wwPDB X-ray Structure Validation Summary Report (i)

Aug 31, 2022 – 07:07 am BST

PDB ID	:	7Q04
Title	:	Crystal structure of TPADO in a substrate-free state
Authors	:	Zahn, M.; Kincannon, W.M.; DuBois, J.L.; McGeehan, J.E.
Deposited on	:	2021-10-14
Resolution	:	2.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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 (i)) were used in the production of this report:

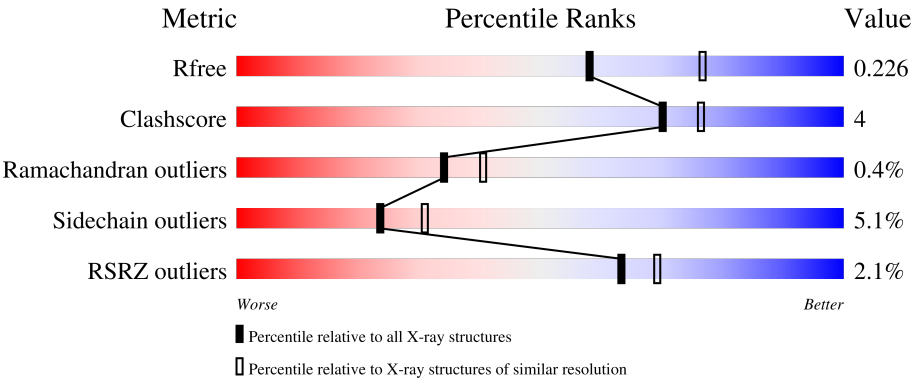
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	89% 10% ·
1	B	154	88% 11% ·
1	C	154	% 86% 14%
2	D	428	4% 79% 8% · 13%
2	E	428	% 82% 9% · 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	428	
3	H	129	

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	FES	E	501	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27325 atoms, of which 13245 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	1	0
			2410	762	1193	211	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	374	Total	C	H	N	O	S	78	0	0
			5775	1852	2842	513	557	11			
2	E	400	Total	C	H	N	O	S	83	0	0
			6181	1986	3035	548	599	13			
2	F	376	Total	C	H	N	O	S	78	0	0
			5797	1856	2853	515	561	12			

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...

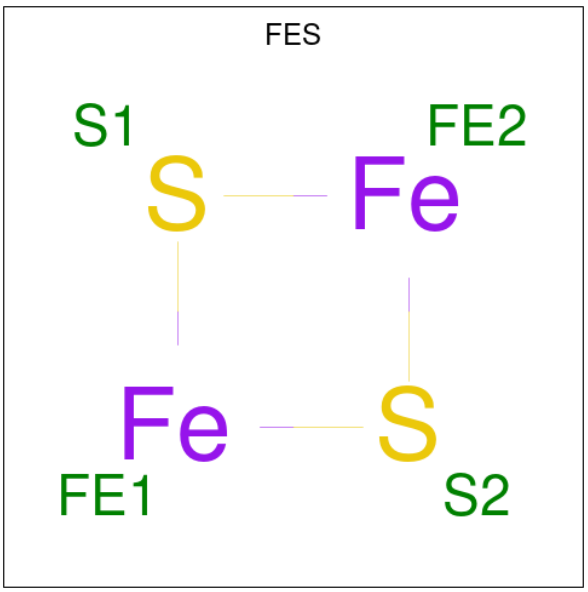
Chain	Residue	Modelled	Actual	Comment	Reference
D	423	HIS	-	expression tag	UNP Q3C1D5
D	424	HIS	-	expression tag	UNP Q3C1D5
D	425	HIS	-	expression tag	UNP Q3C1D5
D	426	HIS	-	expression tag	UNP Q3C1D5
E	-1	MET	-	initiating methionine	UNP Q3C1D5
E	0	GLY	-	expression tag	UNP Q3C1D5
E	414	GLU	-	expression 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)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	F	1	Total Fe S 4 2 2	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Fe 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	53	Total O 53 53	0	0
6	B	61	Total O 61 61	0	0
6	C	43	Total O 43 43	0	0
6	D	41	Total O 41 41	0	0

Continued on next page...

Continued from previous page...

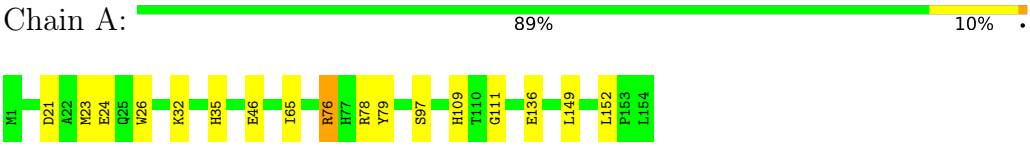
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	108	Total O 108 108	0	0
6	F	77	Total O 77 77	0	0
6	H	25	Total O 25 25	0	0

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.

