



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 11:57 PM JST

PDB ID : 7C8Z
Title : Crystal structure of salicylate 5-hydroxylase NagGH (a Rieske non-heme iron-dependent monooxygenase)
Authors : Li, D.F.; Hou, Y.J.
Deposited on : 2020-06-04
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

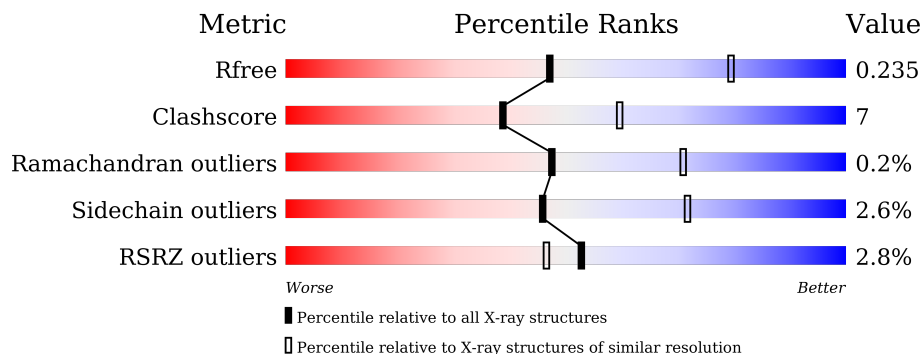
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



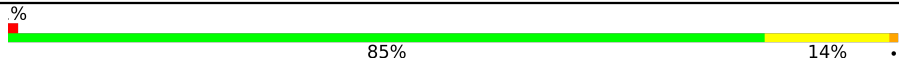

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	442	 2% 70% 16% 13%
1	C	442	 3% 64% 21% 13%
1	E	442	 4% 70% 16% 13%
1	G	442	 4% 70% 15% 13%
2	B	161	 92% 7%
2	D	161	 89% 11%

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Mol	Chain	Length	Quality of chain
2	F	161	 <p>%</p> <p>85% 14%</p>
2	H	161	 <p>88% 12%</p>

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 18150 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 Salicylate 5-hydroxylase, large oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3127	1999	556	557	15	0	0	0
1	C	383	3127	1999	556	557	15	0	0	0
1	E	383	3127	1999	556	557	15	0	0	0
1	G	383	3127	1999	556	557	15	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O52379
A	-17	GLY	-	expression tag	UNP O52379
A	-16	SER	-	expression tag	UNP O52379
A	-15	HIS	-	expression tag	UNP O52379
A	-14	HIS	-	expression tag	UNP O52379
A	-13	HIS	-	expression tag	UNP O52379
A	-12	HIS	-	expression tag	UNP O52379
A	-11	HIS	-	expression tag	UNP O52379
A	-10	HIS	-	expression tag	UNP O52379
A	-9	SER	-	expression tag	UNP O52379
A	-8	SER	-	expression tag	UNP O52379
A	-7	GLY	-	expression tag	UNP O52379
A	-6	LEU	-	expression tag	UNP O52379
A	-5	VAL	-	expression tag	UNP O52379
A	-4	PRO	-	expression tag	UNP O52379
A	-3	ARG	-	expression tag	UNP O52379
A	-2	GLY	-	expression tag	UNP O52379
A	-1	SER	-	expression tag	UNP O52379
A	0	HIS	-	expression tag	UNP O52379
C	-18	MET	-	initiating methionine	UNP O52379
C	-17	GLY	-	expression tag	UNP O52379

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP O52379
C	-15	HIS	-	expression tag	UNP O52379
C	-14	HIS	-	expression tag	UNP O52379
C	-13	HIS	-	expression tag	UNP O52379
C	-12	HIS	-	expression tag	UNP O52379
C	-11	HIS	-	expression tag	UNP O52379
C	-10	HIS	-	expression tag	UNP O52379
C	-9	SER	-	expression tag	UNP O52379
C	-8	SER	-	expression tag	UNP O52379
C	-7	GLY	-	expression tag	UNP O52379
C	-6	LEU	-	expression tag	UNP O52379
C	-5	VAL	-	expression tag	UNP O52379
C	-4	PRO	-	expression tag	UNP O52379
C	-3	ARG	-	expression tag	UNP O52379
C	-2	GLY	-	expression tag	UNP O52379
C	-1	SER	-	expression tag	UNP O52379
C	0	HIS	-	expression tag	UNP O52379
E	-18	MET	-	initiating methionine	UNP O52379
E	-17	GLY	-	expression tag	UNP O52379
E	-16	SER	-	expression tag	UNP O52379
E	-15	HIS	-	expression tag	UNP O52379
E	-14	HIS	-	expression tag	UNP O52379
E	-13	HIS	-	expression tag	UNP O52379
E	-12	HIS	-	expression tag	UNP O52379
E	-11	HIS	-	expression tag	UNP O52379
E	-10	HIS	-	expression tag	UNP O52379
E	-9	SER	-	expression tag	UNP O52379
E	-8	SER	-	expression tag	UNP O52379
E	-7	GLY	-	expression tag	UNP O52379
E	-6	LEU	-	expression tag	UNP O52379
E	-5	VAL	-	expression tag	UNP O52379
E	-4	PRO	-	expression tag	UNP O52379
E	-3	ARG	-	expression tag	UNP O52379
E	-2	GLY	-	expression tag	UNP O52379
E	-1	SER	-	expression tag	UNP O52379
E	0	HIS	-	expression tag	UNP O52379
G	-18	MET	-	initiating methionine	UNP O52379
G	-17	GLY	-	expression tag	UNP O52379
G	-16	SER	-	expression tag	UNP O52379
G	-15	HIS	-	expression tag	UNP O52379
G	-14	HIS	-	expression tag	UNP O52379
G	-13	HIS	-	expression tag	UNP O52379

