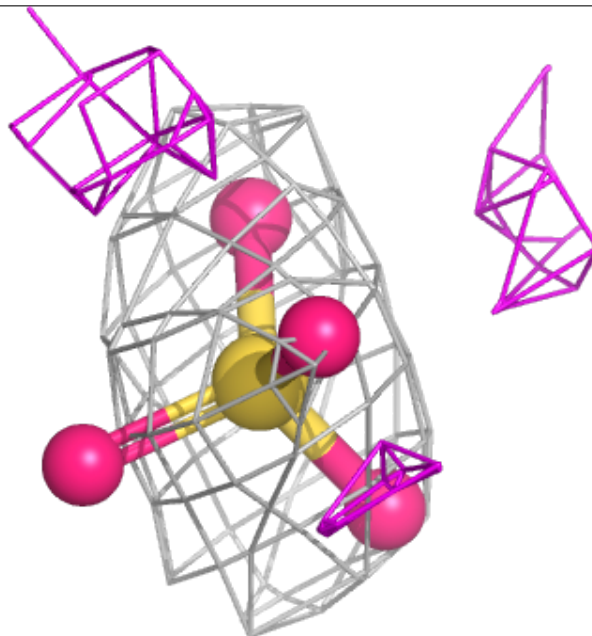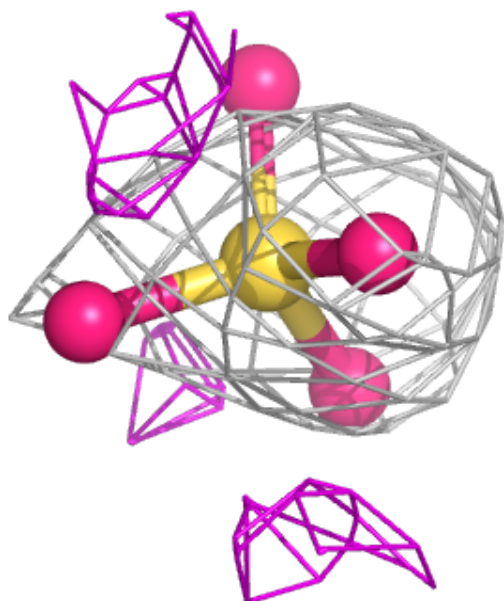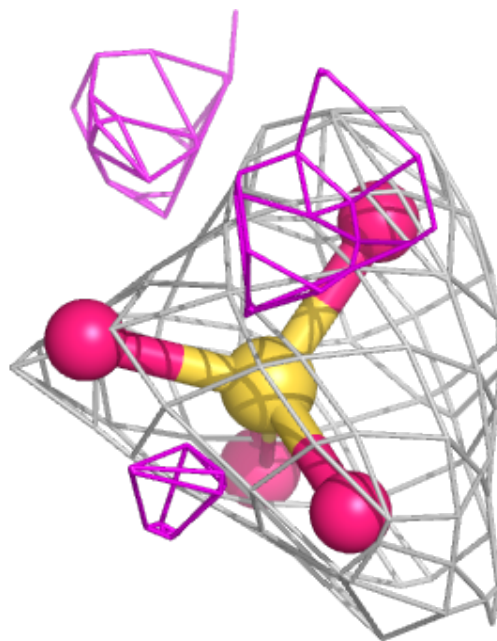
Electron density around SO4 E 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
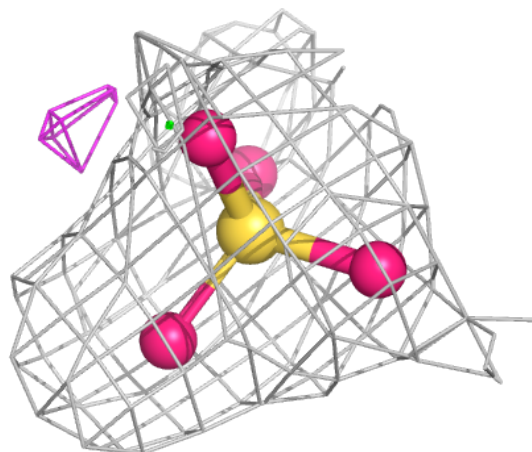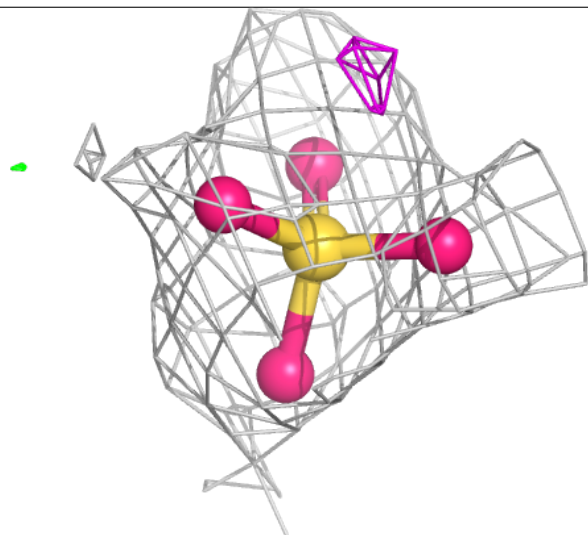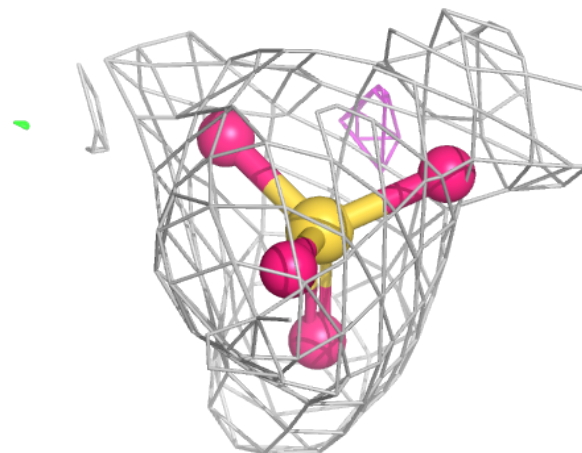
Electron density around SO4 H 202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