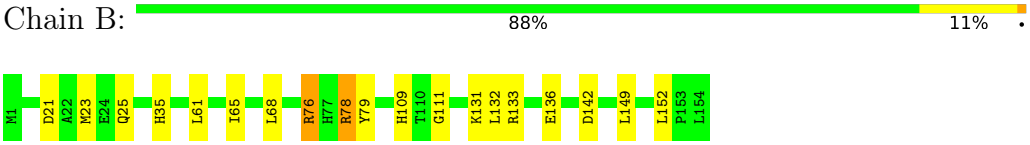
• Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain A:



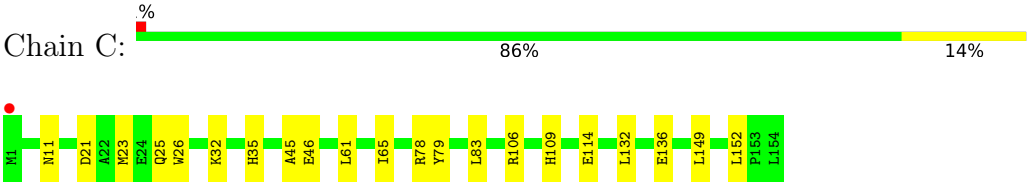
• Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain B:



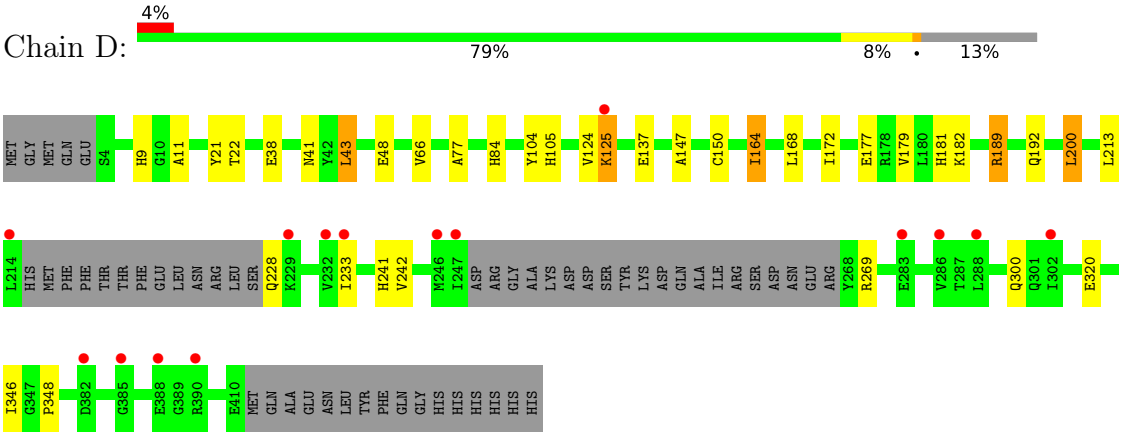
• Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain C:



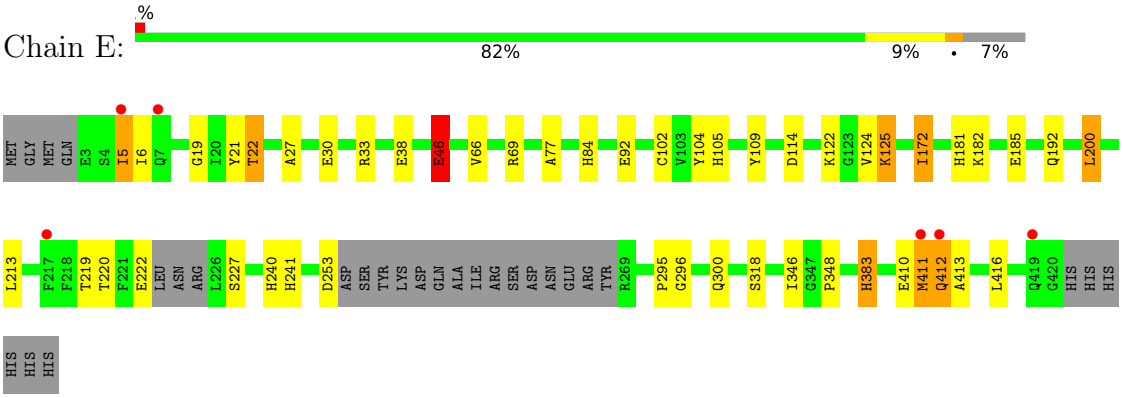
• Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

Chain D:



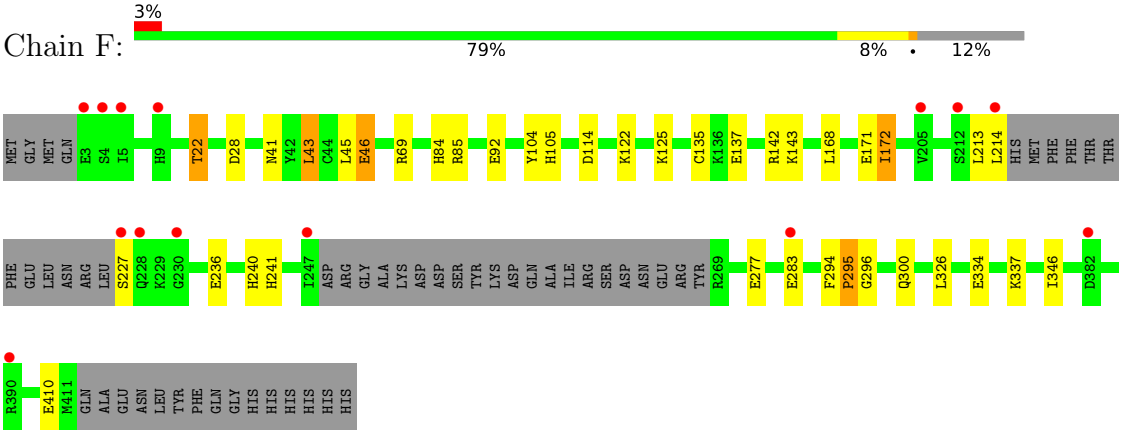
• Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