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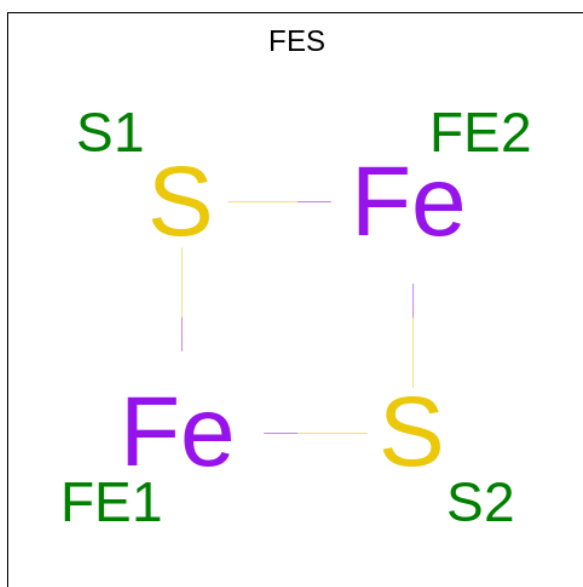
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	HIS	-	expression tag	UNP O52379
G	-11	HIS	-	expression tag	UNP O52379
G	-10	HIS	-	expression tag	UNP O52379
G	-9	SER	-	expression tag	UNP O52379
G	-8	SER	-	expression tag	UNP O52379
G	-7	GLY	-	expression tag	UNP O52379
G	-6	LEU	-	expression tag	UNP O52379
G	-5	VAL	-	expression tag	UNP O52379
G	-4	PRO	-	expression tag	UNP O52379
G	-3	ARG	-	expression tag	UNP O52379
G	-2	GLY	-	expression tag	UNP O52379
G	-1	SER	-	expression tag	UNP O52379
G	0	HIS	-	expression tag	UNP O52379

- Molecule 2 is a protein called Salicylate 5-hydroxylase, small oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	161	1324	849	218	249	8	0	0	0
2	D	161	1324	849	218	249	8	0	0	0
2	F	161	1324	849	218	249	8	0	0	0
2	H	161	1324	849	218	249	8	0	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	G	1	4	2	2	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
4	A	1	1	1	0	0
4	C	1	1	1	0	0
4	E	1	1	1	0	0
4	G	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	71	71	71	0	0

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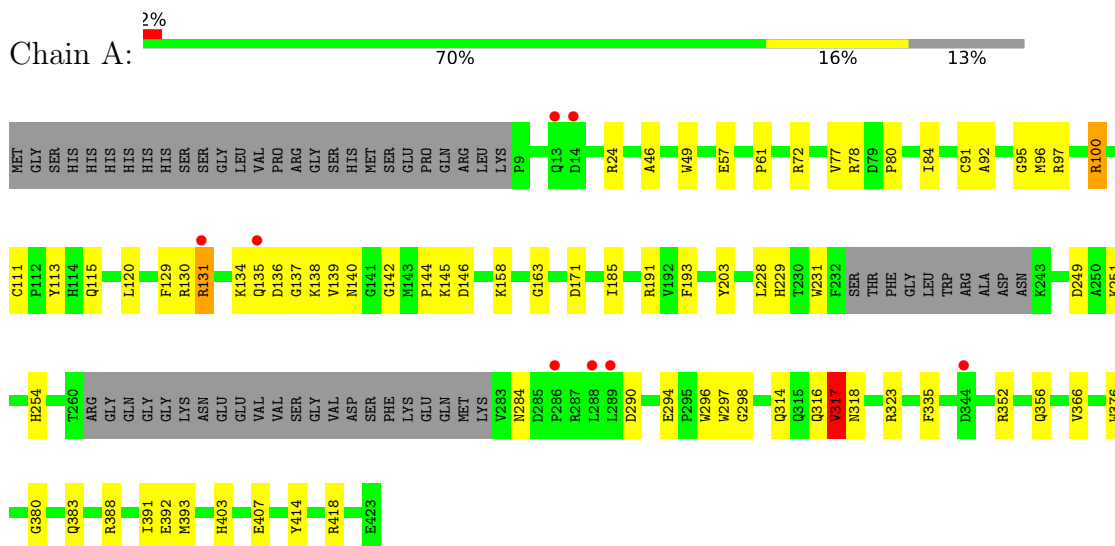
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	38	Total 38	O 38	0	0
5	E	40	Total 40	O 40	0	0
5	G	33	Total 33	O 33	0	0
5	B	38	Total 38	O 38	0	0
5	D	33	Total 33	O 33	0	0
5	F	36	Total 36	O 36	0	0
5	H	37	Total 37	O 37	0	0

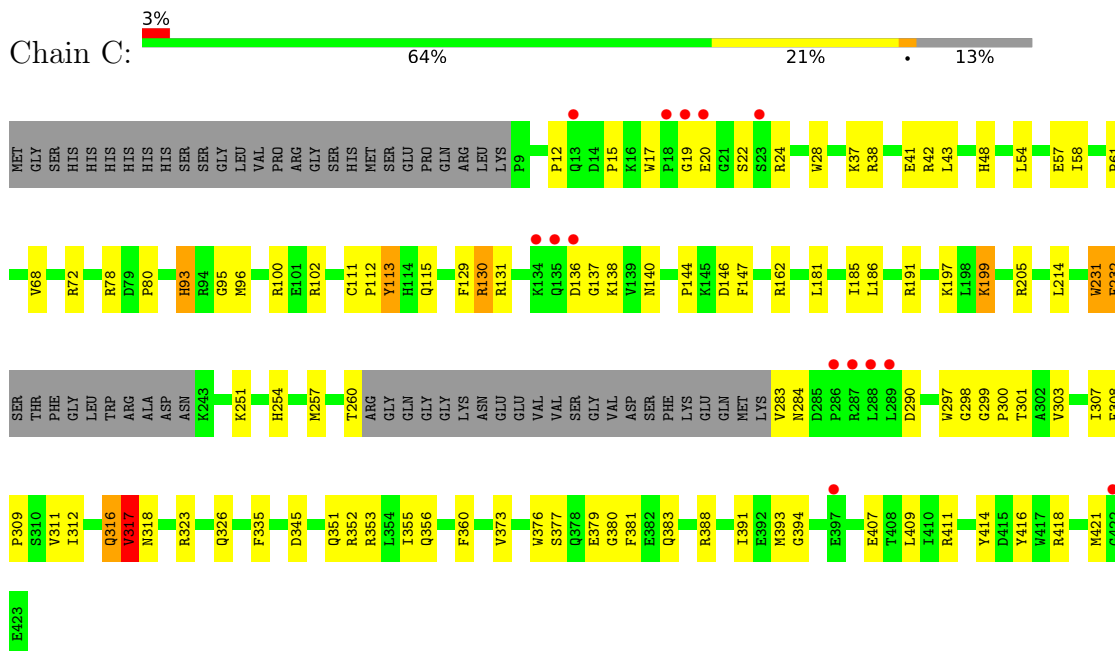
3 Residue-property plots [i](#)

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.

