



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2026 – 09:25 PM JST

PDB ID : 9WTV / pdb_00009wtv
Title : Aquifex aeolicus IscS2 WT - IscU D38A complex
Authors : Kunichika, K.; Fujishiro, T.
Deposited on : 2025-09-17
Resolution : 4.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

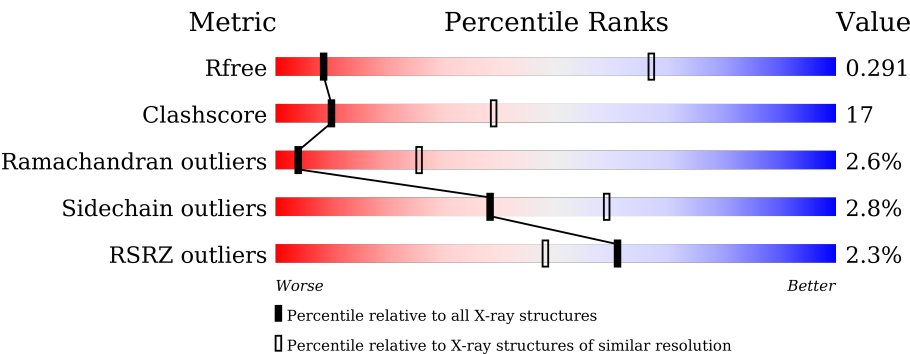
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.40 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}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	
1	E	406	
1	F	406	

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Mol	Chain	Length	Quality of chain
1	G	406	
1	H	406	
1	I	406	
1	J	406	
2	K	157	
2	L	157	
2	M	157	
2	N	157	
2	O	157	
2	P	157	
2	S	157	
2	T	157	
2	U	157	
2	V	157	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	501	-	-	X	-
3	CL	C	501	-	-	X	-
3	CL	F	501	-	-	X	-
3	CL	G	501	-	-	X	-
3	CL	I	501	-	-	X	-
4	FES	M	201	-	-	X	-
4	FES	U	201	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40947 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 cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3086	1963	538	577	8			
1	B	389	Total	C	N	O	S	0	0	0
			3058	1943	534	573	8			
1	C	390	Total	C	N	O	S	0	0	0
			3065	1948	535	574	8			
1	D	389	Total	C	N	O	S	0	0	0
			3058	1943	534	573	8			
1	E	391	Total	C	N	O	S	0	0	0
			3074	1954	537	575	8			
1	F	384	Total	C	N	O	S	0	0	0
			3011	1913	527	563	8			
1	G	385	Total	C	N	O	S	0	0	0
			3018	1918	528	564	8			
1	H	390	Total	C	N	O	S	0	0	0
			3067	1949	536	574	8			
1	I	385	Total	C	N	O	S	0	0	0
			3018	1918	528	564	8			
1	J	391	Total	C	N	O	S	0	0	0
			3079	1958	537	576	8			

- Molecule 2 is a protein called Iron-sulfur cluster assembly scaffold protein IscU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	137	Total	C	N	O	S	0	0	0
			1055	668	175	203	9			
2	L	134	Total	C	N	O	S	0	0	0
			1025	649	172	195	9			
2	M	135	Total	C	N	O	S	0	0	0
			1037	658	173	197	9			
2	N	135	Total	C	N	O	S	0	0	0
			1037	658	173	197	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	133	Total	C	N	O	S	0	0	0
			1017	645	170	193	9			
2	P	135	Total	C	N	O	S	0	0	0
			1037	658	173	197	9			
2	S	133	Total	C	N	O	S	0	0	0
			1017	645	170	193	9			
2	T	135	Total	C	N	O	S	0	0	0
			1037	658	173	197	9			
2	U	135	Total	C	N	O	S	0	0	0
			1037	658	173	197	9			
2	V	138	Total	C	N	O	S	0	0	0
			1064	673	176	206	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	38	ALA	ASP	engineered mutation	UNP O67045
L	38	ALA	ASP	engineered mutation	UNP O67045
M	38	ALA	ASP	engineered mutation	UNP O67045
N	38	ALA	ASP	engineered mutation	UNP O67045
O	38	ALA	ASP	engineered mutation	UNP O67045
P	38	ALA	ASP	engineered mutation	UNP O67045
S	38	ALA	ASP	engineered mutation	UNP O67045
T	38	ALA	ASP	engineered mutation	UNP O67045
U	38	ALA	ASP	engineered mutation	UNP O67045
V	38	ALA	ASP	engineered mutation	UNP O67045

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

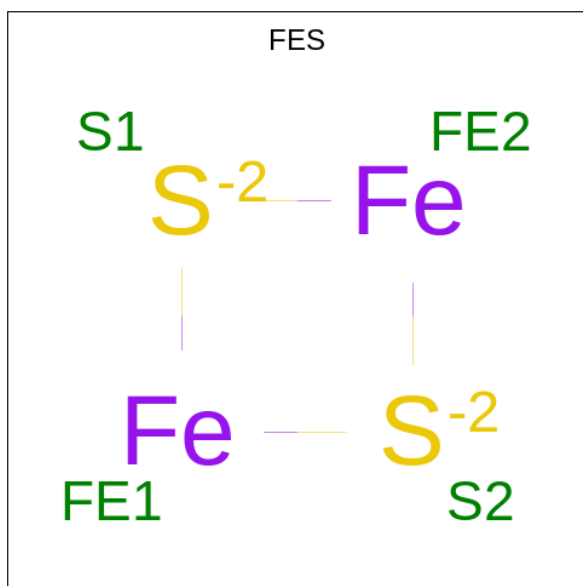
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	J	1	Total 1	Cl 1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 4	Fe 2	S 2	0	0
4	K	1	Total 4	Fe 2	S 2	0	0
4	L	1	Total 4	Fe 2	S 2	0	0
4	M	1	Total 4	Fe 2	S 2	0	0
4	O	1	Total 4	Fe 2	S 2	0	0
4	P	1	Total 4	Fe 2	S 2	0	0
4	S	1	Total 4	Fe 2	S 2	0	0

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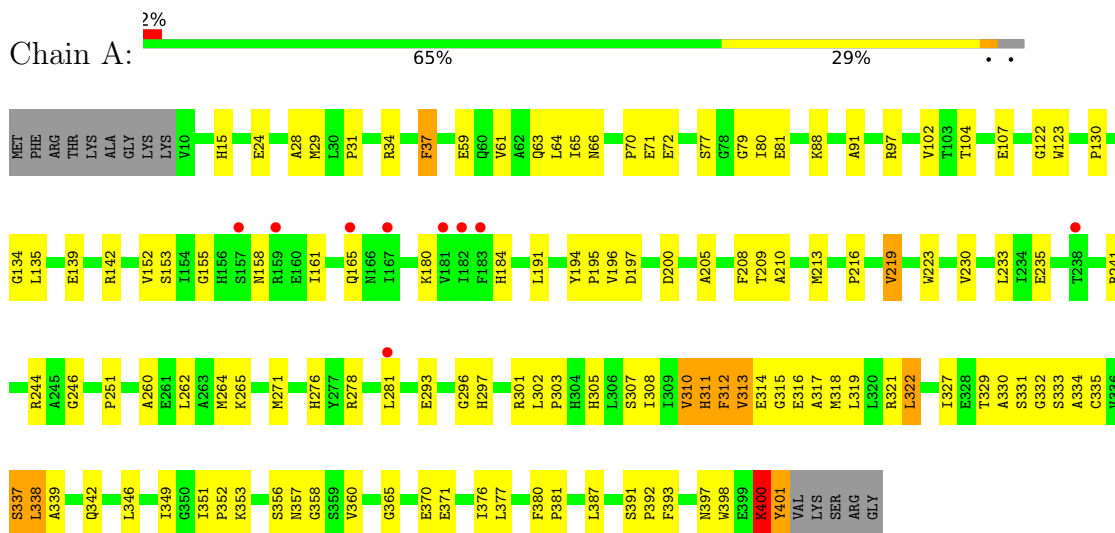
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	Fe	S	0	0
			4	2	2		
4	U	1	Total	Fe	S	0	0
			4	2	2		
4	V	1	Total	Fe	S	0	0
			4	2	2		

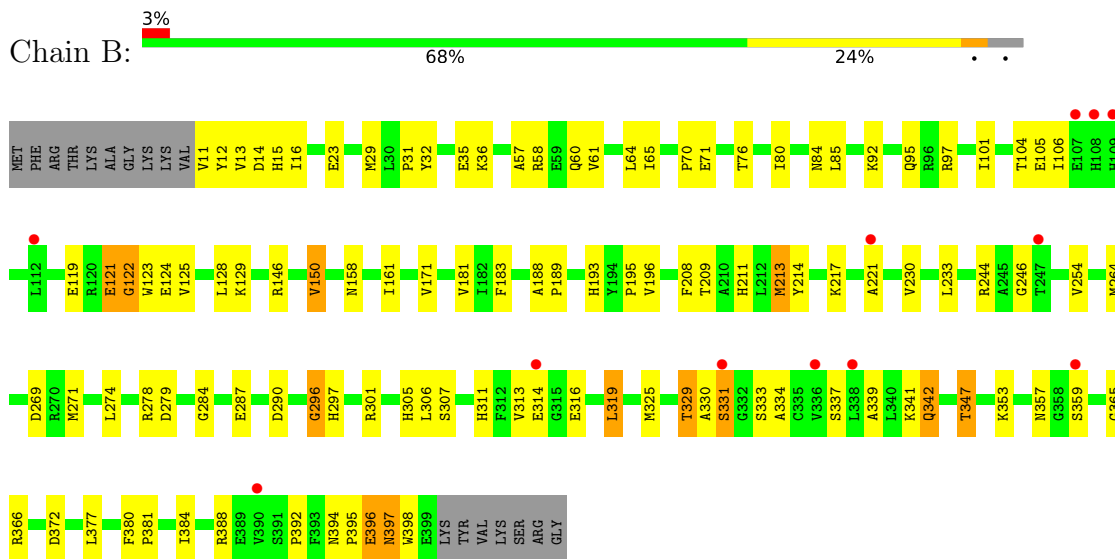
3 Residue-property plots [i](#)