Chain E:



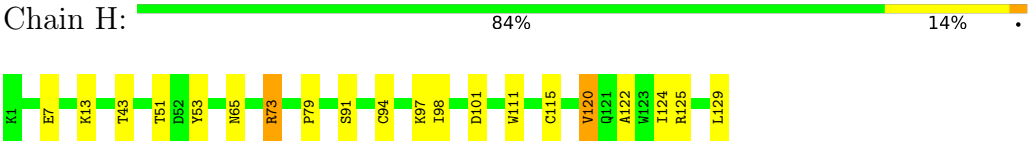
• Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

Chain F:



• Molecule 3: Lysozyme

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	220.81Å 220.81Å 84.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	191.22 – 2.28 191.22 – 2.28	Depositor EDS
% Data completeness (in resolution range)	64.7 (191.22-2.28) 59.6 (191.22-2.28)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.179 , 0.225 0.179 , 0.226	Depositor DCC
R_{free} test set	3392 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27325	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, 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	0.77	0/1243	0.93	0/1685
1	B	0.74	0/1232	0.95	2/1671 (0.1%)
1	C	0.75	1/1232 (0.1%)	0.98	3/1671 (0.2%)
2	D	0.73	1/2998 (0.0%)	0.89	2/4048 (0.0%)
2	E	0.79	1/3216 (0.0%)	0.95	4/4339 (0.1%)
2	F	0.79	2/3008 (0.1%)	0.92	5/4060 (0.1%)
3	H	0.79	0/1021	1.04	1/1379 (0.1%)
All	All	0.77	5/13950 (0.0%)	0.94	17/18853 (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	1
2	E	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	171	GLU	CD-OE2	7.47	1.33	1.25
2	F	410	GLU	CD-OE1	6.38	1.32	1.25
1	C	114	GLU	CD-OE2	5.41	1.31	1.25
2	D	320	GLU	CD-OE2	-5.20	1.20	1.25
2	E	185	GLU	CD-OE1	5.15	1.31	1.25

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	78	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	B	133	ARG	CG-CD-NE	-7.43	96.20	111.80
1	C	78	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	B	76	ARG	NE-CZ-NH1	-7.23	116.69	120.30
2	F	85	ARG	NE-CZ-NH2	-7.11	116.75	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	11	ALA	Peptide
2	E	219	THR	Peptide
2	E	412	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1217	1193	1189	17	0
1	B	1209	1181	1176	14	0
1	C	1209	1181	1176	11	0
2	D	2933	2842	2828	17	0
2	E	3146	3035	3020	22	0
2	F	2944	2853	2838	13	0
3	H	1001	960	959	8	0
4	D	4	0	0	1	0
4	E	4	0	0	2	0
4	F	4	0	0	0	0
5	D	1	0	0	0	0
6	A	53	0	0	3	0
6	B	61	0	0	3	0
6	C	43	0	0	0	0
6	D	41	0	0	0	0
6	E	108	0	0	0	0
6	F	77	0	0	0	0
6	H	25	0	0	1	0
All	All	14080	13245	13186	95	0

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

The worst 5 of 95 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:C:26:TRP:HE3	1:C:65:ILE:HD11	1.29	0.95
1:A:26:TRP:HE3	1:A:65:ILE:HD11	1.31	0.94
2:E:181:HIS:CE1	2:E:182:LYS:HE2	2.17	0.79
1:C:26:TRP:CE3	1:C:65:ILE:HD11	2.20	0.70
1:A:78[A]:ARG:NH1	1:B:142:ASP:OD1	2.24	0.70

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/154 (99%)	146 (95%)	7 (5%)	0	100	100
1	B	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
1	C	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
2	D	368/428 (86%)	354 (96%)	13 (4%)	1 (0%)	41	49
2	E	394/428 (92%)	374 (95%)	17 (4%)	3 (1%)	19	22
2	F	370/428 (86%)	354 (96%)	14 (4%)	2 (0%)	29	34
3	H	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	22
All	All	1716/1875 (92%)	1634 (95%)	75 (4%)	7 (0%)	34	40

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	413	ALA
3	H	120	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	84	HIS
2	D	84	HIS
2	F	84	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/129 (101%)	126 (97%)	4 (3%)	40	53
1	B	129/129 (100%)	124 (96%)	5 (4%)	32	43
1	C	129/129 (100%)	124 (96%)	5 (4%)	32	43
2	D	307/355 (86%)	291 (95%)	16 (5%)	23	30
2	E	329/355 (93%)	309 (94%)	20 (6%)	18	23
2	F	309/355 (87%)	294 (95%)	15 (5%)	25	33
3	H	105/105 (100%)	97 (92%)	8 (8%)	13	15
All	All	1438/1557 (92%)	1365 (95%)	73 (5%)	24	31

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	214	LEU
3	H	124	ILE
2	F	236	GLU
3	H	13	LYS
2	D	179	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	406	HIS
2	E	383	HIS
2	F	406	HIS
3	H	46	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	FES	F	501	2	0,4,4	-	-	-		
4	FES	D	501	2	0,4,4	-	-	-		
4	FES	E	501	2	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	F	501	2	-	-	0/1/1/1
4	FES	D	501	2	-	-	0/1/1/1
4	FES	E	501	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