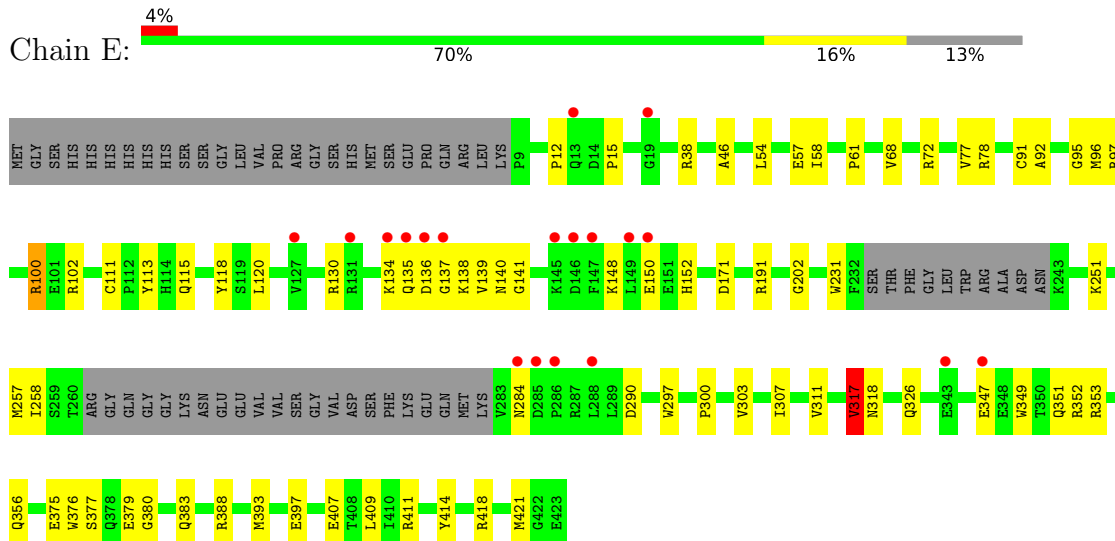
- Molecule 1: Salicylate 5-hydroxylase, large oxygenase component



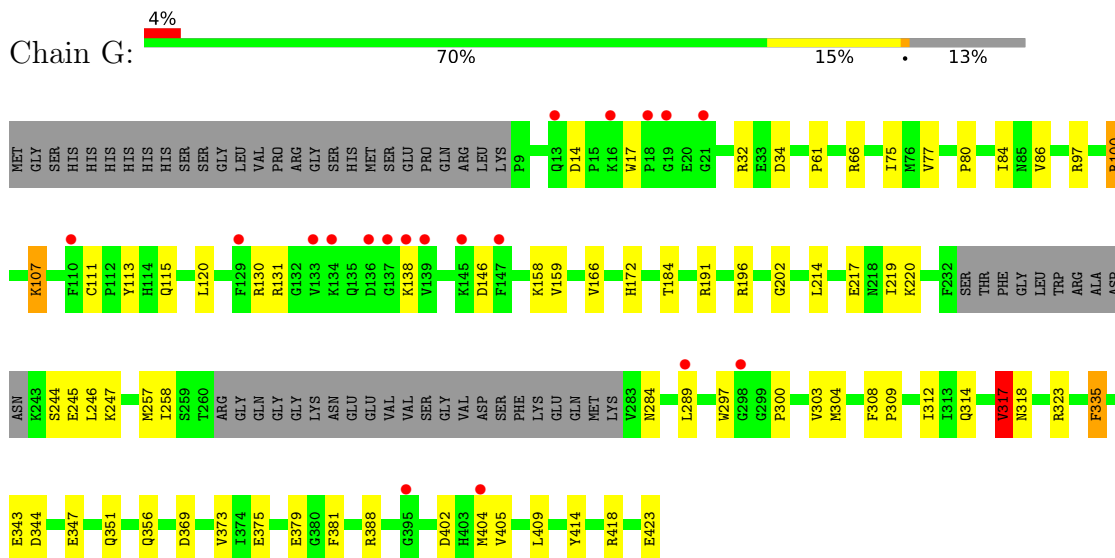
- Molecule 1: Salicylate 5-hydroxylase, large oxygenase component



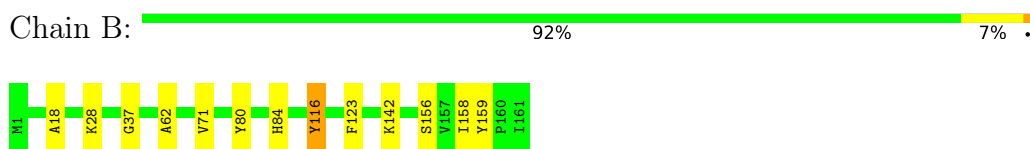
- Molecule 1: Salicylate 5-hydroxylase, large oxygenase component



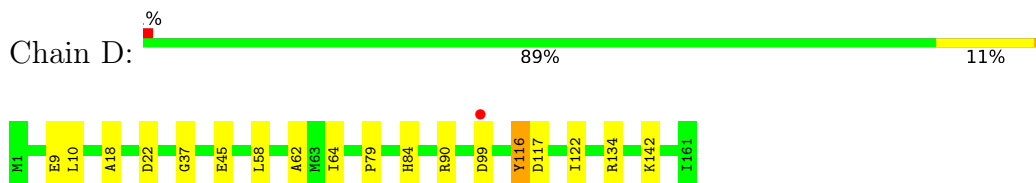
- Molecule 1: Salicylate 5-hydroxylase, large oxygenase component