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: cysteine desulfurase

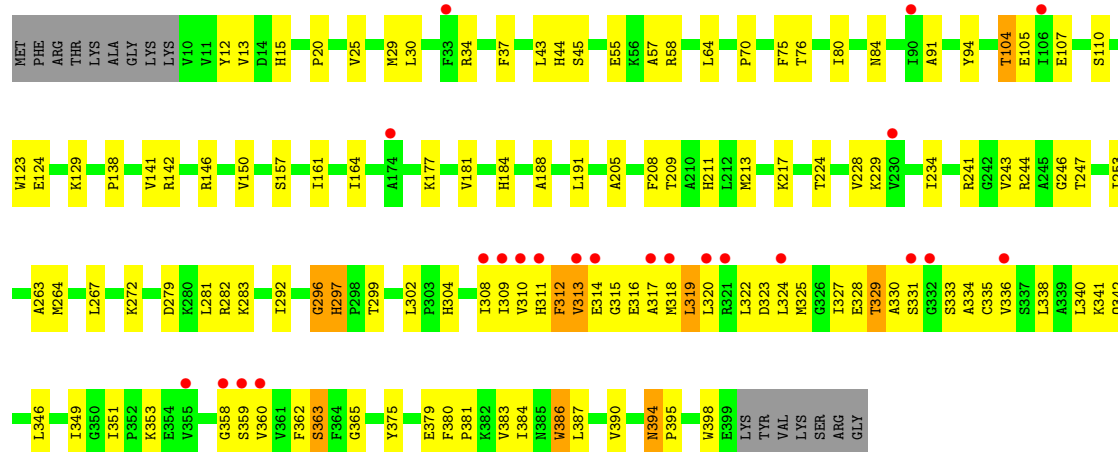


- Molecule 1: cysteine desulfurase

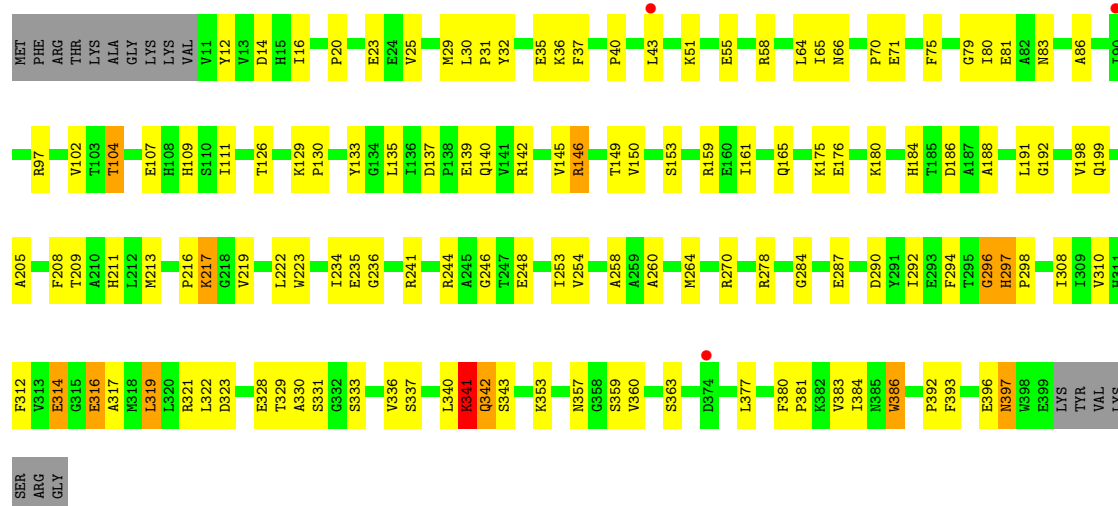


- Molecule 1: cysteine desulfurase

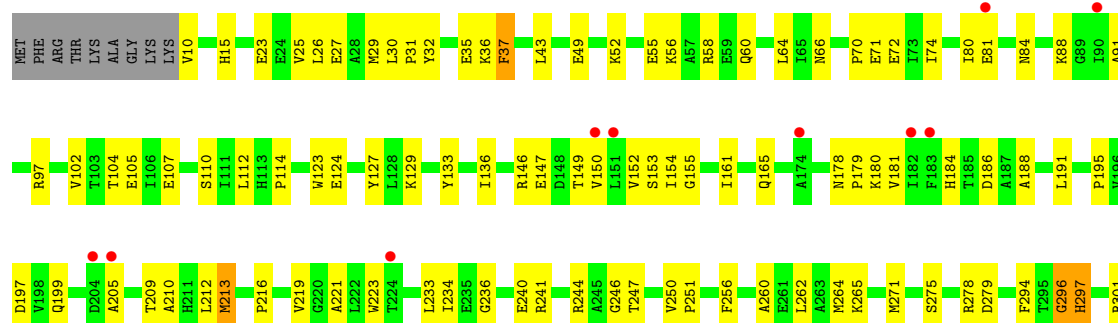


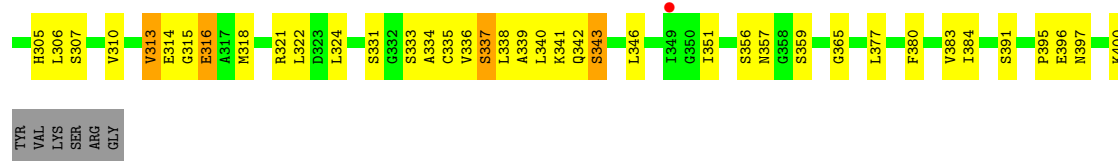


• Molecule 1: cysteine desulfurase

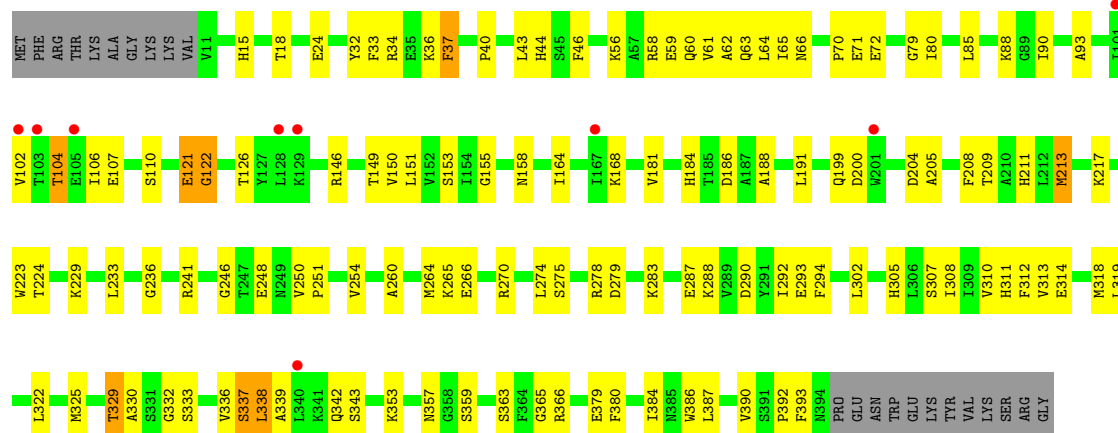


• Molecule 1: cysteine desulfurase

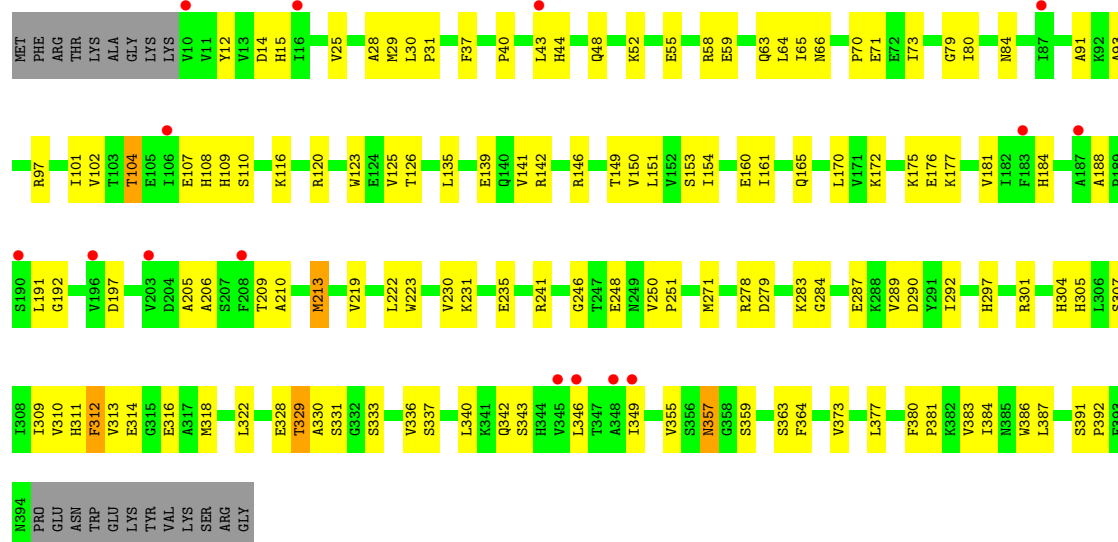




• Molecule 1: cysteine desulfurase

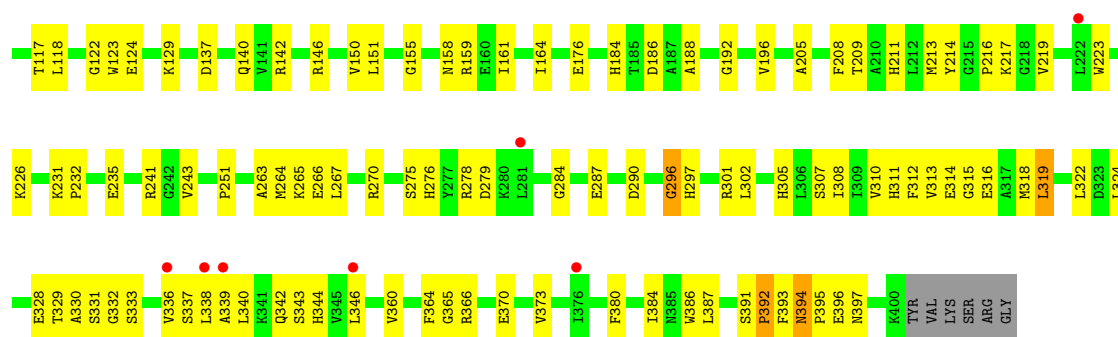


• Molecule 1: cysteine desulfurase

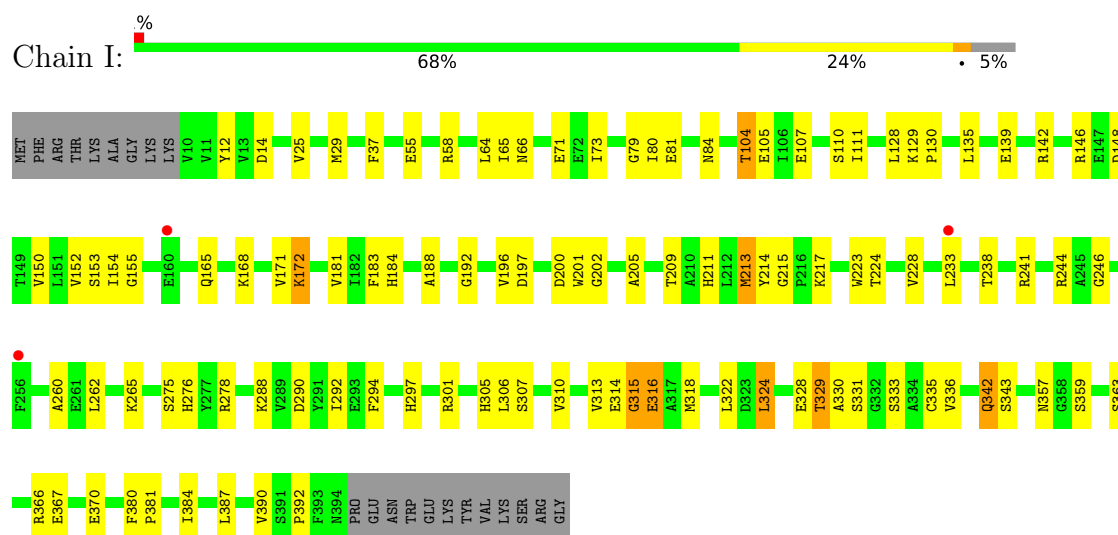


• Molecule 1: cysteine desulfurase

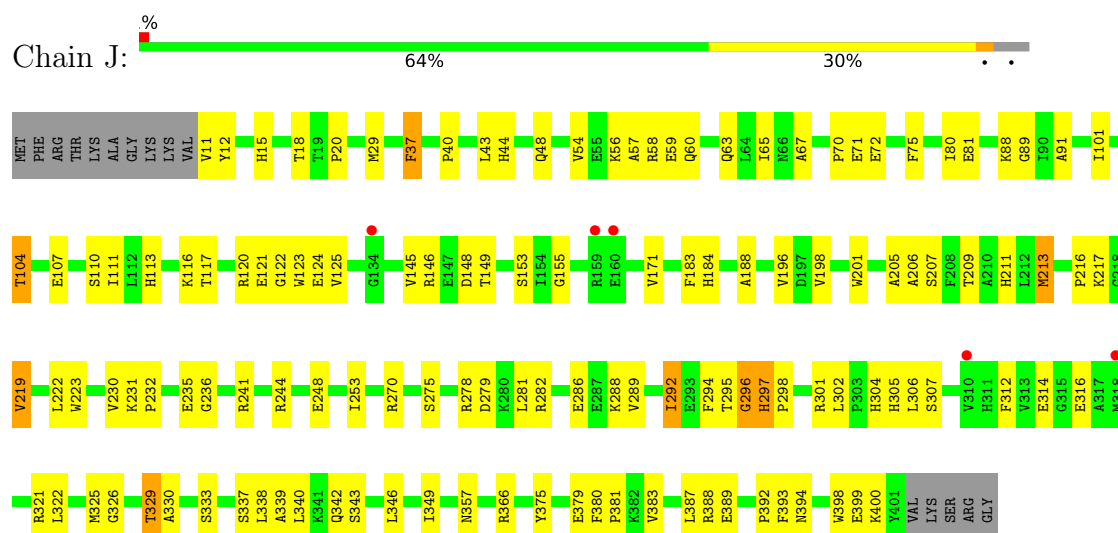




• Molecule 1: cysteine desulfurase



• Molecule 1: cysteine desulfurase

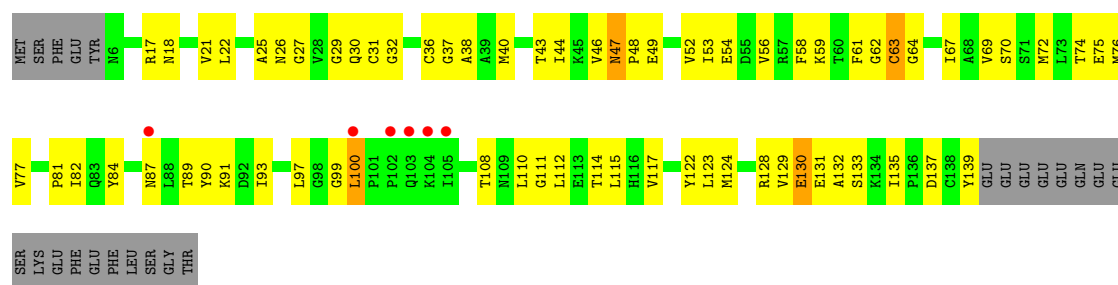
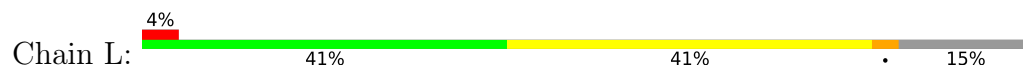


• Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

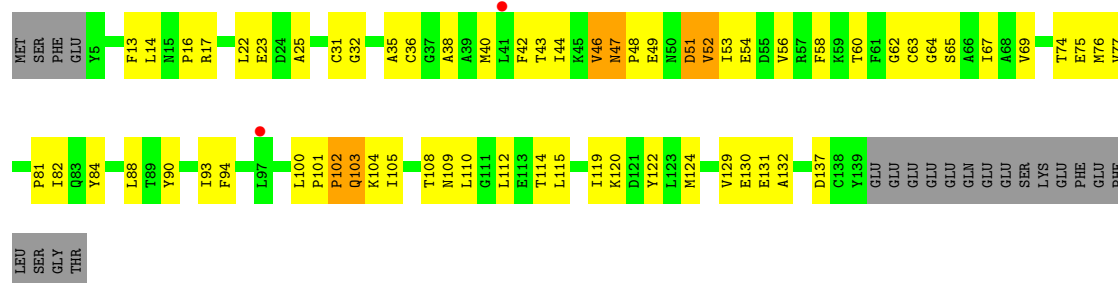
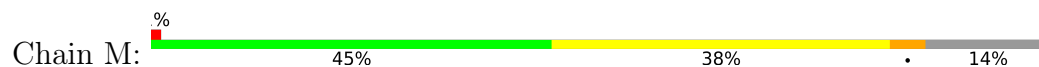




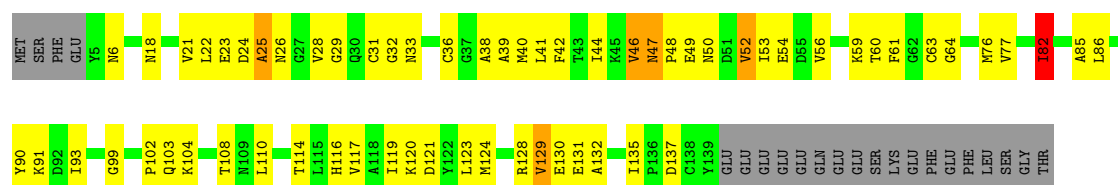
• Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU



• Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

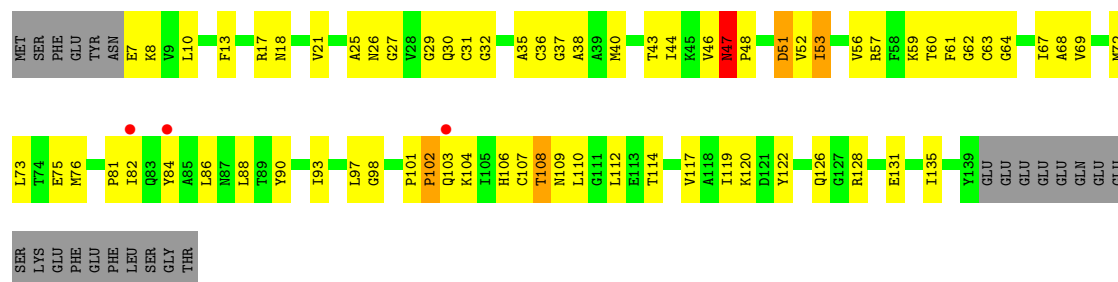


• Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

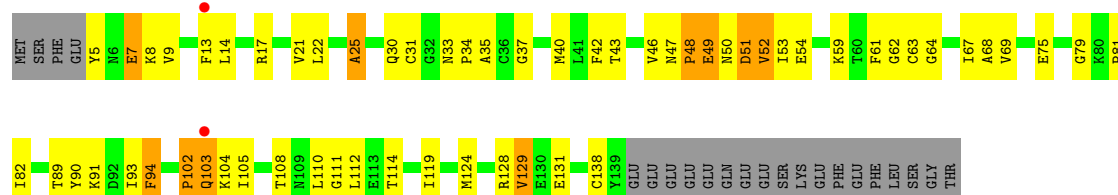


• Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

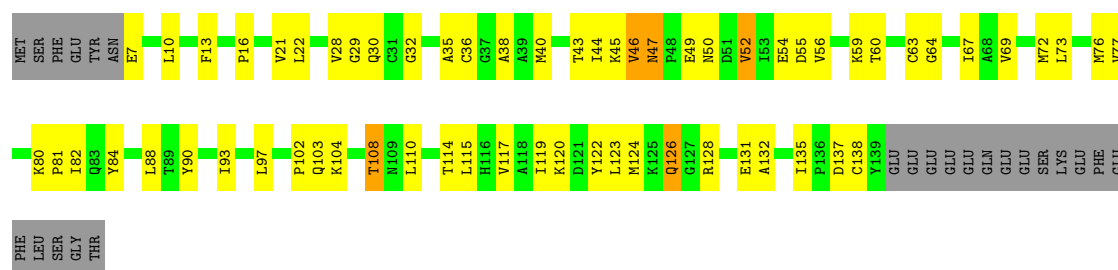




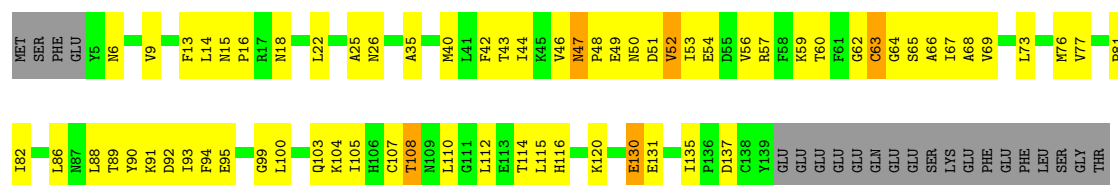
- Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU



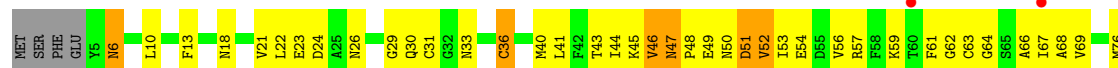
- Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

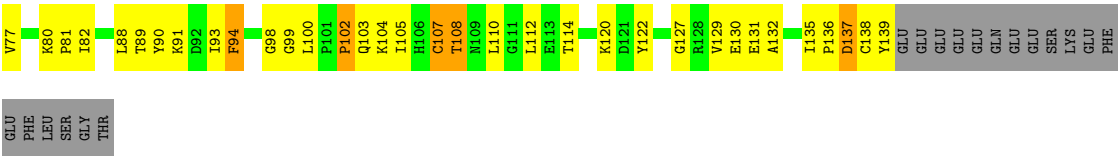


- Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU

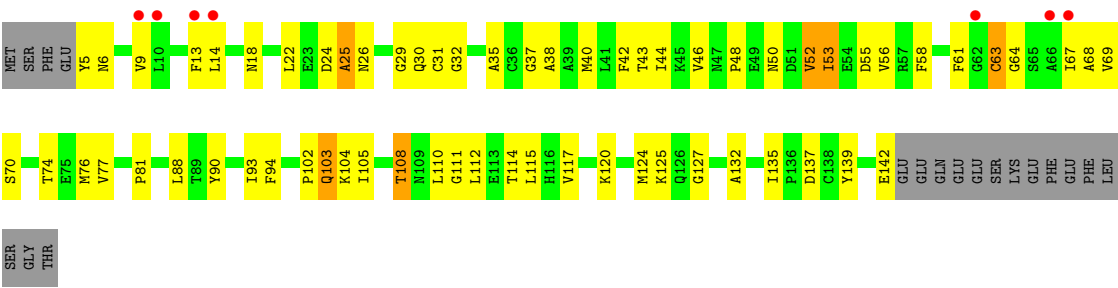


- Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU





● Molecule 2: Iron-sulfur cluster assembly scaffold protein IscU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.50Å 175.84Å 183.06Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	49.36 – 4.40 49.36 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.36-4.40) 99.6 (49.36-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.212 , 0.291 0.212 , 0.291	Depositor DCC
R_{free} test set	2278 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	236.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 264.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.044 for -h,l,k 0.056 for -h,-l,-k 0.058 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	40947	wwPDB-VP
Average B, all atoms (Å ²)	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	10/3154 (0.3%)	0.68	5/4271 (0.1%)
1	B	0.30	0/3125	0.57	1/4232 (0.0%)
1	C	0.30	0/3132	0.57	0/4242
1	D	0.30	0/3125	0.61	4/4232 (0.1%)
1	E	0.26	0/3141	0.55	0/4253
1	F	0.27	0/3075	0.54	1/4162 (0.0%)
1	G	0.25	0/3082	0.53	0/4172
1	H	0.26	0/3134	0.54	0/4243
1	I	0.26	0/3082	0.53	1/4172 (0.0%)
1	J	0.25	0/3147	0.52	0/4261
2	K	0.38	0/1074	0.78	0/1452
2	L	0.31	0/1043	0.67	0/1410
2	M	0.36	0/1056	0.70	0/1428
2	N	0.26	0/1056	0.61	0/1428
2	O	0.31	0/1035	0.68	0/1399
2	P	0.31	0/1056	0.70	0/1428
2	S	0.29	0/1035	0.61	0/1399
2	T	0.33	0/1056	0.64	0/1428
2	U	0.32	0/1056	0.68	0/1428
2	V	0.30	0/1083	0.64	0/1464
All	All	0.31	10/41747 (0.0%)	0.59	12/56504 (0.0%)

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	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
2	U	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	TYR	CD2-CE2	10.42	1.70	1.38
1	A	401	TYR	CD1-CE1	9.92	1.68	1.38
1	A	401	TYR	CZ-OH	8.48	1.55	1.38
1	A	400	LYS	CD-CE	8.47	1.77	1.52
1	A	401	TYR	CE1-CZ	8.32	1.58	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	LYS	CD-CE-NZ	12.13	150.70	111.90
1	A	400	LYS	CG-CD-CE	7.71	129.04	111.30
1	B	122	GLY	N-CA-C	5.49	122.02	111.31
1	I	315	GLY	N-CA-C	5.45	115.17	110.21
1	F	122	GLY	N-CA-C	5.43	119.45	110.97

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLY	Peptide
1	B	121	GLU	Peptide
1	F	121	GLU	Peptide
1	F	122	GLY	Peptide
2	P	138	CYS	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	3086	0	3085	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3058	0	3054	72	0
1	C	3065	0	3063	101	0
1	D	3058	0	3054	101	0
1	E	3074	0	3076	101	0
1	F	3011	0	3019	92	0
1	G	3018	0	3028	100	0
1	H	3067	0	3067	101	0
1	I	3018	0	3028	79	0
1	J	3079	0	3076	95	0
2	K	1055	0	1043	72	0
2	L	1025	0	1022	58	0
2	M	1037	0	1031	58	0
2	N	1037	0	1031	51	0
2	O	1017	0	1016	59	0
2	P	1037	0	1031	48	0
2	S	1017	0	1016	47	0
2	T	1037	0	1031	68	0
2	U	1037	0	1031	71	0
2	V	1064	0	1049	58	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	2	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	3	0
3	G	1	0	0	2	0
3	H	1	0	0	1	0
3	I	1	0	0	2	0
3	J	1	0	0	1	0
4	F	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
4	M	4	0	0	2	0
4	O	4	0	0	0	0
4	P	4	0	0	0	0
4	S	4	0	0	0	0
4	T	4	0	0	1	0
4	U	4	0	0	2	0
4	V	4	0	0	0	0
All	All	40947	0	40851	1421	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 17.