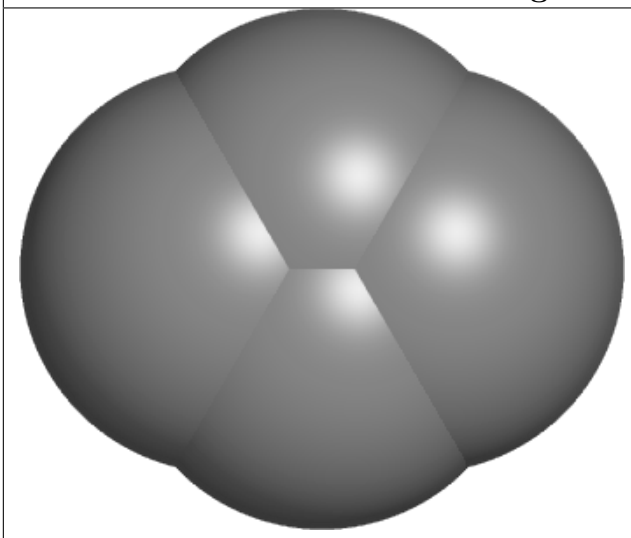
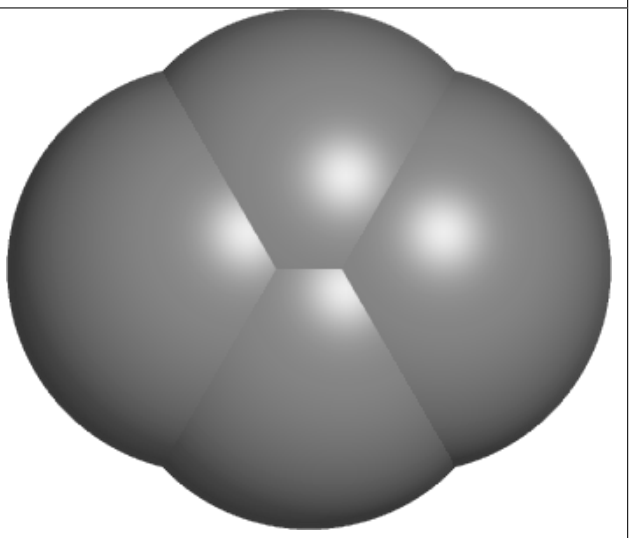
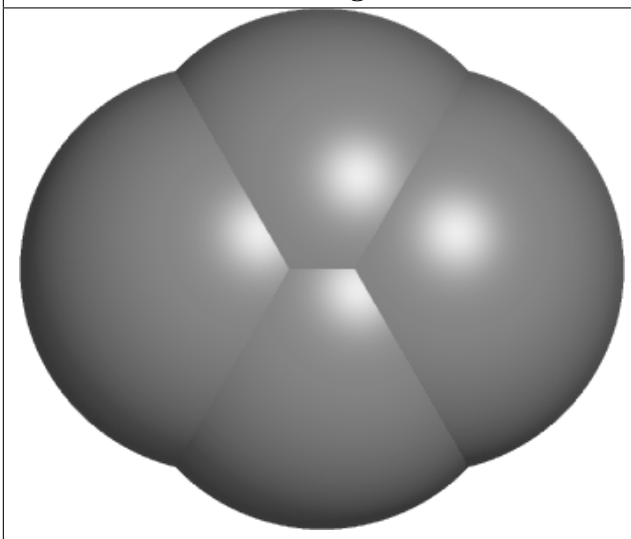
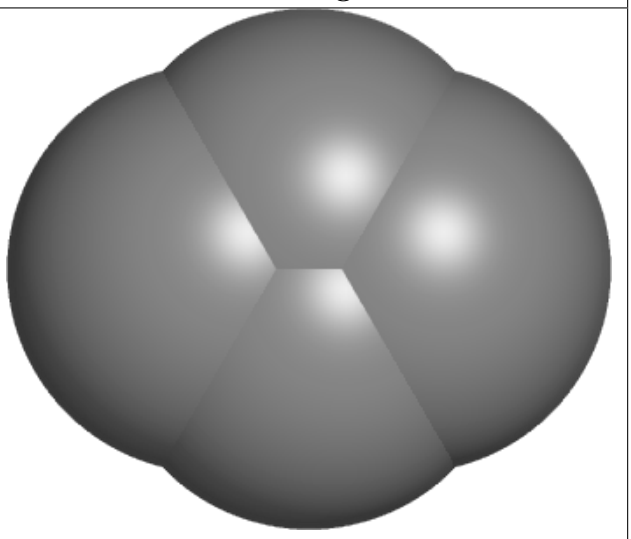
There are no torsion outliers.