- Molecule 2: Salicylate 5-hydroxylase, small oxygenase component



- Molecule 2: Salicylate 5-hydroxylase, small oxygenase component




- Molecule 2: Salicylate 5-hydroxylase, small oxygenase component

Chain F:  % 85% 14%



- Molecule 2: Salicylate 5-hydroxylase, small oxygenase component

Chain H:  % 88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	188.16Å 188.16Å 147.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.28 – 2.60 47.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.28-2.60) 97.6 (47.28-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.192 , 0.237 0.191 , 0.235	Depositor DCC
R_{free} test set	2010 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtrriage
Anisotropy	0.236	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18150	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/3224	0.54	0/4363
1	C	0.31	0/3224	0.52	0/4363
1	E	0.32	0/3224	0.55	0/4363
1	G	0.31	0/3224	0.53	0/4363
2	B	0.31	0/1357	0.54	0/1841
2	D	0.30	0/1357	0.53	0/1841
2	F	0.29	0/1357	0.52	0/1841
2	H	0.29	0/1357	0.52	0/1841
All	All	0.31	0/18324	0.53	0/24816

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3127	0	2983	61	1
1	C	3127	0	2983	76	1
1	E	3127	0	2983	61	0
1	G	3127	0	2983	49	0
2	B	1324	0	1291	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1324	0	1291	10	0
2	F	1324	0	1291	15	0
2	H	1324	0	1291	12	0
3	A	4	0	0	0	0
3	C	4	0	0	1	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	71	0	0	2	0
5	B	38	0	0	1	0
5	C	38	0	0	2	0
5	D	33	0	0	0	0
5	E	40	0	0	0	0
5	F	36	0	0	0	0
5	G	33	0	0	1	0
5	H	37	0	0	2	0
All	All	18150	0	17096	260	1

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 7.