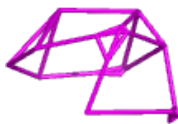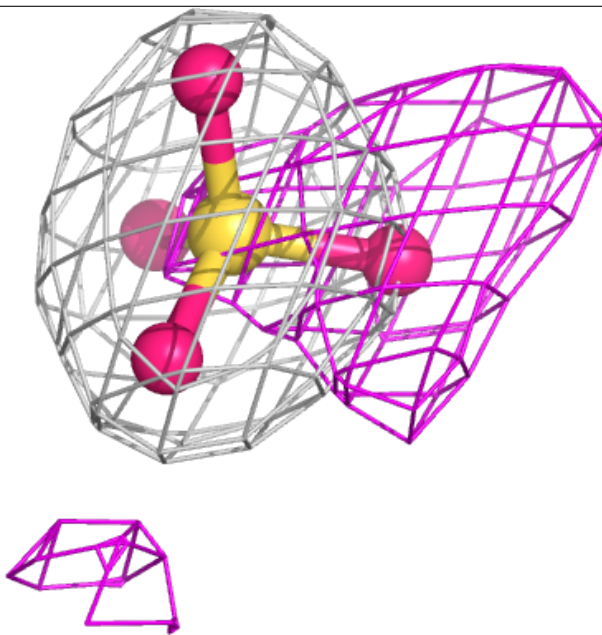$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
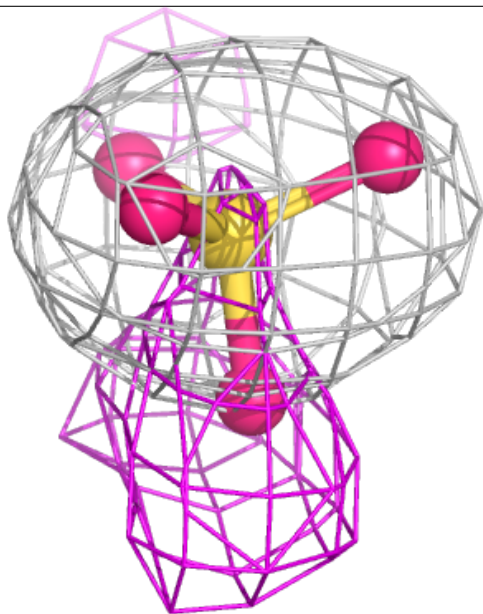and green (positive)
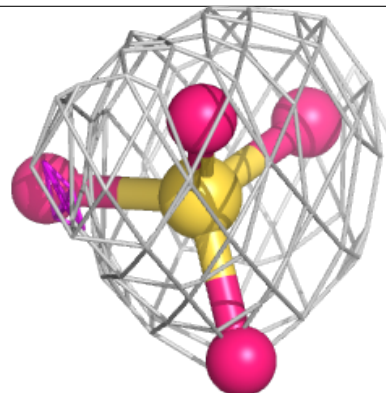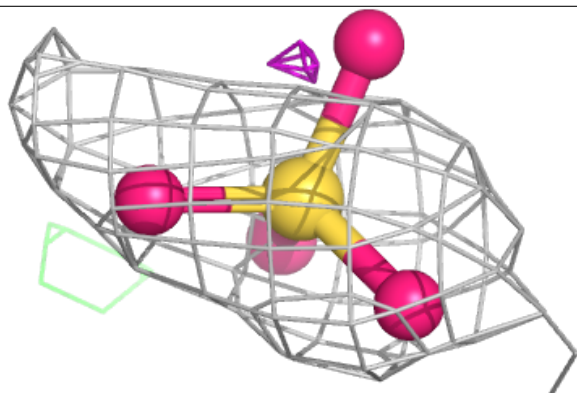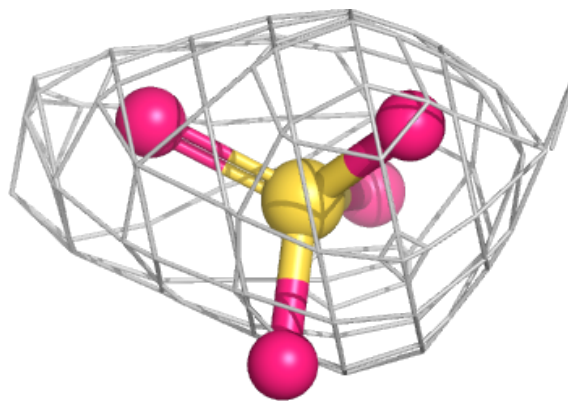
Electron density around FE F 505:

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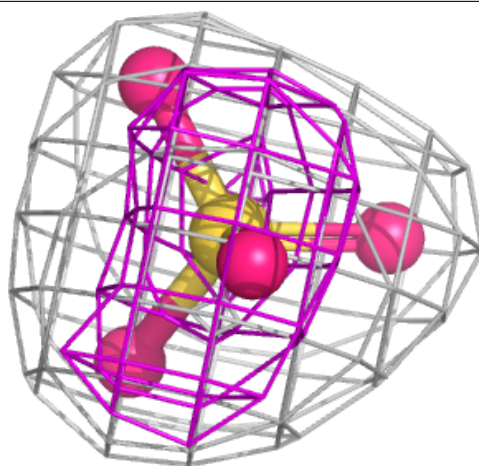and green (positive)

Electron density around FE D 505:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
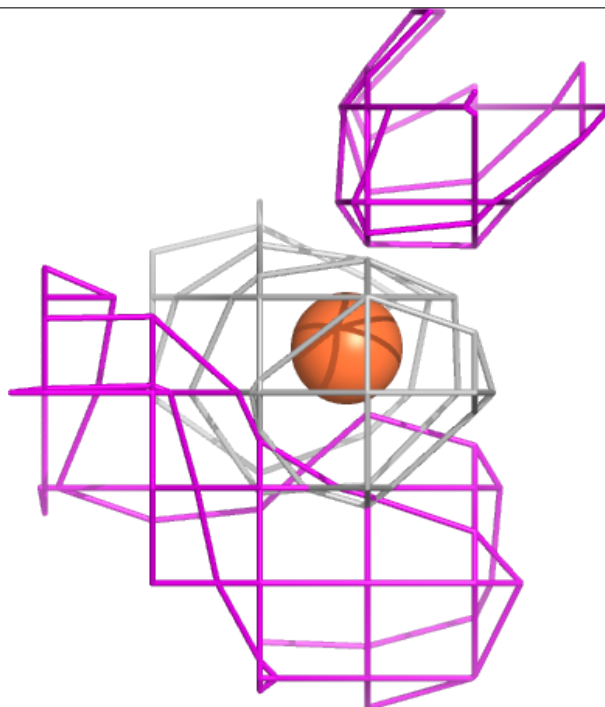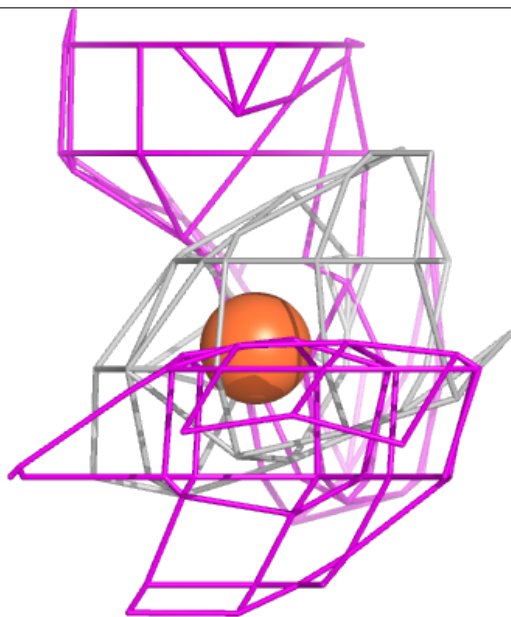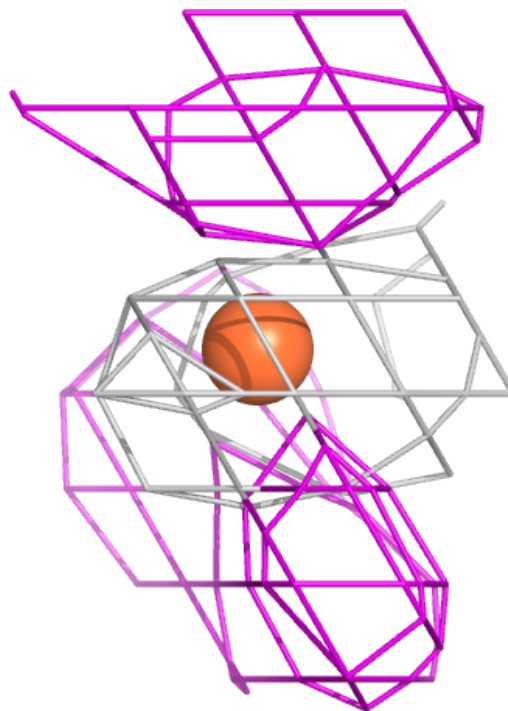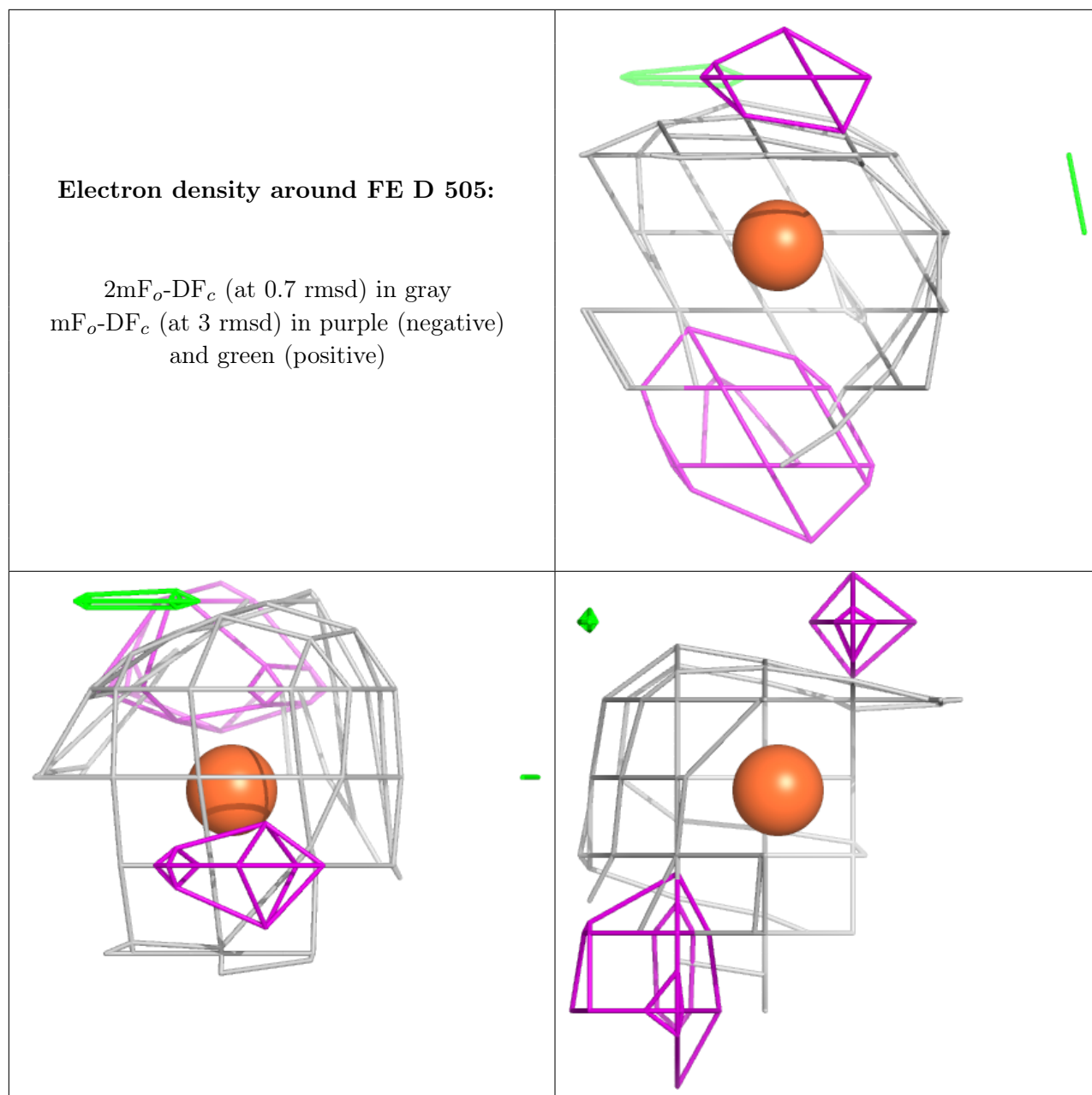
Electron density around SO4 E 504:

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

Electron density around UB7 D 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
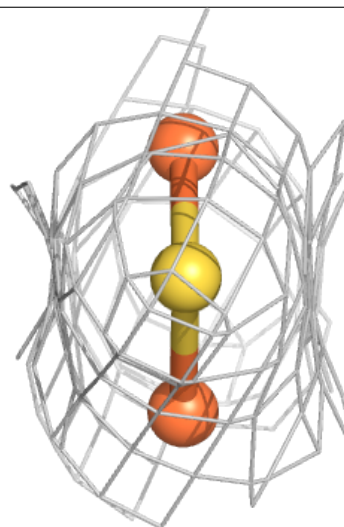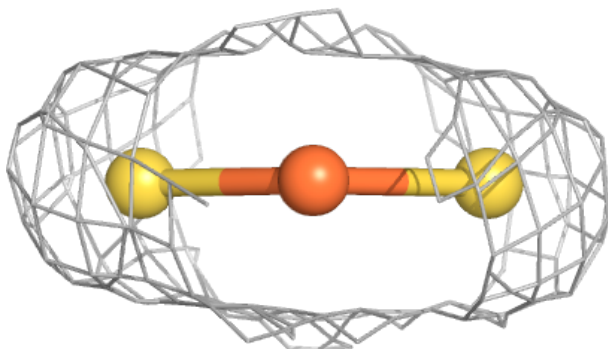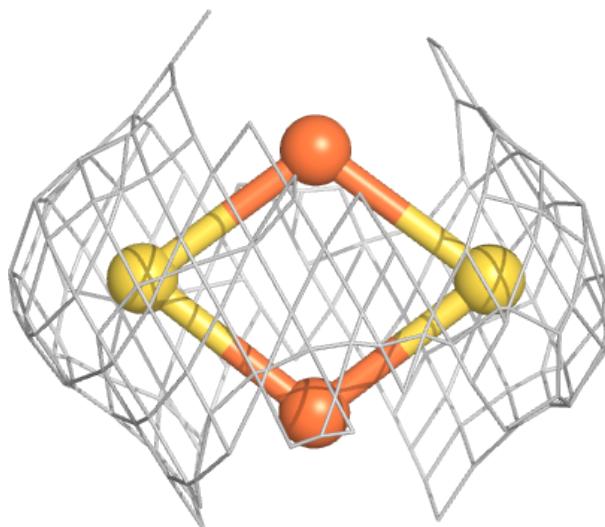and green (positive)