The worst 5 of 1421 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:CE	1:A:400:LYS:CD	1.77	1.61
2:V:40:MET:HB2	2:V:114:THR:HG21	1.44	0.98
2:P:40:MET:HB2	2:P:114:THR:HG21	1.48	0.95
2:U:40:MET:HB2	2:U:114:THR:HG21	1.48	0.95
2:S:40:MET:HB2	2:S:114:THR:HG21	1.46	0.95

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	390/406 (96%)	360 (92%)	24 (6%)	6 (2%)	8	38
1	B	387/406 (95%)	358 (92%)	21 (5%)	8 (2%)	5	29
1	C	388/406 (96%)	350 (90%)	32 (8%)	6 (2%)	8	38
1	D	387/406 (95%)	358 (92%)	23 (6%)	6 (2%)	7	36
1	E	389/406 (96%)	356 (92%)	26 (7%)	7 (2%)	6	33
1	F	382/406 (94%)	357 (94%)	20 (5%)	5 (1%)	9	41
1	G	383/406 (94%)	358 (94%)	23 (6%)	2 (0%)	24	62
1	H	388/406 (96%)	354 (91%)	25 (6%)	9 (2%)	5	28
1	I	383/406 (94%)	358 (94%)	21 (6%)	4 (1%)	12	47
1	J	389/406 (96%)	356 (92%)	28 (7%)	5 (1%)	9	41
2	K	135/157 (86%)	111 (82%)	14 (10%)	10 (7%)	1	10
2	L	132/157 (84%)	116 (88%)	10 (8%)	6 (4%)	2	17
2	M	133/157 (85%)	112 (84%)	14 (10%)	7 (5%)	1	15
2	N	133/157 (85%)	112 (84%)	13 (10%)	8 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	131/157 (83%)	109 (83%)	15 (12%)	7 (5%)	1	15
2	P	133/157 (85%)	111 (84%)	13 (10%)	9 (7%)	1	12
2	S	131/157 (83%)	107 (82%)	17 (13%)	7 (5%)	1	15
2	T	133/157 (85%)	114 (86%)	12 (9%)	7 (5%)	1	15
2	U	133/157 (85%)	112 (84%)	12 (9%)	9 (7%)	1	12
2	V	136/157 (87%)	113 (83%)	17 (12%)	6 (4%)	2	17
All	All	5196/5630 (92%)	4682 (90%)	380 (7%)	134 (3%)	4	25

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	HIS
1	B	397	ASN
1	C	297	HIS
1	C	333	SER
1	D	341	LYS

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	330/341 (97%)	321 (97%)	9 (3%)	39	59
1	B	327/341 (96%)	315 (96%)	12 (4%)	30	51
1	C	328/341 (96%)	319 (97%)	9 (3%)	39	59
1	D	327/341 (96%)	316 (97%)	11 (3%)	32	54
1	E	329/341 (96%)	321 (98%)	8 (2%)	43	63
1	F	322/341 (94%)	314 (98%)	8 (2%)	42	62
1	G	323/341 (95%)	315 (98%)	8 (2%)	42	62
1	H	328/341 (96%)	323 (98%)	5 (2%)	57	70
1	I	323/341 (95%)	315 (98%)	8 (2%)	42	62
1	J	329/341 (96%)	320 (97%)	9 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	116/135 (86%)	108 (93%)	8 (7%)	14	36
2	L	113/135 (84%)	109 (96%)	4 (4%)	32	53
2	M	114/135 (84%)	113 (99%)	1 (1%)	70	76
2	N	114/135 (84%)	110 (96%)	4 (4%)	32	53
2	O	112/135 (83%)	108 (96%)	4 (4%)	31	52
2	P	114/135 (84%)	109 (96%)	5 (4%)	25	47
2	S	112/135 (83%)	109 (97%)	3 (3%)	39	59
2	T	114/135 (84%)	113 (99%)	1 (1%)	70	76
2	U	114/135 (84%)	110 (96%)	4 (4%)	32	53
2	V	117/135 (87%)	115 (98%)	2 (2%)	53	67
All	All	4406/4760 (93%)	4283 (97%)	123 (3%)	38	59

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	104	THR
2	P	63	CYS
1	I	172	LYS
2	P	49	GLU
2	U	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	113	HIS
1	I	158	ASN
2	U	33	ASN
2	P	47	ASN
1	G	158	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	V	201	2,1	0,4,4	-	-	-		
4	FES	O	201	2,1	0,4,4	-	-	-		
4	FES	L	201	2,1	0,4,4	-	-	-		
4	FES	K	201	2,1	0,4,4	-	-	-		
4	FES	U	201	2,1	0,4,4	-	-	-		
4	FES	P	201	2,1	0,4,4	-	-	-		
4	FES	S	201	2,1	0,4,4	-	-	-		
4	FES	M	201	2,1	0,4,4	-	-	-		
4	FES	F	502	2,1	0,4,4	-	-	-		
4	FES	T	201	2,1	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	V	201	2,1	-	-	0/1/1/1
4	FES	O	201	2,1	-	-	0/1/1/1
4	FES	L	201	2,1	-	-	0/1/1/1
4	FES	K	201	2,1	-	-	0/1/1/1
4	FES	U	201	2,1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	P	201	2,1	-	-	0/1/1/1
4	FES	S	201	2,1	-	-	0/1/1/1
4	FES	M	201	2,1	-	-	0/1/1/1
4	FES	F	502	2,1	-	-	0/1/1/1
4	FES	T	201	2,1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

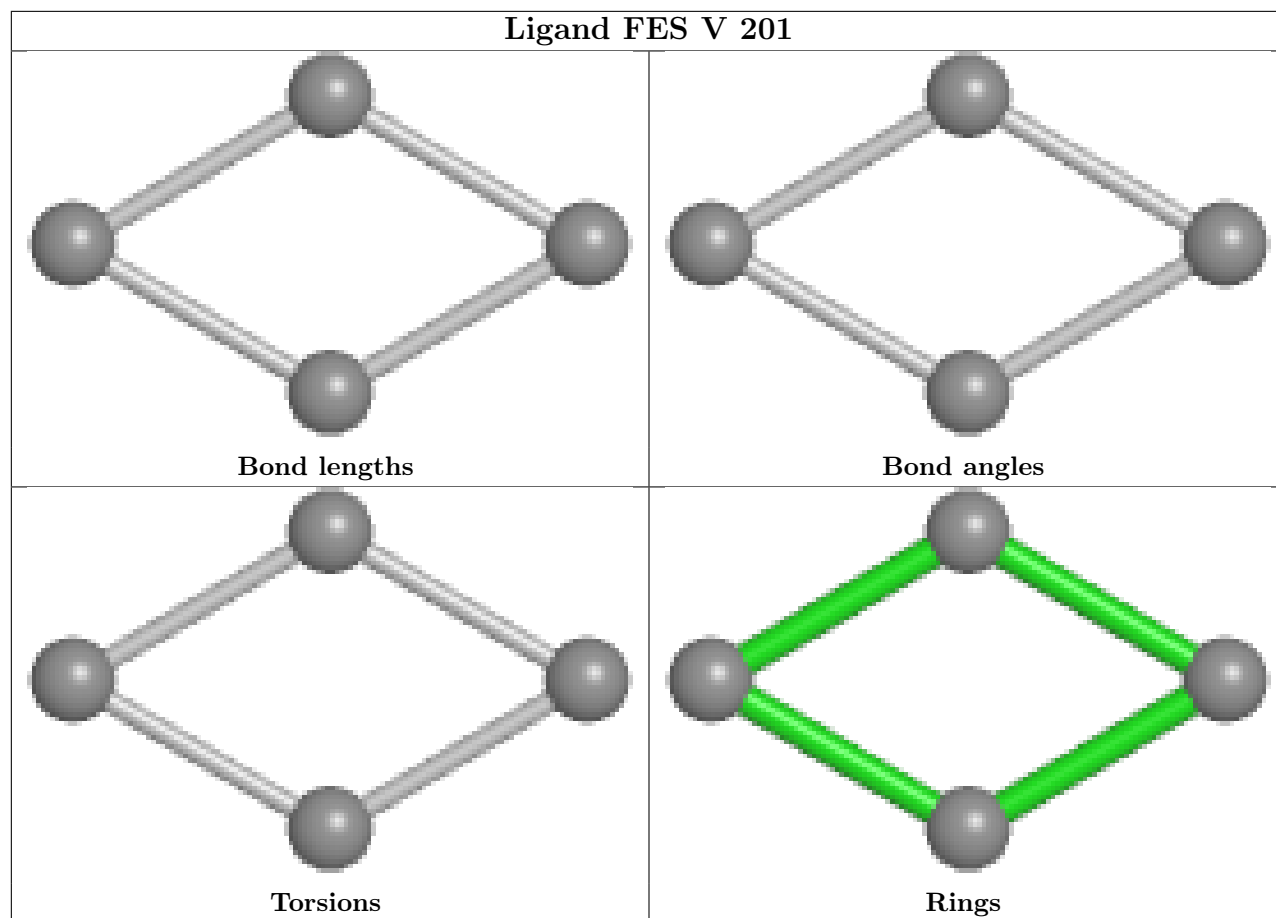
There are no torsion outliers.

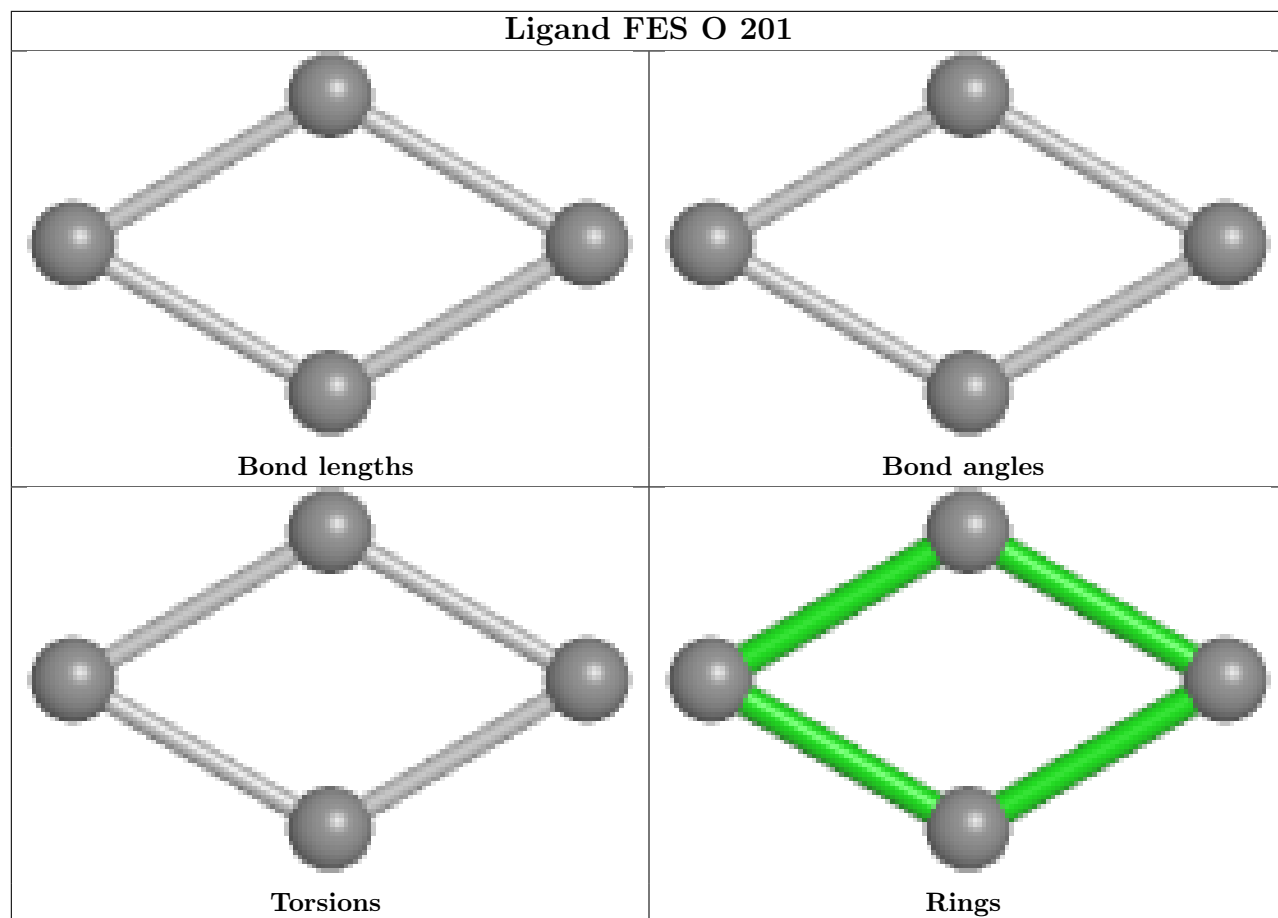
There are no ring outliers.