All (260) 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:G:317:VAL:CG2	1:G:318:ASN:H	1.49	1.23
1:E:317:VAL:CG2	1:E:318:ASN:H	1.53	1.20
1:C:317:VAL:CG2	1:C:318:ASN:H	1.51	1.19
1:A:317:VAL:CG2	1:A:318:ASN:H	1.54	1.17
1:A:317:VAL:HG23	1:A:318:ASN:H	1.12	1.10
1:G:317:VAL:HG23	1:G:318:ASN:H	1.02	1.10
1:A:317:VAL:HG23	1:A:356:GLN:HE22	1.17	1.10
1:C:317:VAL:HG23	1:C:318:ASN:H	1.07	1.10
1:E:317:VAL:HG23	1:E:318:ASN:H	1.11	1.07
1:G:317:VAL:HG23	1:G:318:ASN:N	1.68	1.06
1:G:317:VAL:CG2	1:G:356:GLN:OE1	2.04	1.05
1:A:317:VAL:HG23	1:A:318:ASN:N	1.71	1.04
1:G:317:VAL:HG23	1:G:356:GLN:OE1	1.55	1.03
1:C:317:VAL:CG2	1:C:356:GLN:OE1	2.06	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:CG2	1:A:356:GLN:NE2	2.22	1.02
1:C:317:VAL:HG23	1:C:318:ASN:N	1.68	1.02
1:E:317:VAL:HG23	1:E:318:ASN:N	1.71	1.00
1:A:317:VAL:CG2	1:A:356:GLN:HE22	1.77	0.97
1:G:317:VAL:CG2	1:G:318:ASN:N	2.22	0.96
1:C:317:VAL:CG2	1:C:318:ASN:N	2.23	0.93
1:E:317:VAL:CG2	1:E:318:ASN:N	2.24	0.92
1:C:317:VAL:HG23	1:C:356:GLN:OE1	1.71	0.88
1:A:317:VAL:CG2	1:A:318:ASN:N	2.25	0.88
1:G:246:LEU:HD22	1:G:257:MET:HG2	1.60	0.84
1:E:317:VAL:HG21	1:E:356:GLN:NE2	1.93	0.83
1:E:397:GLU:O	1:E:411:ARG:NH2	2.10	0.83
1:A:317:VAL:HG22	1:A:318:ASN:H	1.45	0.81
1:C:317:VAL:HG22	1:C:318:ASN:H	1.45	0.80
1:E:191:ARG:NE	1:E:297:TRP:O	2.16	0.79
1:A:131:ARG:HD3	1:A:145:LYS:HE3	1.64	0.79
1:G:191:ARG:NE	1:G:297:TRP:O	2.18	0.77
1:E:317:VAL:HG22	1:E:318:ASN:H	1.46	0.76
1:A:317:VAL:HG21	1:A:356:GLN:NE2	2.00	0.76
1:C:317:VAL:HG21	1:C:356:GLN:OE1	1.85	0.75
1:C:377:SER:OG	1:E:96:MET:HE2	1.85	0.75
1:G:317:VAL:HG22	1:G:318:ASN:H	1.47	0.75
1:A:317:VAL:HG23	1:A:356:GLN:NE2	1.92	0.75
1:A:294:GLU:OE1	1:A:296:TRP:NE1	2.19	0.74
1:E:284:ASN:HB3	2:F:62:ALA:HB1	1.70	0.74
1:C:284:ASN:HB3	2:D:62:ALA:HB1	1.70	0.73
1:A:72:ARG:HG2	1:E:383:GLN:HG3	1.72	0.71
1:A:185:ILE:HD13	1:A:254:HIS:HB2	1.71	0.70
2:D:9:GLU:OE1	2:D:134:ARG:NH2	2.24	0.70
1:E:290:ASP:OD2	1:E:352:ARG:NH1	2.24	0.70
1:G:317:VAL:HG21	1:G:356:GLN:OE1	1.89	0.70
1:C:283:VAL:N	5:C:601:HOH:O	2.25	0.69
1:E:12:PRO:HB2	1:E:15:PRO:HG3	1.74	0.69
1:C:316:GLN:HG2	1:C:360:PHE:HZ	1.58	0.69
1:A:393:MET:HB3	1:A:407:GLU:HG3	1.73	0.68
1:E:318:ASN:HB2	1:E:356:GLN:OE1	1.94	0.68
2:F:37:GLY:HA2	2:F:142:LYS:O	1.94	0.67
1:E:297:TRP:HZ2	1:E:317:VAL:O	1.78	0.66
1:C:191:ARG:NE	1:C:297:TRP:O	2.25	0.66
1:E:297:TRP:CZ2	1:E:317:VAL:O	2.50	0.65
1:C:111:CYS:O	1:C:115:GLN:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:MET:HB3	1:C:407:GLU:HG3	1.79	0.64
1:C:373:VAL:HB	1:E:96:MET:HE1	1.79	0.64
2:D:37:GLY:HA2	2:D:142:LYS:O	1.98	0.64
1:G:111:CYS:O	1:G:115:GLN:HA	1.98	0.63
1:E:317:VAL:CG2	1:E:356:GLN:NE2	2.61	0.63
1:C:130:ARG:NH2	1:C:147:PHE:O	2.32	0.63
2:H:37:GLY:HA2	2:H:142:LYS:O	1.99	0.63
1:A:191:ARG:NE	1:A:297:TRP:O	2.32	0.62
1:A:376:TRP:CE2	1:C:100:ARG:HD2	2.34	0.62
1:A:131:ARG:CD	1:A:145:LYS:HE3	2.29	0.62
1:A:290:ASP:OD2	1:A:352:ARG:NH1	2.31	0.62
1:C:345:ASP:OD2	1:C:353:ARG:NH1	2.32	0.62
1:G:258:ILE:HG23	1:G:300:PRO:HB3	1.82	0.61
1:A:185:ILE:HD12	1:A:249:ASP:HB3	1.82	0.61
1:C:58:ILE:O	1:C:78:ARG:NH1	2.34	0.61
1:E:58:ILE:O	1:E:78:ARG:NH1	2.34	0.60
1:G:77:VAL:HG21	1:G:120:LEU:HD22	1.84	0.60
1:C:379:GLU:OE1	1:E:100:ARG:NH2	2.28	0.59
1:C:231:TRP:O	1:C:232:PHE:HB2	2.02	0.59
2:B:37:GLY:HA2	2:B:142:LYS:O	2.02	0.59
1:G:184:THR:HG21	1:G:247:LYS:HD3	1.83	0.58
1:A:61:PRO:HB3	1:A:80:PRO:HA	1.84	0.58
1:C:22:SER:O	1:C:411:ARG:HG3	2.03	0.58
2:H:97:ASP:HB3	5:H:202:HOH:O	2.03	0.58
1:E:111:CYS:O	1:E:115:GLN:HA	2.04	0.58
1:C:316:GLN:HG2	1:C:360:PHE:CZ	2.39	0.58
1:E:61:PRO:HA	1:E:78:ARG:HG2	1.86	0.58
1:A:91:CYS:SG	1:A:92:ALA:N	2.76	0.57
1:C:351:GLN:OE1	1:C:355:ILE:HG13	2.04	0.57
1:A:251:LYS:NZ	5:A:607:HOH:O	2.36	0.57
1:A:318:ASN:HB2	1:A:356:GLN:NE2	2.20	0.57
1:E:138:LYS:HG2	1:E:139:VAL:O	2.04	0.56
1:A:383:GLN:HG3	1:C:72:ARG:HG2	1.86	0.56
1:C:290:ASP:OD2	1:C:352:ARG:NH1	2.39	0.56
1:G:284:ASN:HB3	2:H:62:ALA:HB1	1.86	0.56
1:A:111:CYS:O	1:A:115:GLN:HA	2.05	0.56
1:G:158:LYS:HG3	1:G:172:HIS:ND1	2.21	0.56
1:G:304:MET:HE1	1:G:314:GLN:HG3	1.88	0.56
1:G:107:LYS:NZ	5:G:602:HOH:O	2.34	0.56
1:C:38:ARG:HB3	1:C:421:MET:HE3	1.87	0.56
1:E:102:ARG:NH2	2:D:117:ASP:OD1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:HB3	2:B:62:ALA:HB1	1.87	0.55
1:E:77:VAL:HG21	1:E:120:LEU:HD22	1.88	0.55
1:A:228:LEU:HD13	1:C:113:TYR:HA	1.88	0.55
1:A:376:TRP:CZ2	1:C:100:ARG:HD2	2.42	0.55
2:F:22:ASP:OD1	2:F:84:HIS:ND1	2.40	0.54
1:C:383:GLN:HG3	1:E:72:ARG:HG2	1.90	0.54
1:G:246:LEU:CD2	1:G:257:MET:HG2	2.35	0.54
2:D:122:ILE:HD11	2:F:122:ILE:HD11	1.90	0.54
1:E:97:ARG:HD2	1:E:100:ARG:NH2	2.22	0.54
1:A:297:TRP:HZ2	1:A:317:VAL:O	1.91	0.53
1:G:217:GLU:OE2	1:G:414:TYR:OH	2.17	0.53
1:E:148:LYS:HG2	1:E:150:GLU:OE2	2.09	0.53
1:C:12:PRO:HB2	1:C:15:PRO:HG3	1.91	0.53
1:E:393:MET:HB3	1:E:407:GLU:HG3	1.91	0.52
1:A:135:GLN:OE1	1:A:140:ASN:ND2	2.39	0.52
2:H:79:PRO:HB2	2:H:116:TYR:CE2	2.45	0.52
1:C:181:LEU:HD23	1:C:185:ILE:HG22	1.90	0.52
1:C:377:SER:OG	1:E:96:MET:CE	2.56	0.51
1:C:214:LEU:HD21	1:C:381:PHE:HE2	1.75	0.51
1:C:257:MET:O	1:C:303:VAL:HA	2.11	0.51
1:C:376:TRP:CE2	1:E:100:ARG:HD2	2.46	0.51
1:C:307:ILE:HB	1:C:311:VAL:HG12	1.92	0.51
1:A:97:ARG:HD3	5:A:626:HOH:O	2.11	0.51
1:G:323:ARG:HB3	1:G:335:PHE:CZ	2.46	0.51
2:H:80:TYR:CD2	2:H:113:ARG:HG3	2.46	0.51
1:A:78:ARG:HH22	1:A:84:ILE:HD11	1.75	0.50
1:A:297:TRP:CZ2	1:A:317:VAL:O	2.64	0.50
1:C:111:CYS:O	1:C:115:GLN:CA	2.59	0.50
1:C:22:SER:O	1:C:22:SER:OG	2.28	0.50
1:A:134:LYS:HA	1:A:139:VAL:HA	1.94	0.50
1:G:245:GLU:HB3	1:G:402:ASP:HA	1.93	0.50
1:G:146:ASP:OD1	1:G:146:ASP:N	2.44	0.49
1:A:317:VAL:CG2	1:A:356:GLN:HE21	2.22	0.49
2:H:22:ASP:OD1	2:H:84:HIS:ND1	2.44	0.49