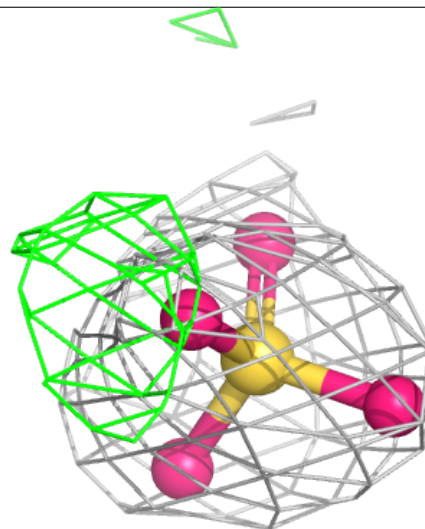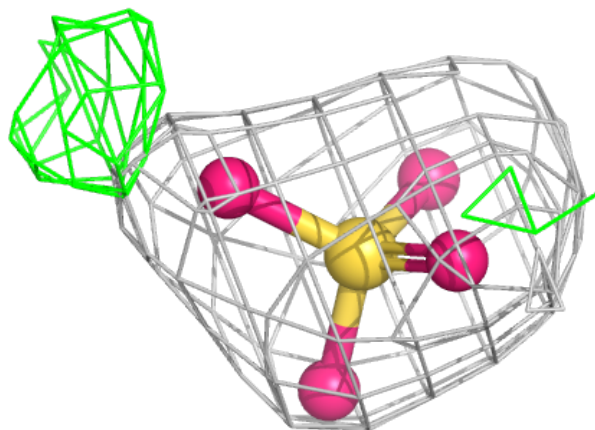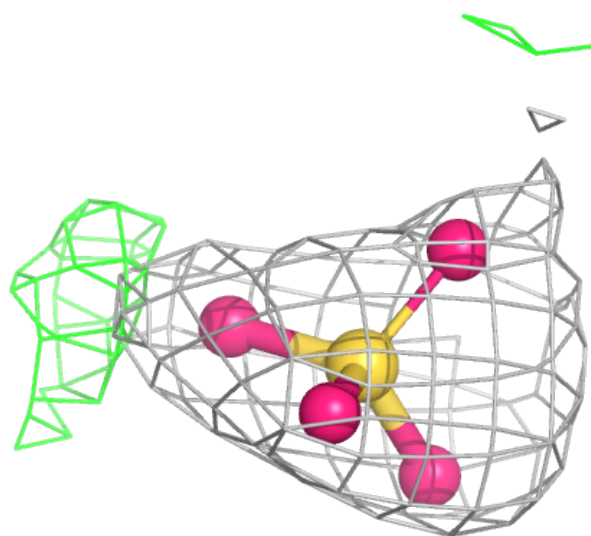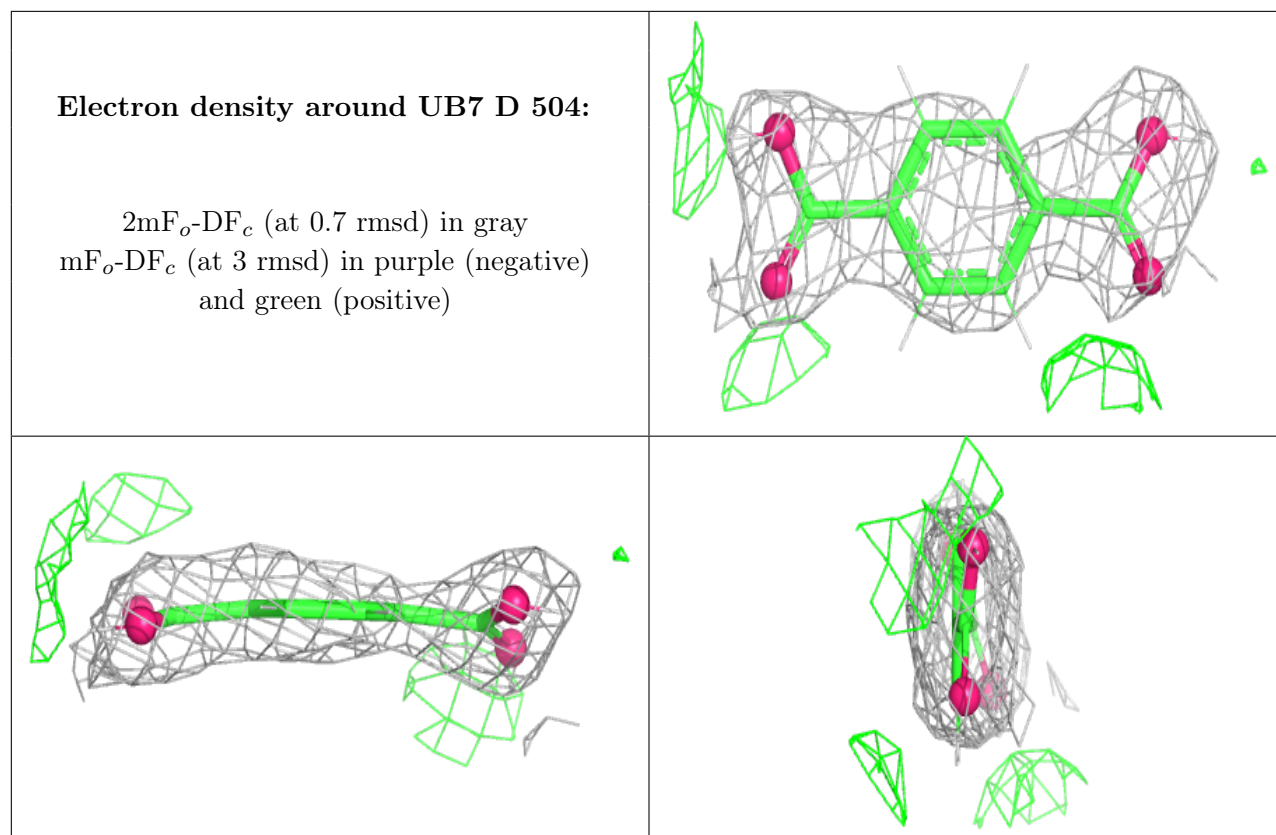
Electron density around SO4 E 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
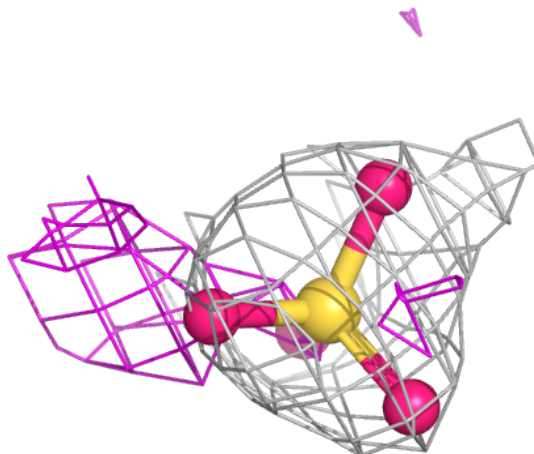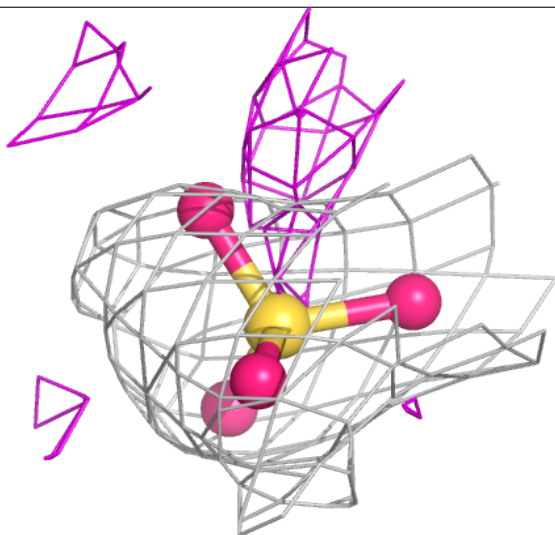