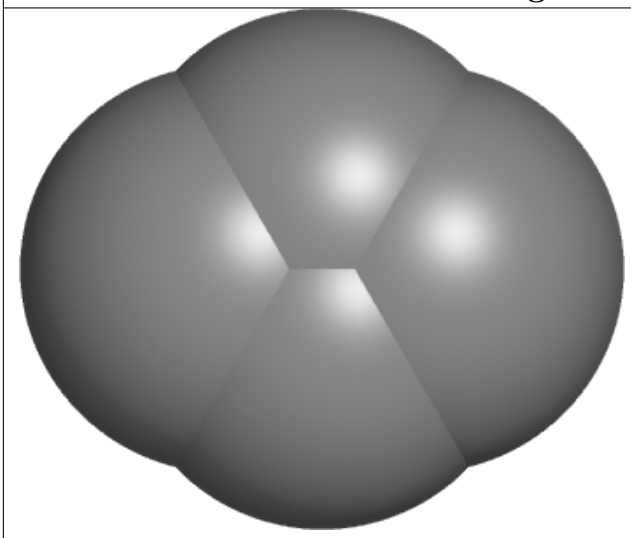
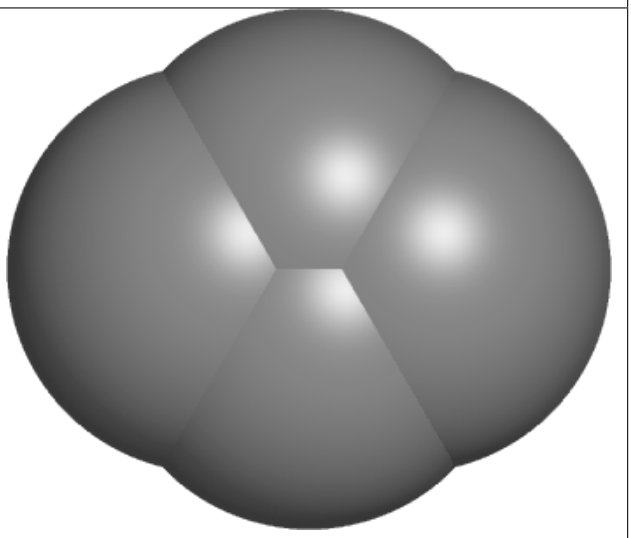
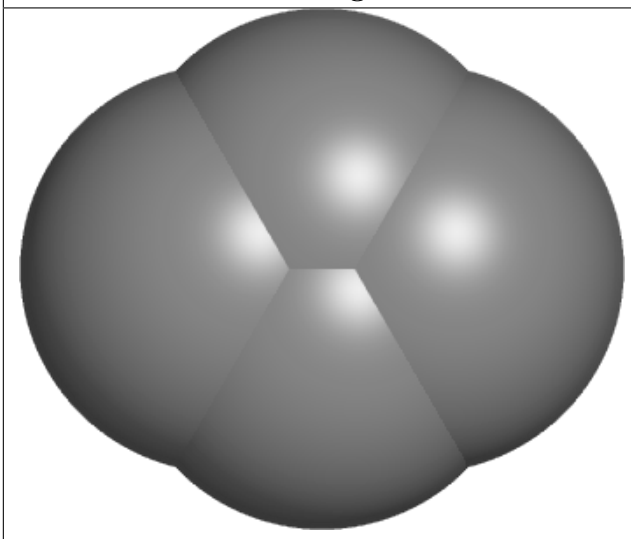
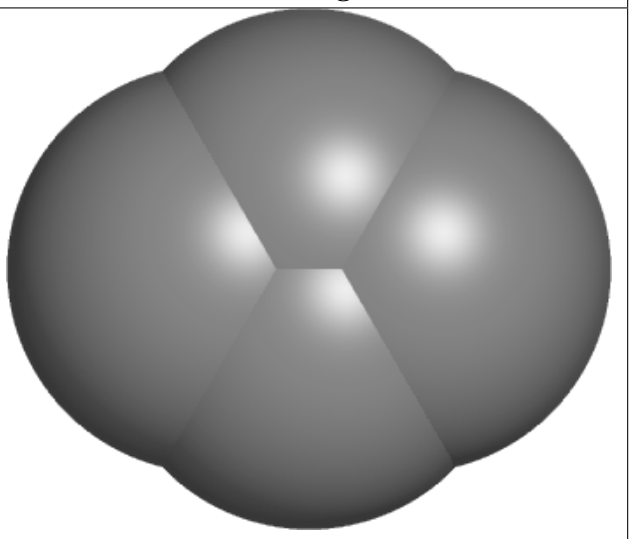
There are no ring outliers.