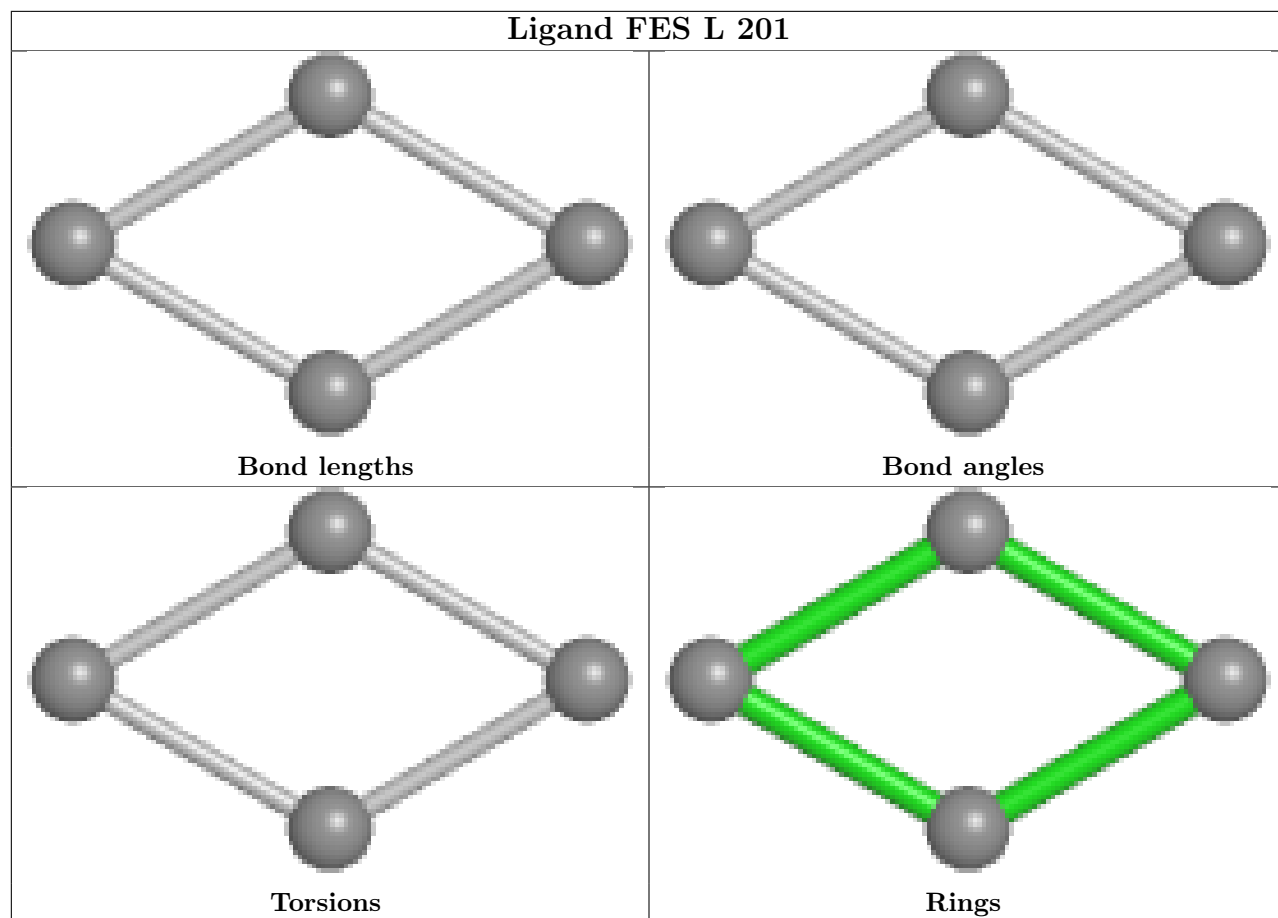
3 monomers are involved in 5 short contacts:

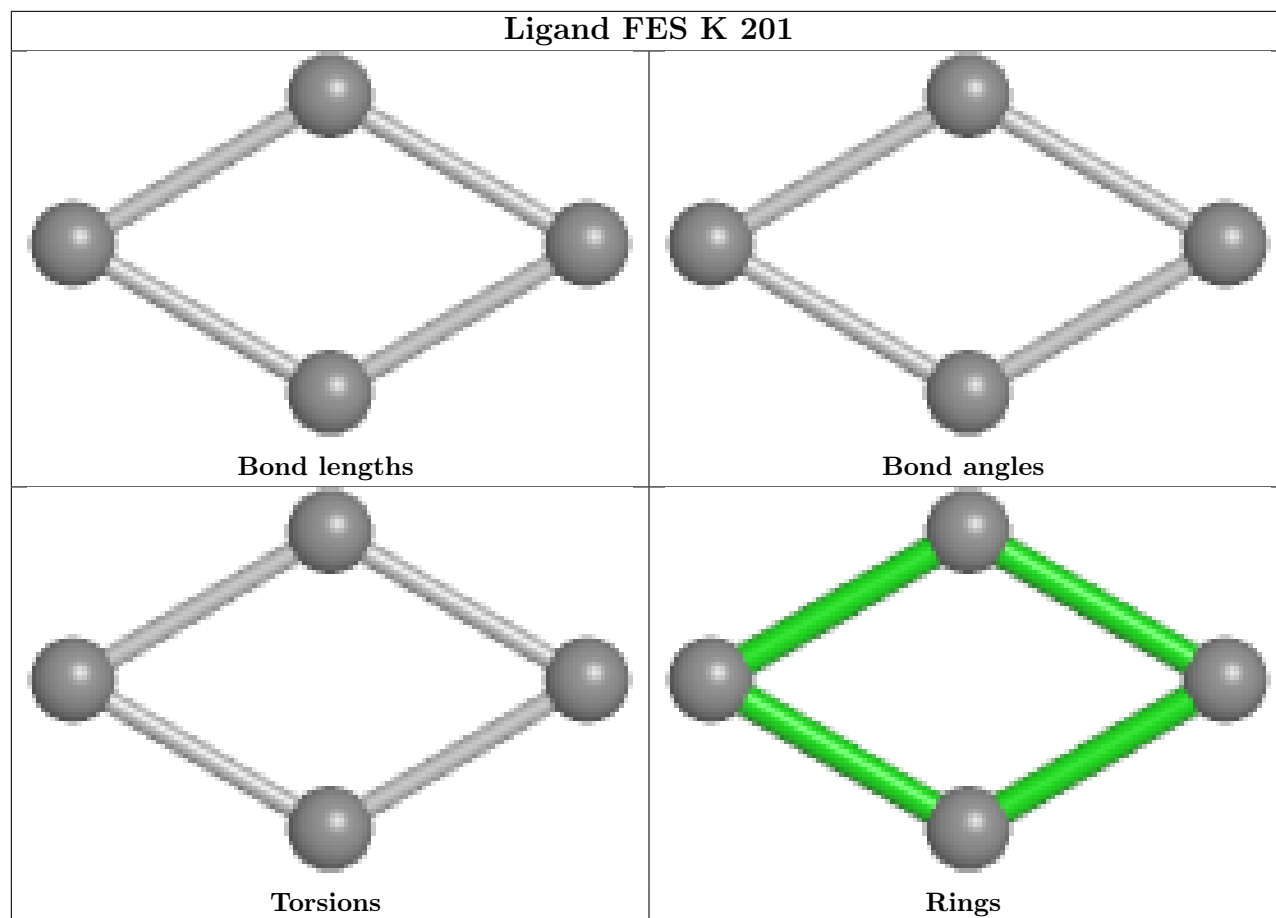
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	201	FES	2	0
4	M	201	FES	2	0
4	T	201	FES	1	0

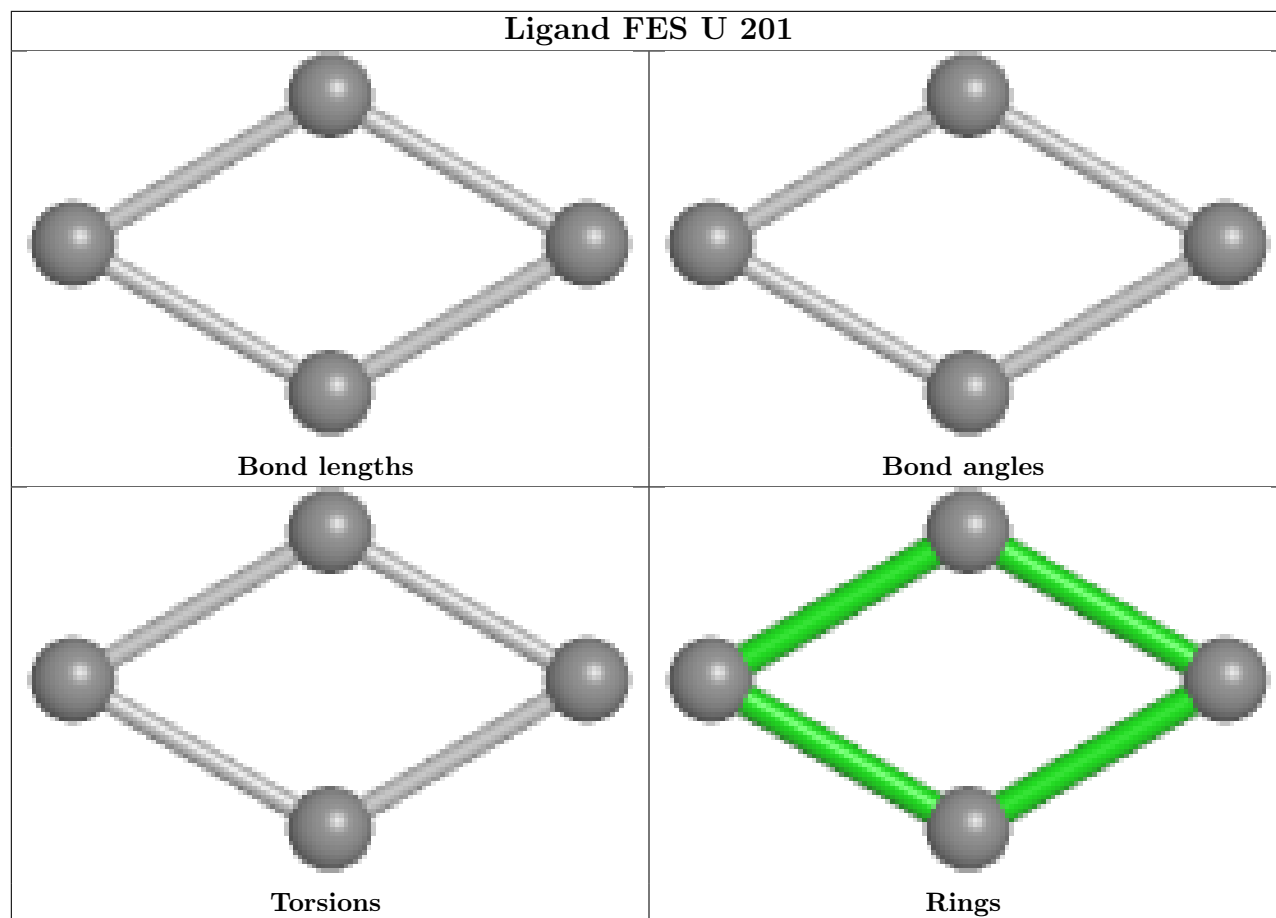
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