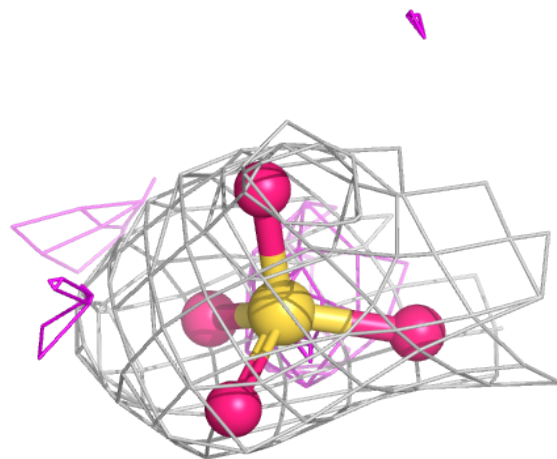
Electron density around SO4 E 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
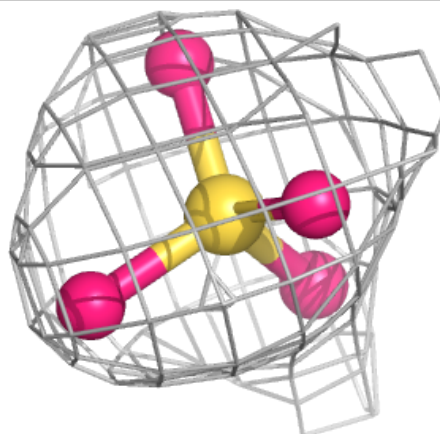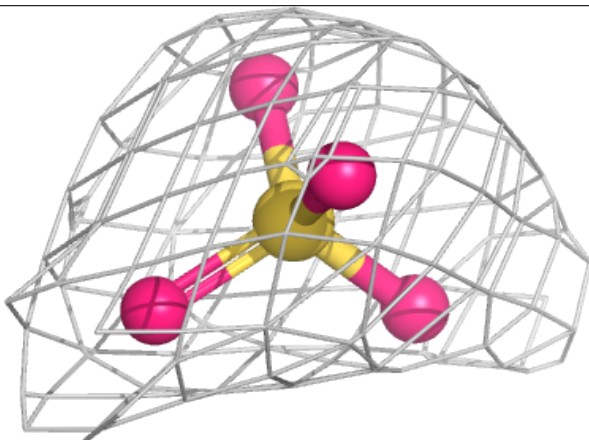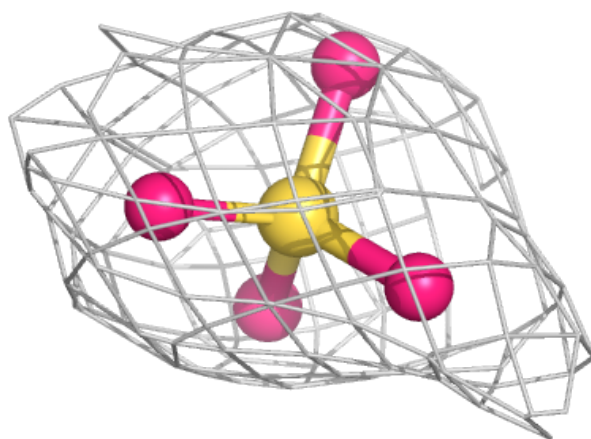
Electron density around SO4 D 502:

$2mF_o\text{-}DF_c$ (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 503:

$2mF_o\text{-}DF_c$ (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 502:

$2mF_o$-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 H 201:

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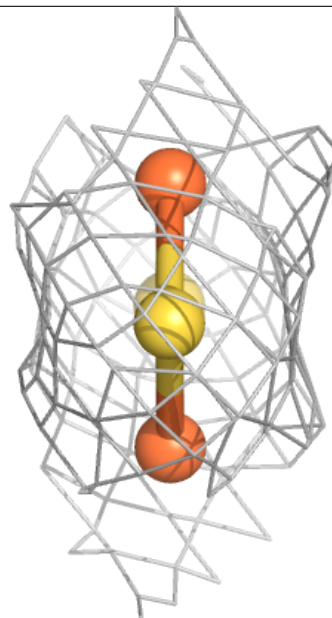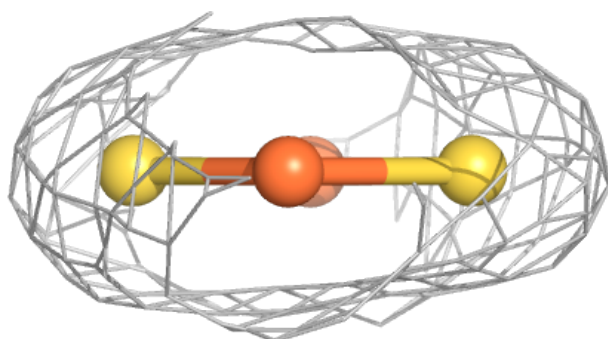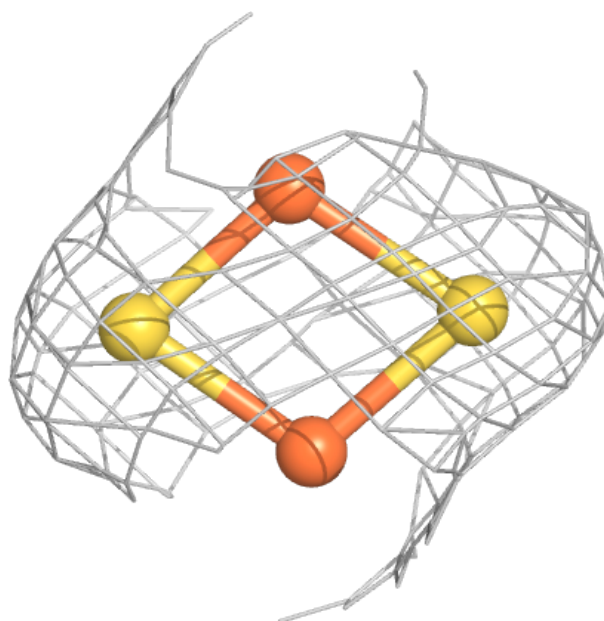and green (positive)