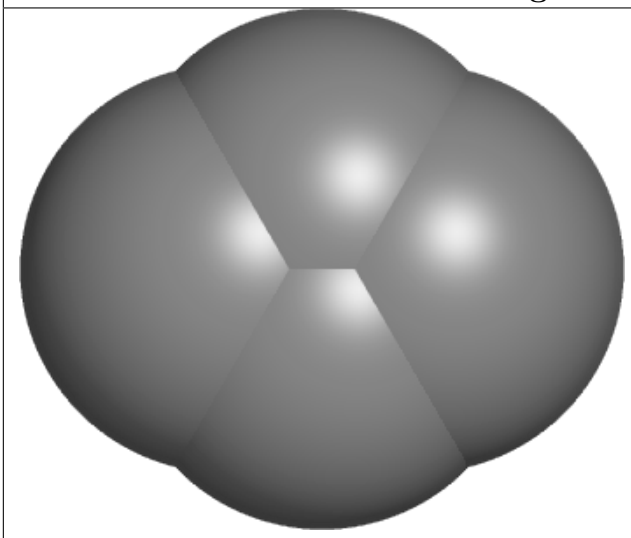
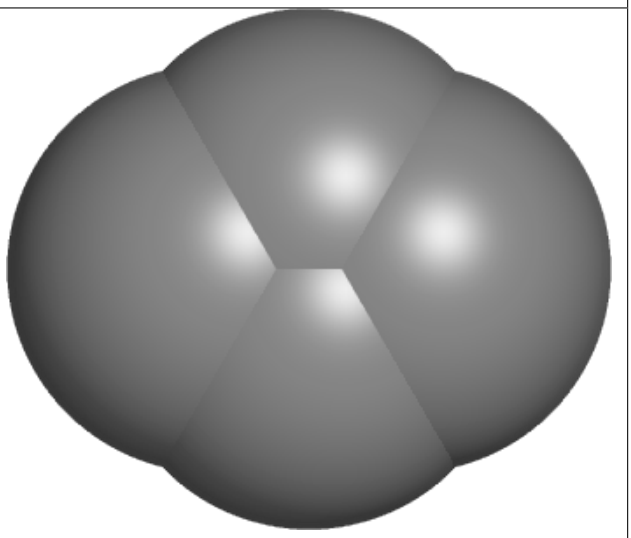
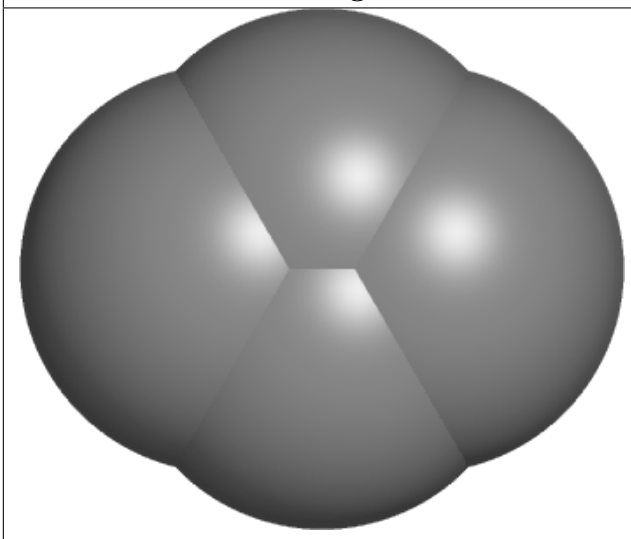
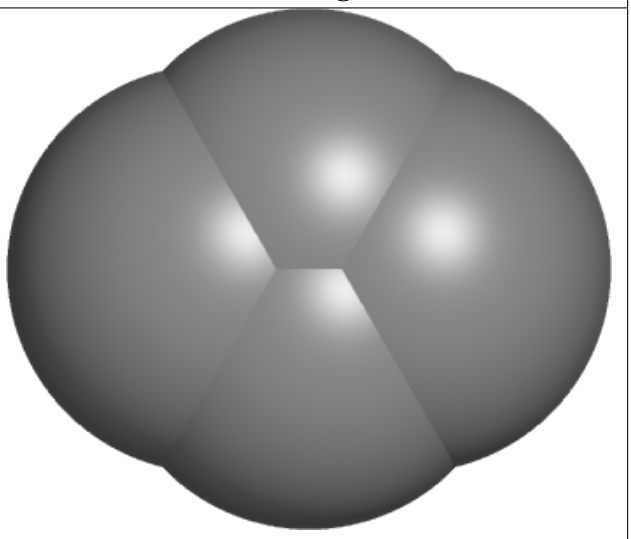
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	FES	1	0
4	E	501	FES	2	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 FES F 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand FES D 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand FES E 501	
	
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, 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	A	154/154 (100%)	-0.06	0 100 100	29, 39, 65, 83	0
1	B	154/154 (100%)	-0.14	0 100 100	29, 40, 67, 101	0
1	C	154/154 (100%)	-0.12	1 (0%) 89 91	29, 44, 70, 105	0
2	D	374/428 (87%)	0.11	15 (4%) 38 43	39, 59, 100, 130	0
2	E	400/428 (93%)	-0.11	6 (1%) 73 78	30, 44, 84, 118	0
2	F	376/428 (87%)	0.01	14 (3%) 41 47	31, 48, 88, 121	0
3	H	129/129 (100%)	-0.15	0 100 100	34, 47, 79, 94	0
All	All	1741/1875 (92%)	-0.04	36 (2%) 63 69	29, 47, 87, 130	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	382	ASP	5.8
2	F	5	ILE	4.2
2	D	283	GLU	4.1
2	D	288	LEU	4.0
2	D	247	ILE	3.9

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)

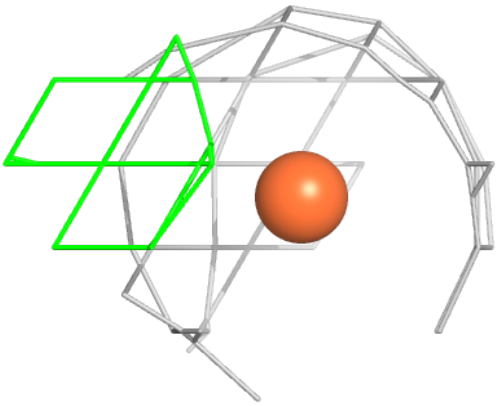
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

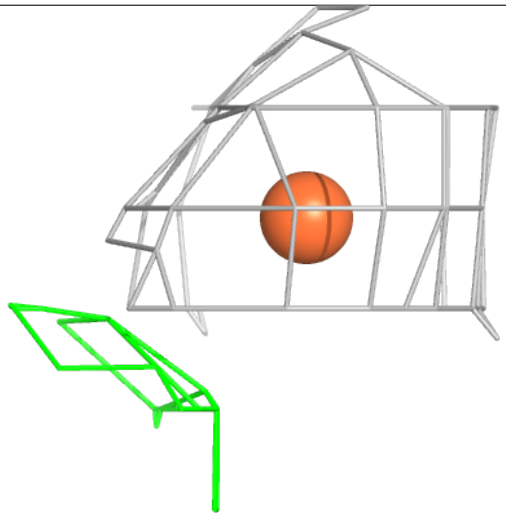
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FE	D	502	1/1	0.81	0.06	122,122,122,122	0
4	FES	E	501	4/4	0.98	0.12	50,51,52,53	0
4	FES	F	501	4/4	0.99	0.17	36,37,38,41	0
4	FES	D	501	4/4	0.99	0.15	48,49,50,51	0