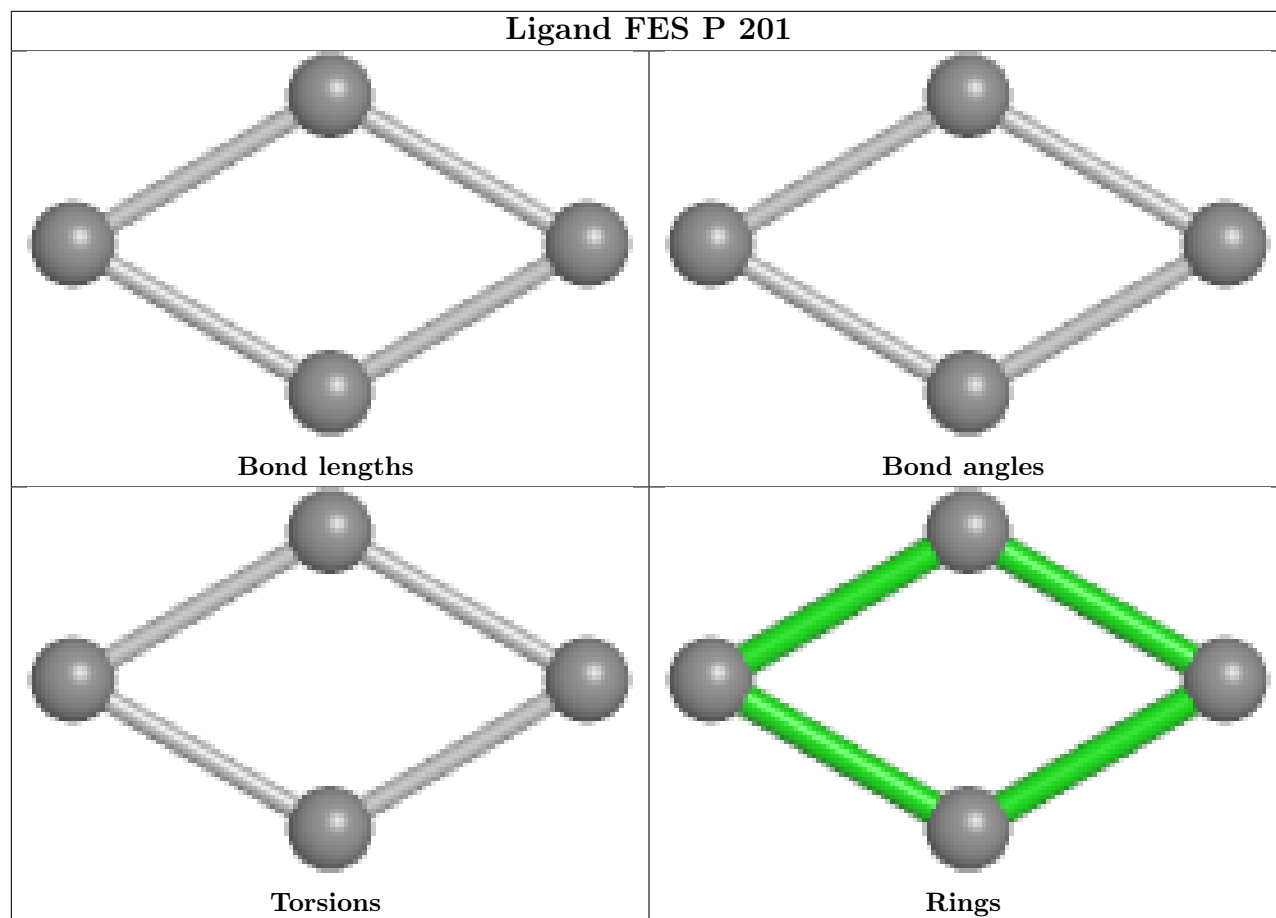


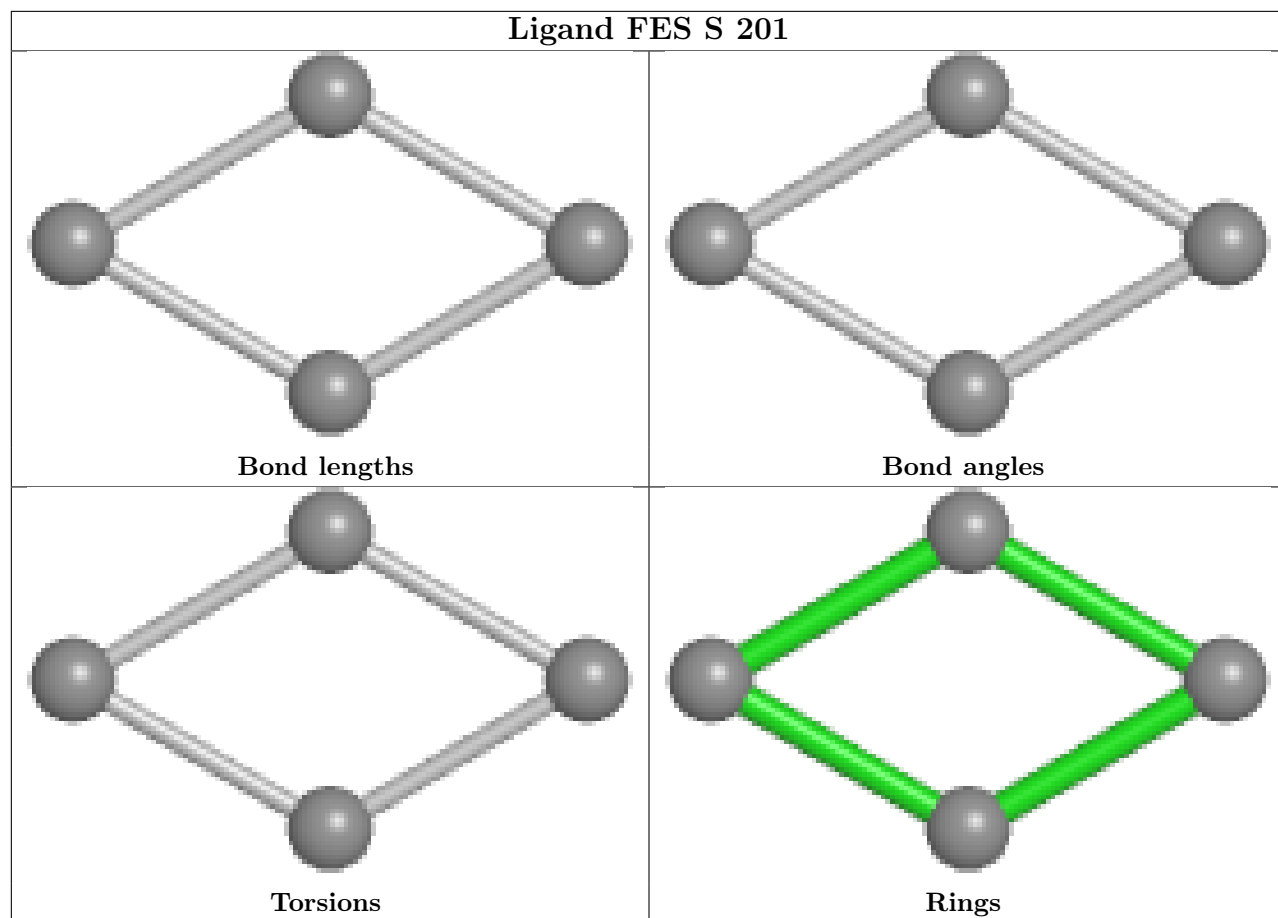


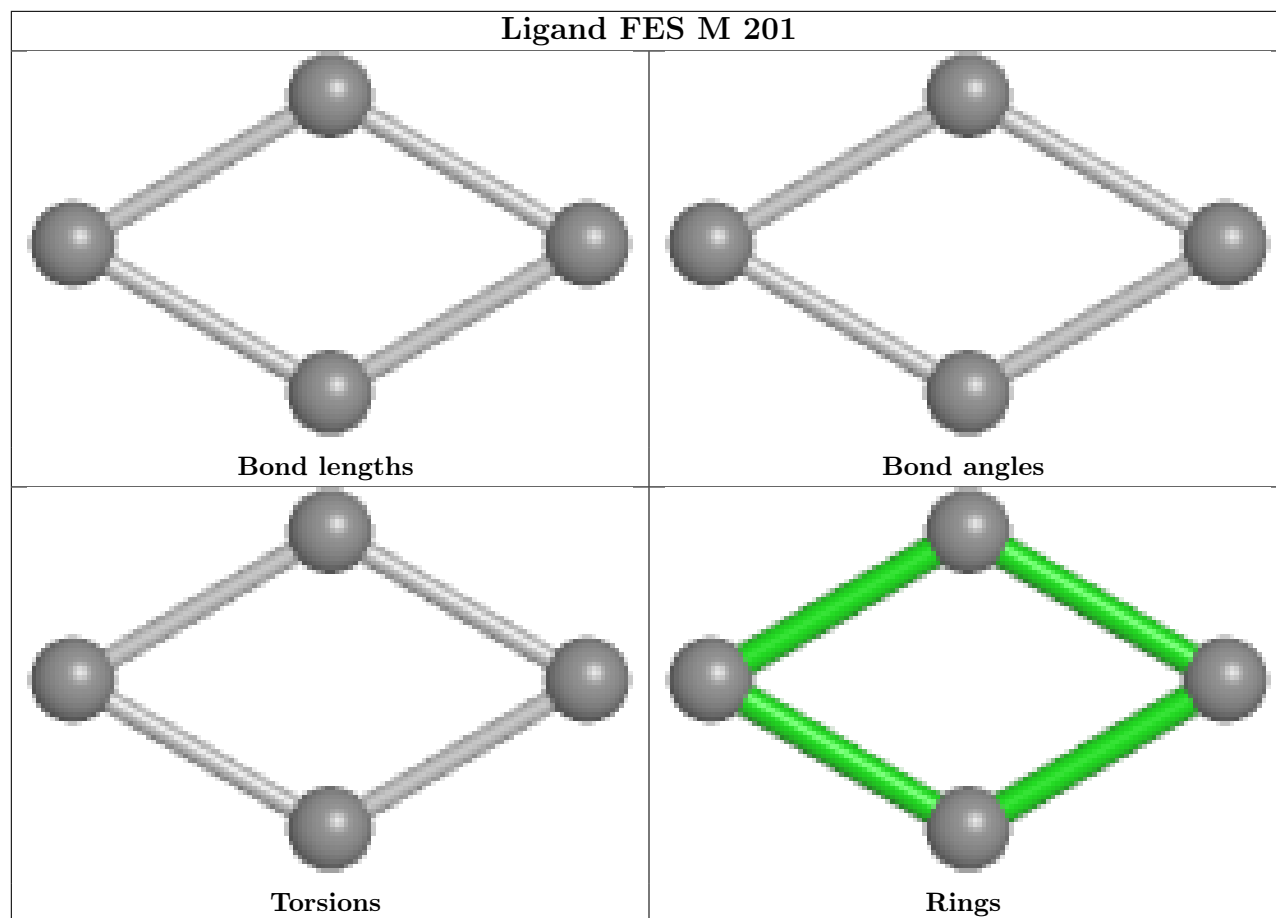


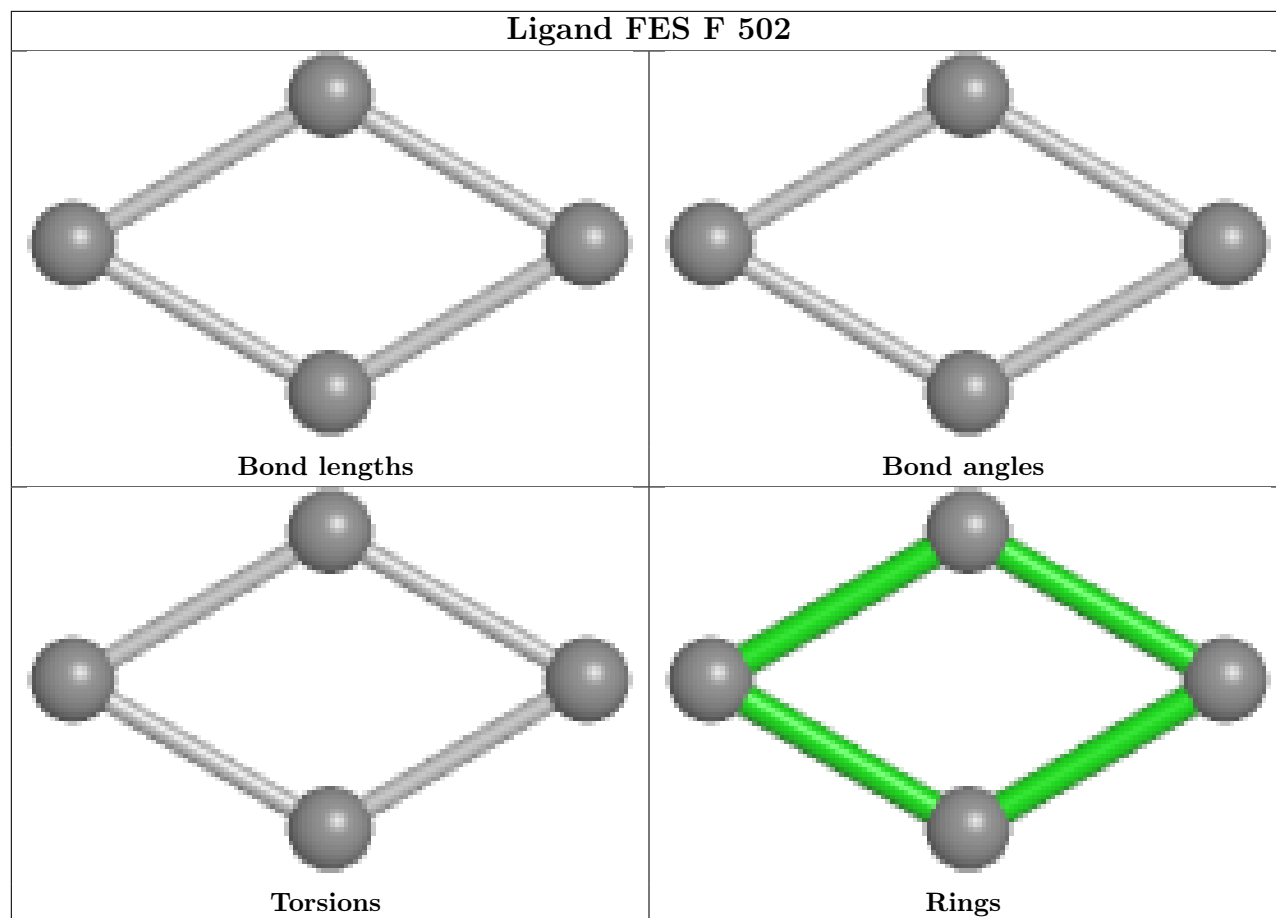


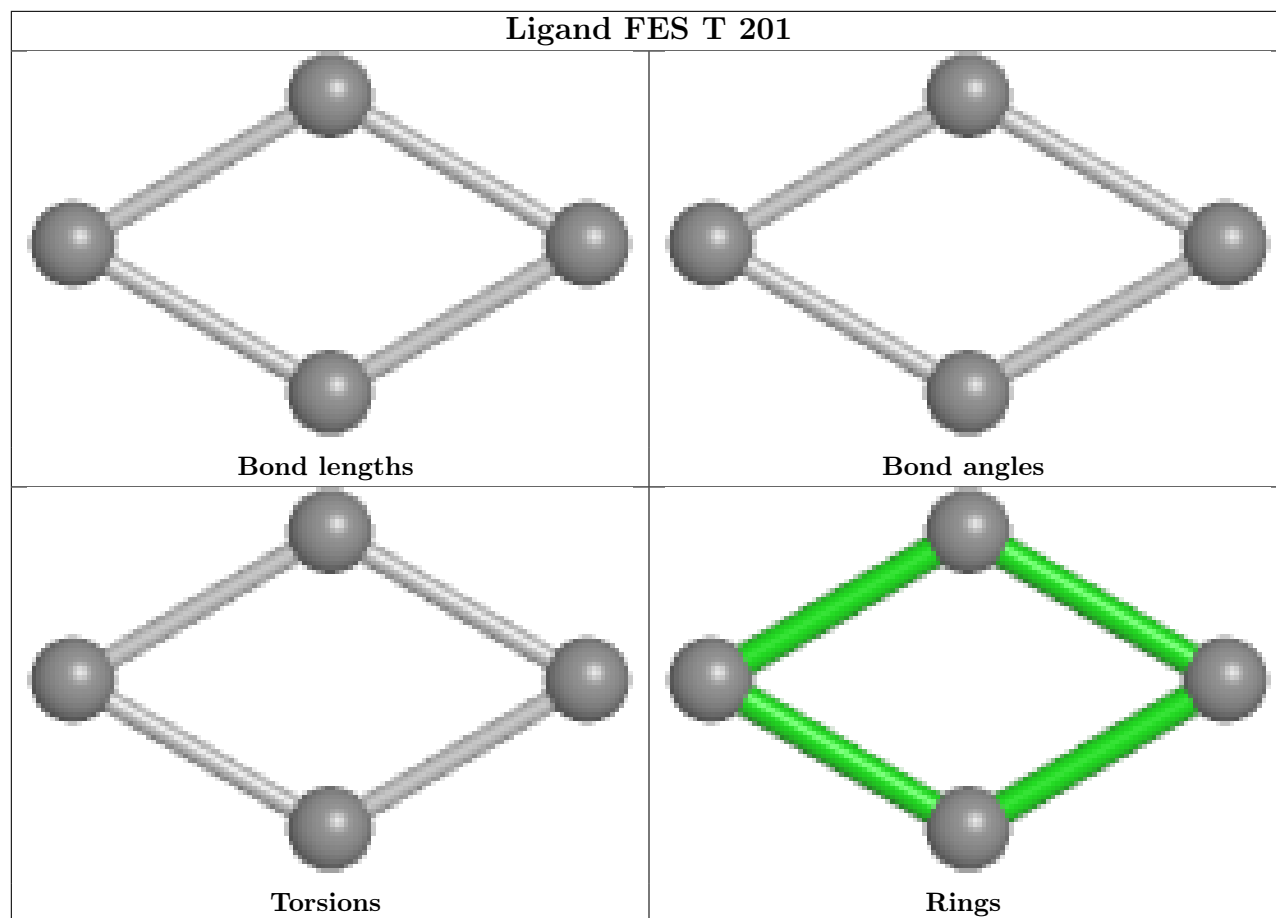












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	392/406 (96%)	-0.20	9 (2%) 61 48	89, 189, 242, 313	0
1	B	389/406 (95%)	-0.13	12 (3%) 51 40	132, 210, 272, 365	0
1	C	390/406 (96%)	0.01	23 (5%) 28 28	135, 206, 264, 317	0
1	D	389/406 (95%)	-0.28	3 (0%) 82 69	137, 201, 259, 330	0
1	E	391/406 (96%)	-0.18	11 (2%) 55 43	146, 230, 276, 339	0
1	F	384/406 (94%)	-0.24	9 (2%) 61 48	150, 232, 313, 456	0
1	G	385/406 (94%)	-0.09	15 (3%) 43 36	167, 243, 309, 353	0
1	H	390/406 (96%)	-0.27	7 (1%) 67 53	166, 245, 299, 360	0
1	I	385/406 (94%)	-0.22	3 (0%) 82 69	181, 256, 310, 351	0
1	J	391/406 (96%)	-0.27	5 (1%) 75 60	167, 248, 345, 394	0
2	K	137/157 (87%)	-0.21	2 (1%) 72 56	144, 204, 272, 359	0
2	L	134/157 (85%)	-0.19	6 (4%) 38 33	178, 240, 316, 365	0
2	M	135/157 (85%)	-0.20	2 (1%) 72 56	170, 238, 319, 370	0
2	N	135/157 (85%)	-0.46	0 100 100	294, 364, 427, 525	0
2	O	133/157 (84%)	-0.29	3 (2%) 61 48	219, 278, 347, 385	0
2	P	135/157 (85%)	-0.29	2 (1%) 72 56	173, 245, 319, 395	0
2	S	133/157 (84%)	-0.54	0 100 100	302, 390, 440, 459	0
2	T	135/157 (85%)	-0.41	0 100 100	194, 259, 347, 374	0
2	U	135/157 (85%)	-0.39	2 (1%) 72 56	193, 273, 337, 405	0
2	V	138/157 (87%)	-0.26	7 (5%) 33 31	168, 250, 300, 395	0