Electron density around FES D 501:

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

Electron density around FES E 501:

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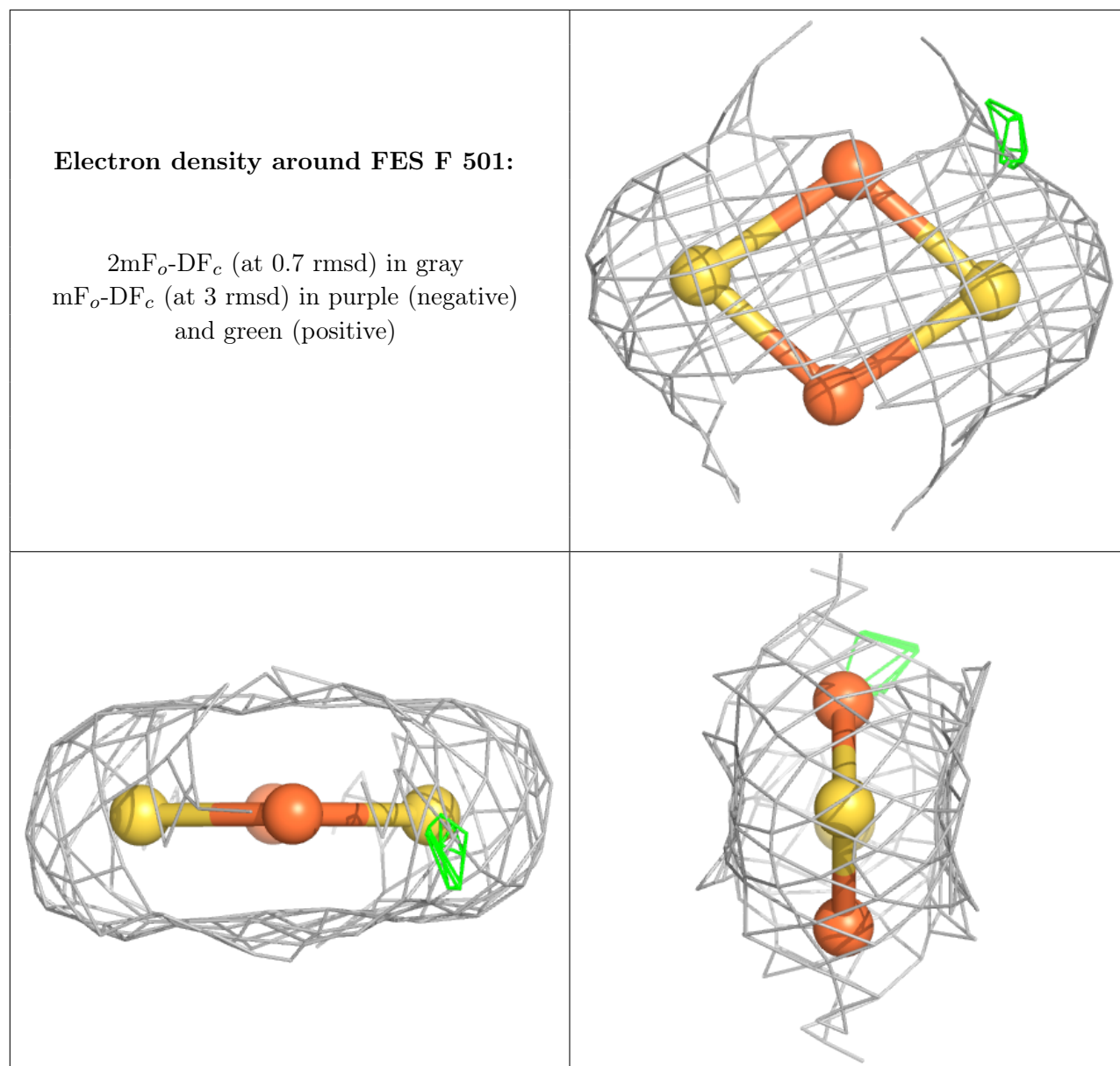and green (positive)

Electron density around FES F 501:

$2mF_o$-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 ⓘ

There are no such residues in this entry.