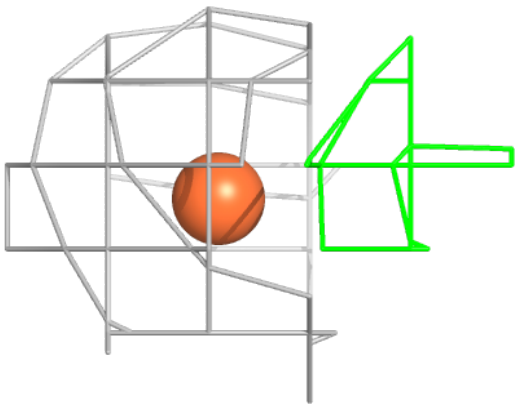
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FE D 502:

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

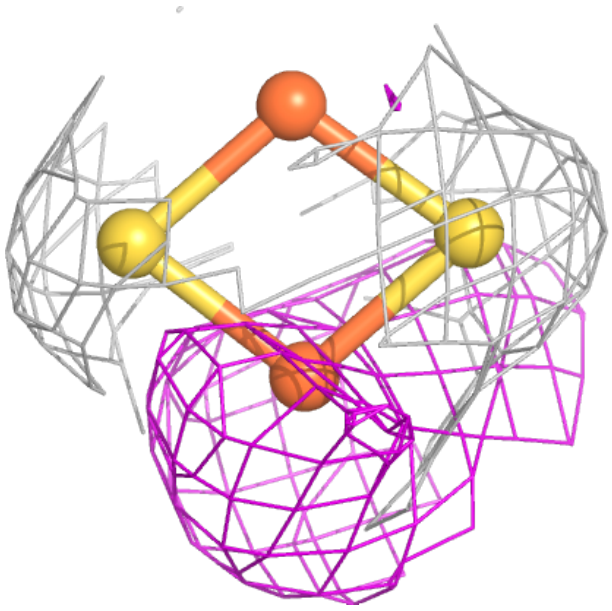


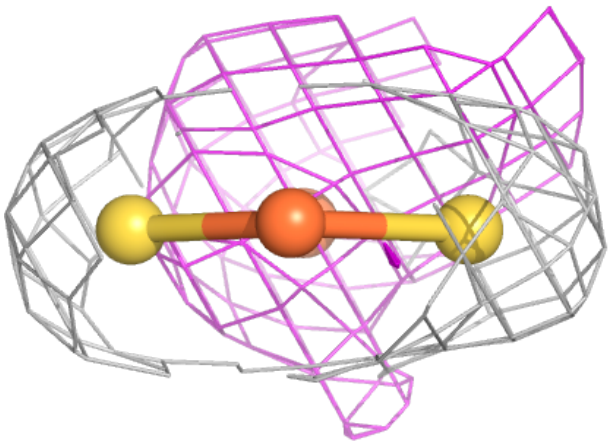


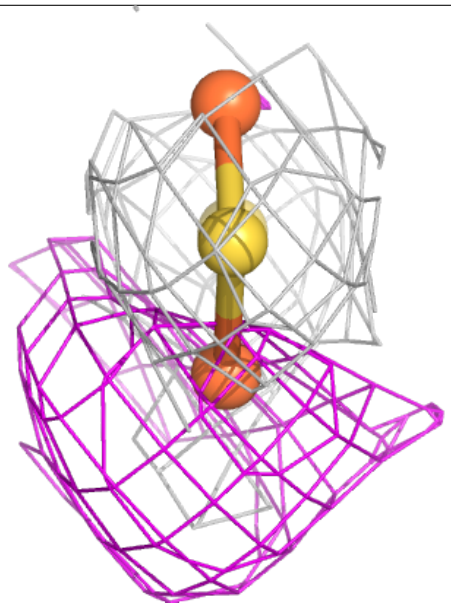


Electron density around FES E 501:

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

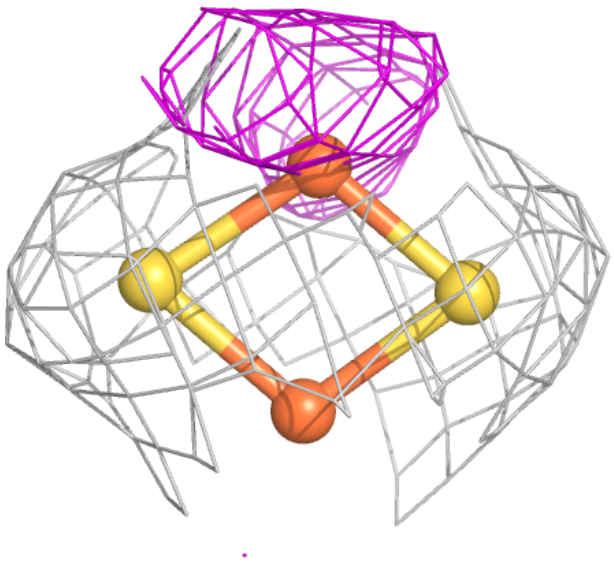


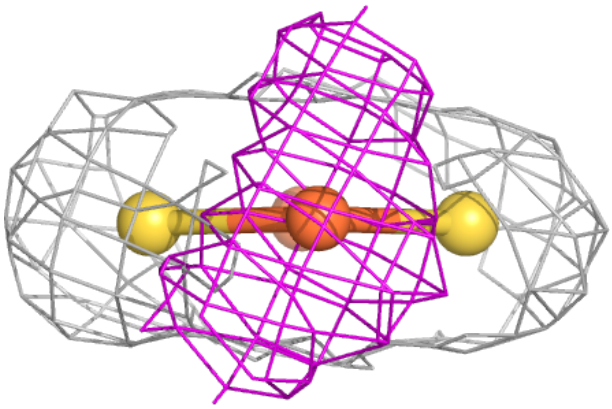


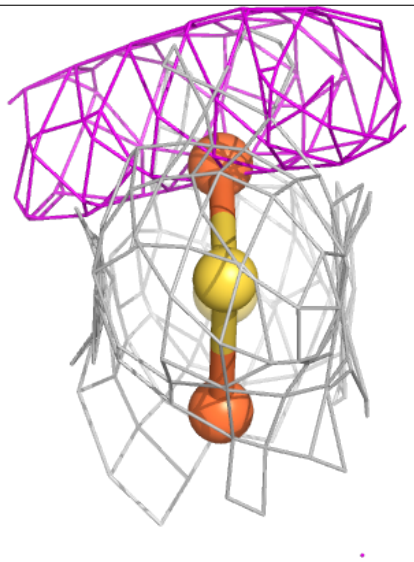


Electron density around FES F 501:

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

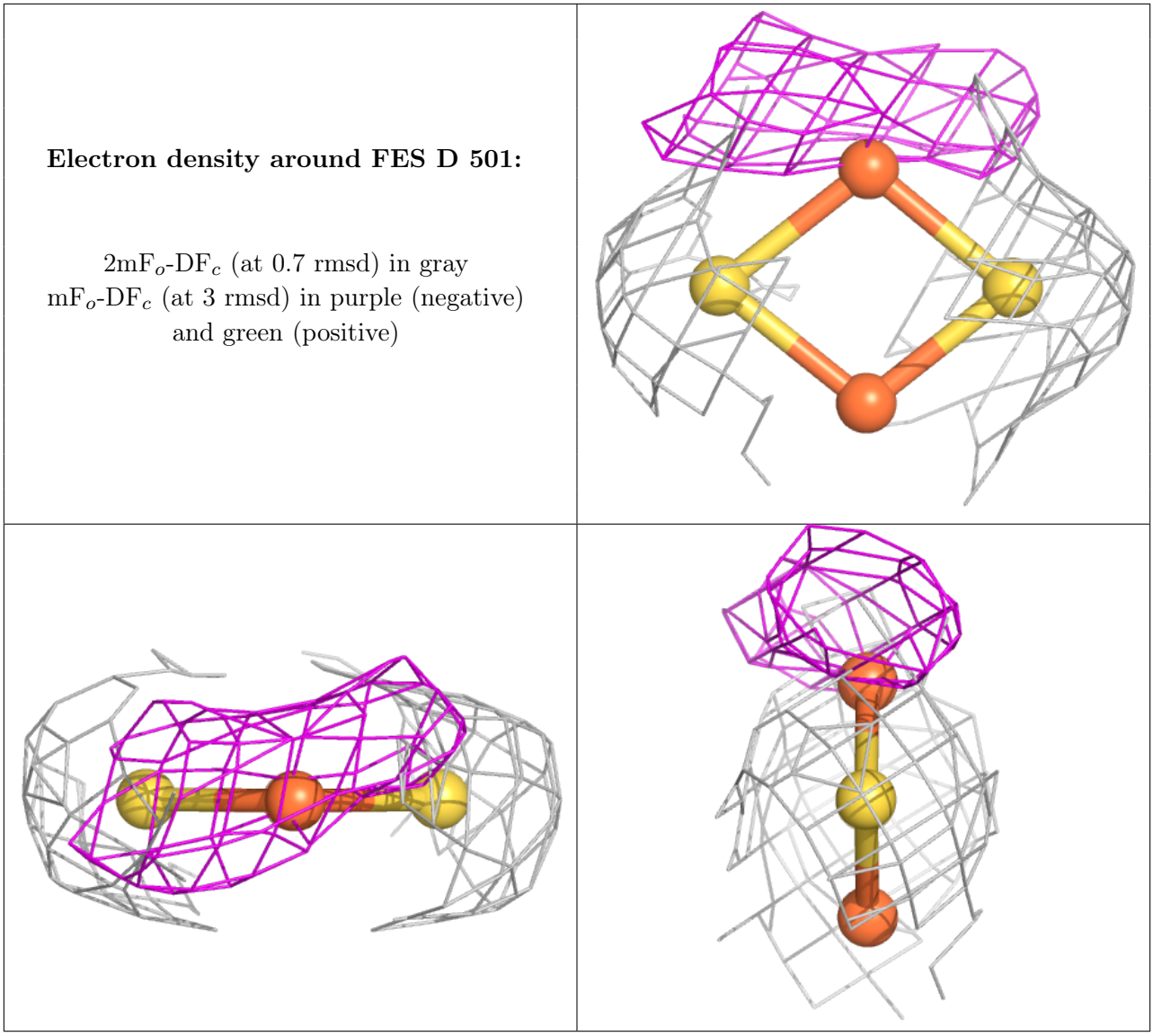






Electron density around FES D 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.