1:E:134:LYS:HA	1:E:138:LYS:O	2.13	0.48
2:H:97:ASP:HB2	2:H:99:ASP:OD1	2.12	0.48
1:G:318:ASN:HB2	1:G:356:GLN:OE1	2.13	0.48
1:G:196:ARG:NH1	1:G:344:ASP:OD2	2.38	0.48
2:F:126:GLY:HA3	2:F:148:TYR:HA	1.96	0.48
1:C:96:MET:HE2	1:C:112:PRO:HD2	1.96	0.48
1:C:257:MET:HE3	1:C:409:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TRP:HB2	1:C:298:GLY:HA2	1.96	0.47
1:G:258:ILE:HG13	1:G:303:VAL:HG22	1.96	0.47
2:F:30:PRO:HG3	2:F:64:ILE:HG22	1.96	0.47
1:A:403:HIS:CG	1:C:140:ASN:HB3	2.50	0.47
2:D:58:LEU:HD13	2:D:64:ILE:HA	1.97	0.47
1:C:181:LEU:HA	1:C:254:HIS:HD2	1.79	0.47
1:G:130:ARG:HH21	1:G:131:ARG:HE	1.63	0.47
2:F:30:PRO:O	2:F:61:LYS:HE3	2.15	0.47
5:C:608:HOH:O	1:E:152:HIS:HD2	1.98	0.47
1:E:202:GLY:HA3	2:F:53:LEU:HB3	1.97	0.47
1:A:138:LYS:NZ	1:A:139:VAL:HG12	2.30	0.46
1:G:61:PRO:HB3	1:G:80:PRO:HA	1.98	0.46
1:A:95:GLY:O	1:E:380:GLY:HA3	2.16	0.46
1:E:91:CYS:SG	1:E:92:ALA:N	2.89	0.46
1:E:91:CYS:SG	1:E:118:TYR:OH	2.61	0.46
1:C:323:ARG:HB3	1:C:335:PHE:CZ	2.51	0.46
1:G:75:ILE:O	1:G:86:VAL:HA	2.16	0.46
1:C:318:ASN:HB2	1:C:356:GLN:OE1	2.16	0.46
1:E:257:MET:HE3	1:E:409:LEU:HD12	1.98	0.46
2:F:58:LEU:HD13	2:F:64:ILE:HA	1.97	0.46
1:E:257:MET:O	1:E:303:VAL:HA	2.15	0.45
1:C:345:ASP:CG	1:C:353:ARG:HH12	2.18	0.45
1:E:284:ASN:H	2:F:66:ASP:CG	2.20	0.45
1:A:97:ARG:HD2	1:A:100:ARG:NH2	2.32	0.45
1:C:394:GLY:HA2	1:E:141:GLY:HA2	1.98	0.45
1:E:38:ARG:NH1	1:E:421:MET:O	2.50	0.45
1:G:84:ILE:O	1:G:159:VAL:HG11	2.16	0.45
1:G:111:CYS:O	1:G:115:GLN:CA	2.63	0.45
2:D:79:PRO:HB2	2:D:116:TYR:CZ	2.51	0.45
1:A:393:MET:CE	1:C:129:PHE:HB2	2.47	0.45
1:E:54:LEU:HB2	1:E:57:GLU:HG3	1.98	0.45
1:E:414:TYR:O	1:E:418:ARG:HG3	2.17	0.45
2:B:123:PHE:HZ	2:B:156:SER:O	1.99	0.45
1:G:418:ARG:NH2	1:G:423:GLU:O	2.46	0.44
1:A:414:TYR:O	1:A:418:ARG:HG3	2.18	0.44
1:C:391:ILE:O	1:C:411:ARG:HD2	2.17	0.44
1:A:297:TRP:HB2	1:A:298:GLY:HA2	2.00	0.44
1:E:96:MET:HE3	1:E:96:MET:HB2	1.91	0.44
2:H:98:ALA:N	5:H:202:HOH:O	2.36	0.44
1:A:111:CYS:O	1:A:115:GLN:CA	2.66	0.44
1:A:229:HIS:CD2	1:A:366:VAL:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:TRP:O	1:C:19:GLY:N	2.50	0.44
1:E:251:LYS:HE2	1:E:251:LYS:HA	2.00	0.44
1:A:318:ASN:HB2	1:A:356:GLN:HE22	1.81	0.44
1:C:61:PRO:HB3	1:C:80:PRO:HA	2.00	0.43
1:A:163:GLY:O	1:A:193:PHE:HB3	2.18	0.43
1:C:93:HIS:HB3	3:C:501:FES:S2	2.58	0.43
1:G:369:ASP:O	1:G:373:VAL:HG13	2.18	0.43
1:G:405:VAL:HG12	1:G:405:VAL:O	2.19	0.43
1:C:299:GLY:H	1:C:300:PRO:HD2	1.83	0.43
1:C:380:GLY:HA3	1:E:95:GLY:O	2.18	0.43
1:G:244:SER:CB	1:G:404:MET:HG3	2.49	0.43
1:C:15:PRO:HB2	1:C:28:TRP:CE2	2.53	0.43
1:E:68:VAL:HG11	1:E:326:GLN:HB3	2.00	0.43
1:A:391:ILE:HG22	1:A:407:GLU:OE1	2.19	0.43
1:A:77:VAL:HG21	1:A:120:LEU:HD22	2.00	0.43
1:A:323:ARG:HB3	1:A:335:PHE:CZ	2.53	0.43
2:B:80:TYR:CZ	2:B:159:TYR:HD2	2.37	0.43
2:F:80:TYR:CD1	2:F:113:ARG:HG3	2.54	0.43
2:F:123:PHE:HZ	2:F:156:SER:O	2.01	0.43
1:E:111:CYS:O	1:E:115:GLN:CA	2.67	0.43
1:E:135:GLN:N	1:E:138:LYS:O	2.41	0.43
1:E:136:ASP:HA	1:E:137:GLY:HA2	1.74	0.43
2:B:28:LYS:NZ	5:B:207:HOH:O	2.52	0.43
1:C:414:TYR:O	1:C:418:ARG:HG3	2.18	0.42
1:C:308:PHE:HA	1:C:309:PRO:HA	1.78	0.42
1:G:97:ARG:HD2	1:G:100:ARG:NH2	2.34	0.42
1:C:43:LEU:HA	1:C:48:HIS:CE1	2.54	0.42
1:C:205:ARG:HD2	2:D:45:GLU:OE2	2.20	0.42
1:C:251:LYS:HD3	1:C:416:TYR:HE1	1.83	0.42
1:G:220:LYS:HB3	1:G:409:LEU:HB2	2.01	0.42
2:H:79:PRO:HB2	2:H:116:TYR:CZ	2.54	0.42
1:C:42:ARG:HH11	1:C:421:MET:HA	1.85	0.42
1:C:102:ARG:NH2	2:B:116:TYR:O	2.52	0.42
1:E:46:ALA:HA	1:E:171:ASP:HB2	2.02	0.42
1:E:307:ILE:HB	1:E:311:VAL:HG12	2.00	0.42
1:G:202:GLY:HA3	2:H:53:LEU:HB3	2.00	0.42
1:A:96:MET:HA	1:E:377:SER:HA	2.01	0.42
1:G:84:ILE:HG21	1:G:166:VAL:HG11	2.02	0.42
2:H:43:PRO:HG3	2:H:148:TYR:OH	2.19	0.42
1:G:308:PHE:HA	1:G:309:PRO:HA	1.79	0.42
1:A:100:ARG:NH2	1:E:379:GLU:OE1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LEU:HB2	1:C:57:GLU:HG3	2.01	0.41
1:G:214:LEU:HD21	1:G:381:PHE:HE2	1.84	0.41
1:G:246:LEU:HB3	1:G:409:LEU:HD11	2.02	0.41
1:A:136:ASP:HA	1:A:137:GLY:HA2	1.78	0.41
1:G:219:ILE:HG13	1:G:312:ILE:HD13	2.02	0.41
2:F:29:TRP:CE2	2:F:160:PRO:HB3	2.55	0.41
2:F:79:PRO:HB2	2:F:116:TYR:CZ	2.55	0.41
1:A:380:GLY:HA3	1:C:95:GLY:O	2.20	0.41
1:C:136:ASP:HA	1:C:137:GLY:HA2	1.75	0.41
1:C:351:GLN:O	1:C:352:ARG:C	2.57	0.41
1:G:32:ARG:NH2	1:G:34:ASP:OD2	2.32	0.41
2:F:113:ARG:HB2	2:F:123:PHE:HB2	2.03	0.41
1:C:199:LYS:HB3	1:C:199:LYS:HE3	1.85	0.41
1:A:57:GLU:OE1	1:A:203:TYR:OH	2.25	0.41
1:A:100:ARG:HD2	1:E:376:TRP:CE2	2.55	0.41
1:C:68:VAL:HG11	1:C:326:GLN:HB3	2.02	0.41
1:A:129:PHE:O	1:A:142:GLY:HA2	2.21	0.41
1:A:144:PRO:HB2	1:A:146:ASP:OD1	2.20	0.41
1:C:138:LYS:HD2	1:C:138:LYS:HA	1.80	0.41
1:E:258:ILE:HG23	1:E:300:PRO:HB3	2.03	0.41
1:E:375:GLU:O	1:E:379:GLU:HG3	2.21	0.41
1:G:375:GLU:O	1:G:379:GLU:HG3	2.20	0.41
1:C:312:ILE:HB	1:C:323:ARG:HB2	2.03	0.41
1:E:138:LYS:HE3	1:E:140:ASN:OD1	2.20	0.41
1:G:66:ARG:NH2	1:G:100:ARG:O	2.53	0.41
2:D:18:ALA:HB1	2:D:84:HIS:HB2	2.02	0.41
1:E:349:TRP:O	1:E:353:ARG:HG3	2.22	0.41
1:A:46:ALA:HA	1:A:171:ASP:HB2	2.02	0.40
1:A:49:TRP:HH2	1:A:158:LYS:HG2	1.86	0.40
1:C:37:LYS:O	1:C:41:GLU:HG2	2.20	0.40
1:C:162:ARG:NE	1:C:186:LEU:HD11	2.37	0.40
2:B:18:ALA:HB1	2:B:84:HIS:HB2	2.03	0.40
2:B:71:VAL:HG13	2:B:158:ILE:HG23	2.02	0.40
1:E:347:GLU:O	1:E:351:GLN:HG2	2.21	0.40
1:G:304:MET:HE2	1:G:314:GLN:HA	2.03	0.40
1:G:347:GLU:O	1:G:351:GLN:HG2	2.21	0.40
2:D:22:ASP:OD1	2:D:84:HIS:ND1	2.52	0.40
1:C:260:THR:HA	1:C:301:THR:HB	2.03	0.40
2:H:30:PRO:HG3	2:H:64:ILE:HG22	2.04	0.40
1:A:392:GLU:O	1:C:144:PRO:HD3	2.21	0.40
1:G:17:TRP:CE2	1:G:418:ARG:HD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:O	1:C:131:ARG:NH1[6_554]	2.19	0.01