All	All	5236/5630 (93%)	-0.22	121 (2%) 61 48	89, 234, 351, 525	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	GLU	6.3
1	B	336	VAL	6.2
1	C	310	VAL	5.9
1	A	167	ILE	5.3
1	C	318	MET	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

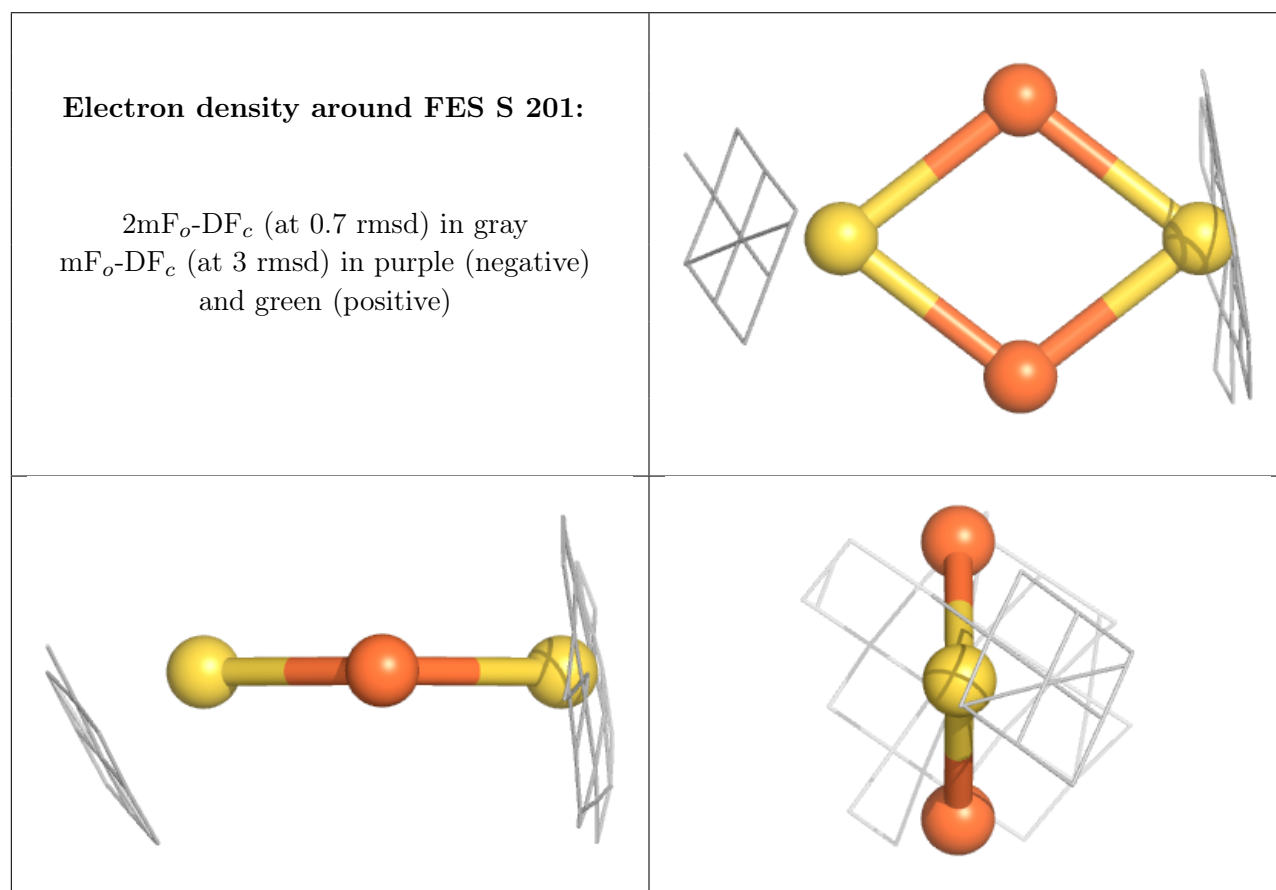
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	F	501	1/1	0.50	0.31	187,187,187,187	0
3	CL	D	501	1/1	0.76	0.28	115,115,115,115	0
3	CL	I	501	1/1	0.81	0.21	146,146,146,146	0
3	CL	A	501	1/1	0.83	0.20	85,85,85,85	0
3	CL	H	501	1/1	0.85	0.19	128,128,128,128	0
3	CL	G	501	1/1	0.85	0.15	138,138,138,138	0
4	FES	S	201	4/4	0.87	0.09	359,359,359,359	0
3	CL	C	501	1/1	0.88	0.14	110,110,110,110	0
4	FES	F	502	4/4	0.91	0.06	311,311,311,311	0
3	CL	J	501	1/1	0.92	0.17	151,151,151,151	0
3	CL	E	501	1/1	0.94	0.15	121,121,121,121	0
4	FES	L	201	4/4	0.96	0.07	203,203,203,203	0
4	FES	O	201	4/4	0.97	0.05	303,303,303,303	0
4	FES	P	201	4/4	0.97	0.04	275,275,275,275	0
3	CL	B	501	1/1	0.97	0.09	95,95,95,95	0
4	FES	U	201	4/4	0.97	0.04	254,254,254,254	0
4	FES	V	201	4/4	0.98	0.04	223,223,223,223	0
4	FES	T	201	4/4	0.99	0.03	237,237,237,237	0
4	FES	M	201	4/4	0.99	0.04	211,211,211,211	0

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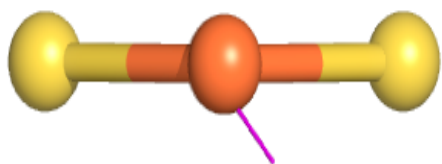
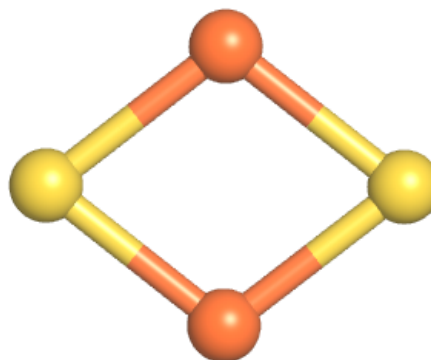
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FES	K	201	4/4	0.99	0.05	169,176,177,188	0

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.