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	377/442 (85%)	359 (95%)	17 (4%)	1 (0%)	41 64
1	C	377/442 (85%)	360 (96%)	16 (4%)	1 (0%)	41 64
1	E	377/442 (85%)	357 (95%)	19 (5%)	1 (0%)	41 64
1	G	377/442 (85%)	352 (93%)	24 (6%)	1 (0%)	41 64
2	B	159/161 (99%)	156 (98%)	3 (2%)	0	100 100
2	D	159/161 (99%)	154 (97%)	5 (3%)	0	100 100
2	F	159/161 (99%)	154 (97%)	5 (3%)	0	100 100
2	H	159/161 (99%)	155 (98%)	4 (2%)	0	100 100
All	All	2144/2412 (89%)	2047 (96%)	93 (4%)	4 (0%)	47 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	VAL
1	C	317	VAL
1	E	317	VAL
1	G	317	VAL

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	329/380 (87%)	319 (97%)	10 (3%)	41	67
1	C	329/380 (87%)	316 (96%)	13 (4%)	31	57
1	E	329/380 (87%)	323 (98%)	6 (2%)	59	80
1	G	329/380 (87%)	319 (97%)	10 (3%)	41	67
2	B	144/144 (100%)	143 (99%)	1 (1%)	84	94
2	D	144/144 (100%)	140 (97%)	4 (3%)	43	69
2	F	144/144 (100%)	141 (98%)	3 (2%)	53	77
2	H	144/144 (100%)	142 (99%)	2 (1%)	67	85
All	All	1892/2096 (90%)	1843 (97%)	49 (3%)	46	72