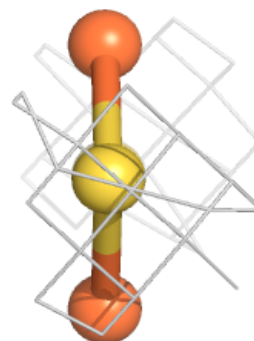
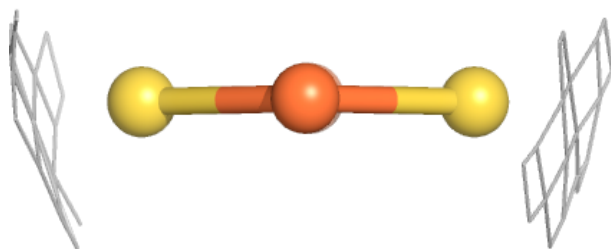
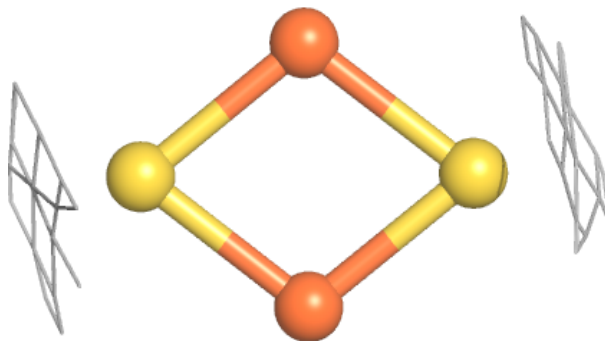
Electron density around FES F 502:

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

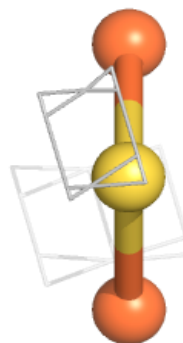
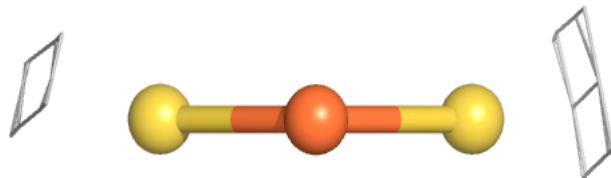
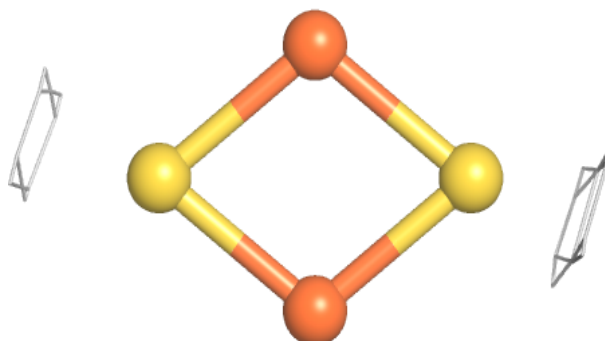


Electron density around FES L 201:

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

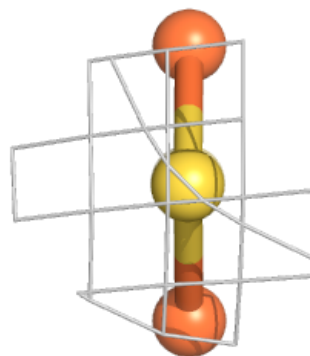
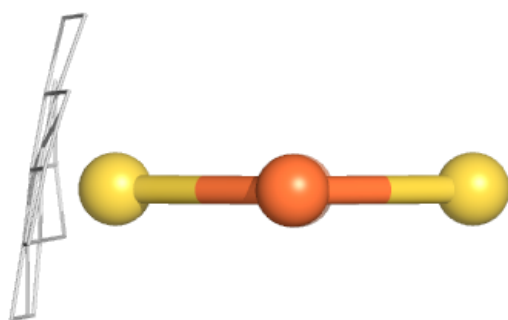
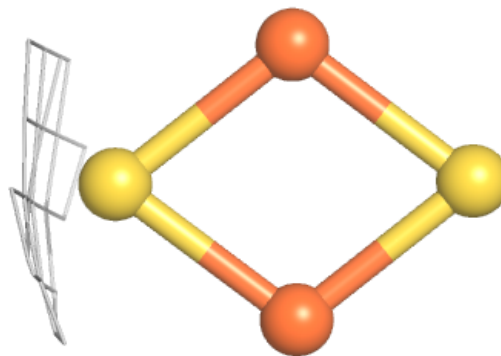
**Electron density around FES O 201:**

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

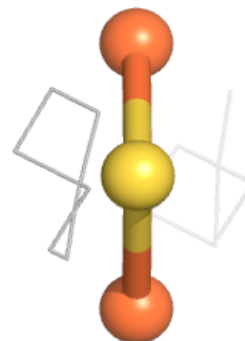
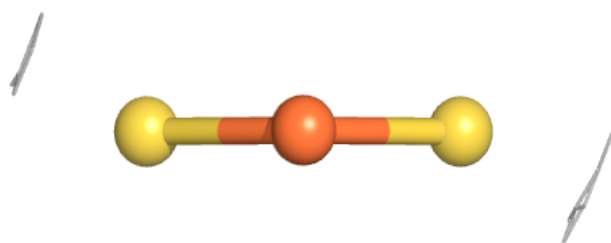
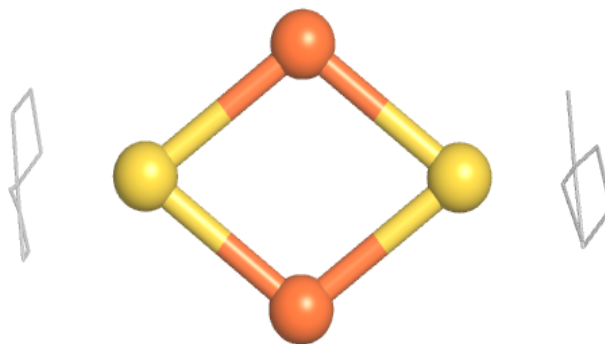


Electron density around FES P 201:

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

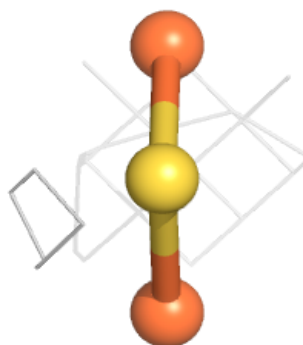
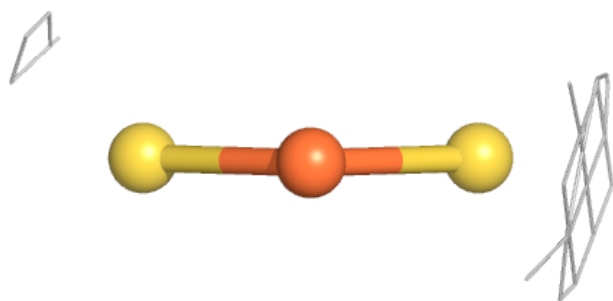
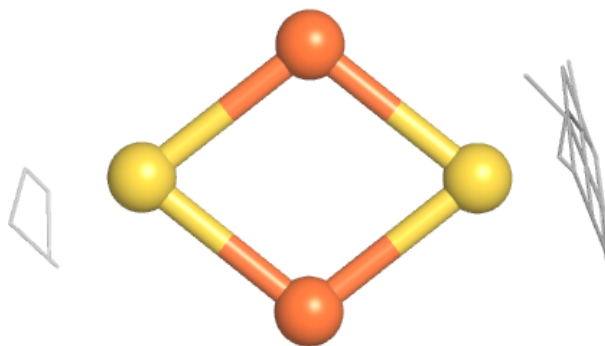
**Electron density around FES U 201:**

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

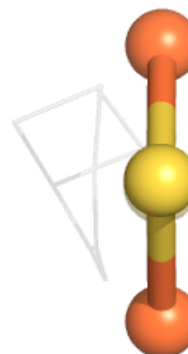
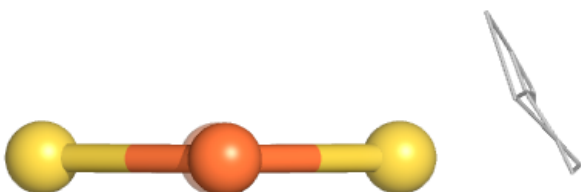
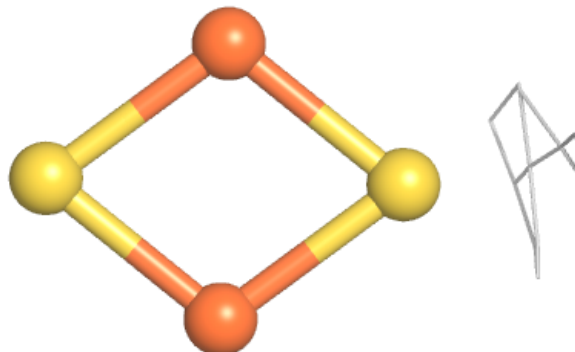


Electron density around FES V 201:

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

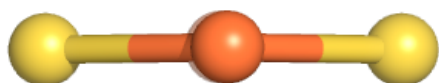
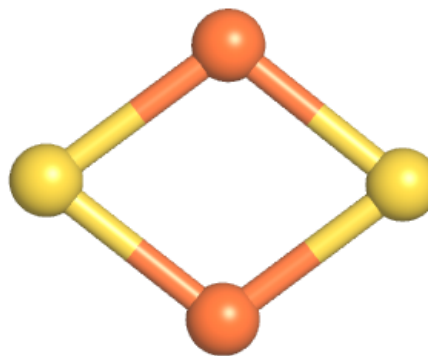
**Electron density around FES T 201:**

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

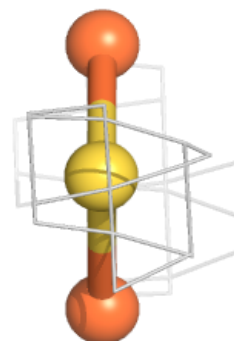
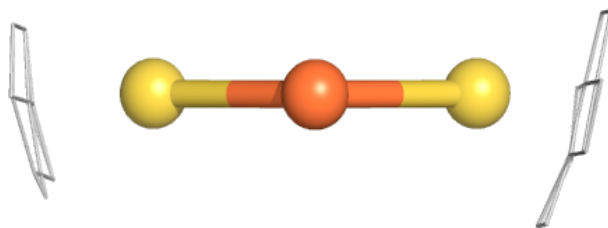
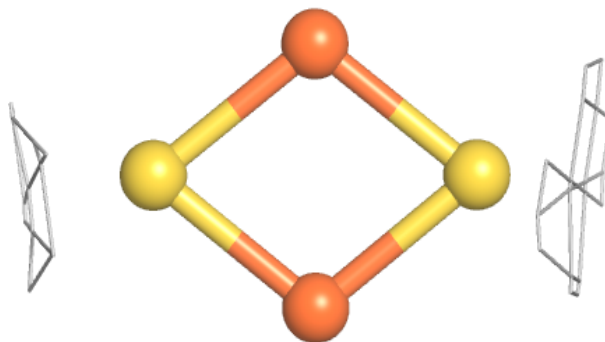


Electron density around FES M 201:

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

**Electron density around FES K 201:**

$2mF_o - DF_c$ (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.