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	100	ARG
1	A	113	TYR
1	A	130	ARG
1	A	131	ARG
1	A	231	TRP
1	A	314	GLN
1	A	316	GLN
1	A	317	VAL
1	A	388	ARG
1	C	20	GLU
1	C	24	ARG
1	C	93	HIS
1	C	113	TYR
1	C	130	ARG
1	C	146	ASP
1	C	197	LYS
1	C	199	LYS
1	C	231	TRP
1	C	232	PHE
1	C	316	GLN
1	C	317	VAL
1	C	388	ARG

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Mol	Chain	Res	Type
1	E	100	ARG
1	E	113	TYR
1	E	130	ARG
1	E	231	TRP
1	E	317	VAL
1	E	388	ARG
1	G	14	ASP
1	G	100	ARG
1	G	107	LYS
1	G	113	TYR
1	G	138	LYS
1	G	289	LEU
1	G	317	VAL
1	G	335	PHE
1	G	343	GLU
1	G	388	ARG
2	B	116	TYR
2	D	10	LEU
2	D	90	ARG
2	D	99	ASP
2	D	116	TYR
2	F	10	LEU
2	F	90	ARG
2	F	116	TYR
2	H	10	LEU
2	H	90	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	356	GLN
1	E	316	GLN
1	G	13	GLN
1	G	125	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	FES	A	501	1	0,4,4	-	-	-		
3	FES	C	501	1	0,4,4	-	-	-		
3	FES	E	501	1	0,4,4	-	-	-		
3	FES	G	501	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
3	FES	A	501	1	-	-	0/1/1/1
3	FES	C	501	1	-	-	0/1/1/1
3	FES	E	501	1	-	-	0/1/1/1
3	FES	G	501	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

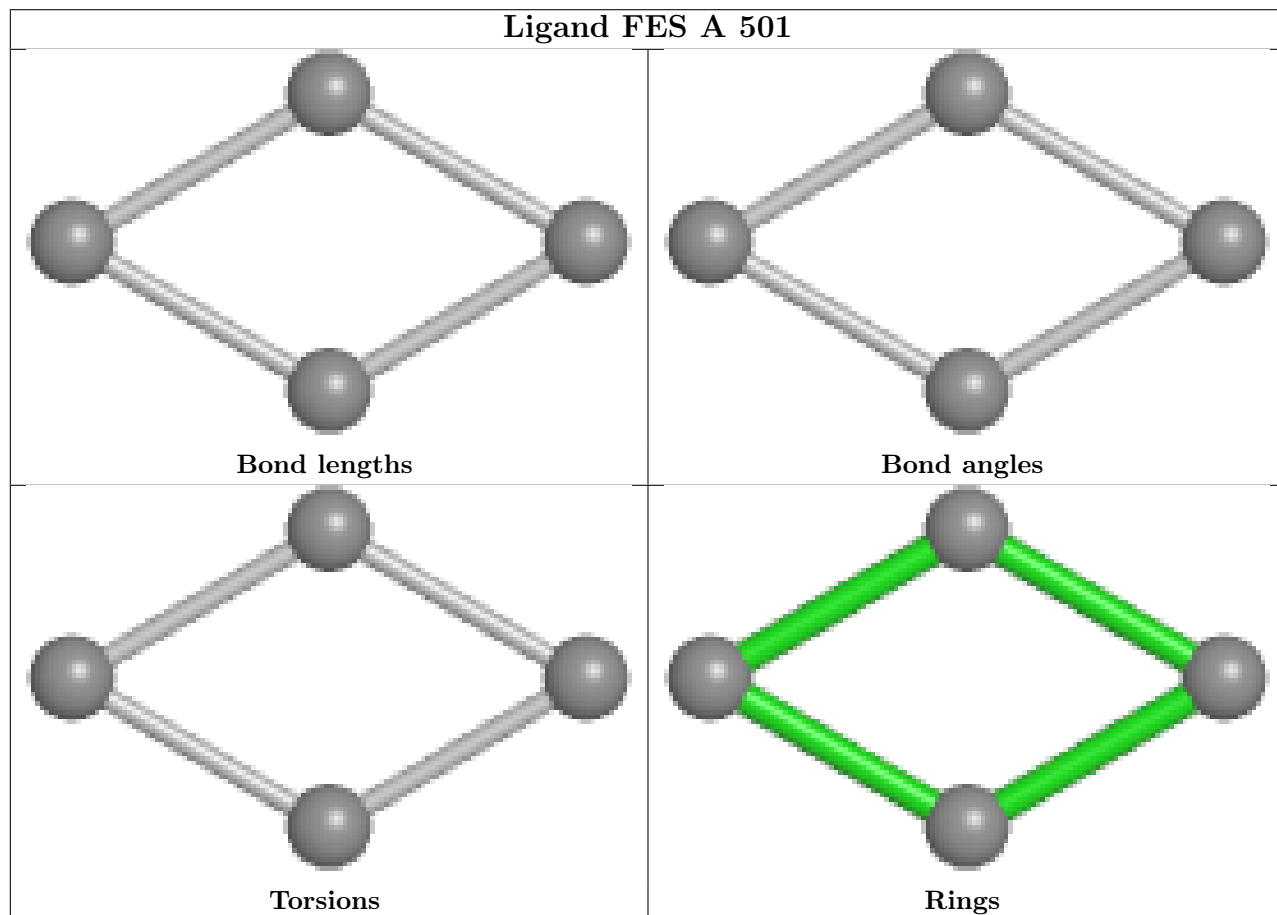
There are no torsion outliers.

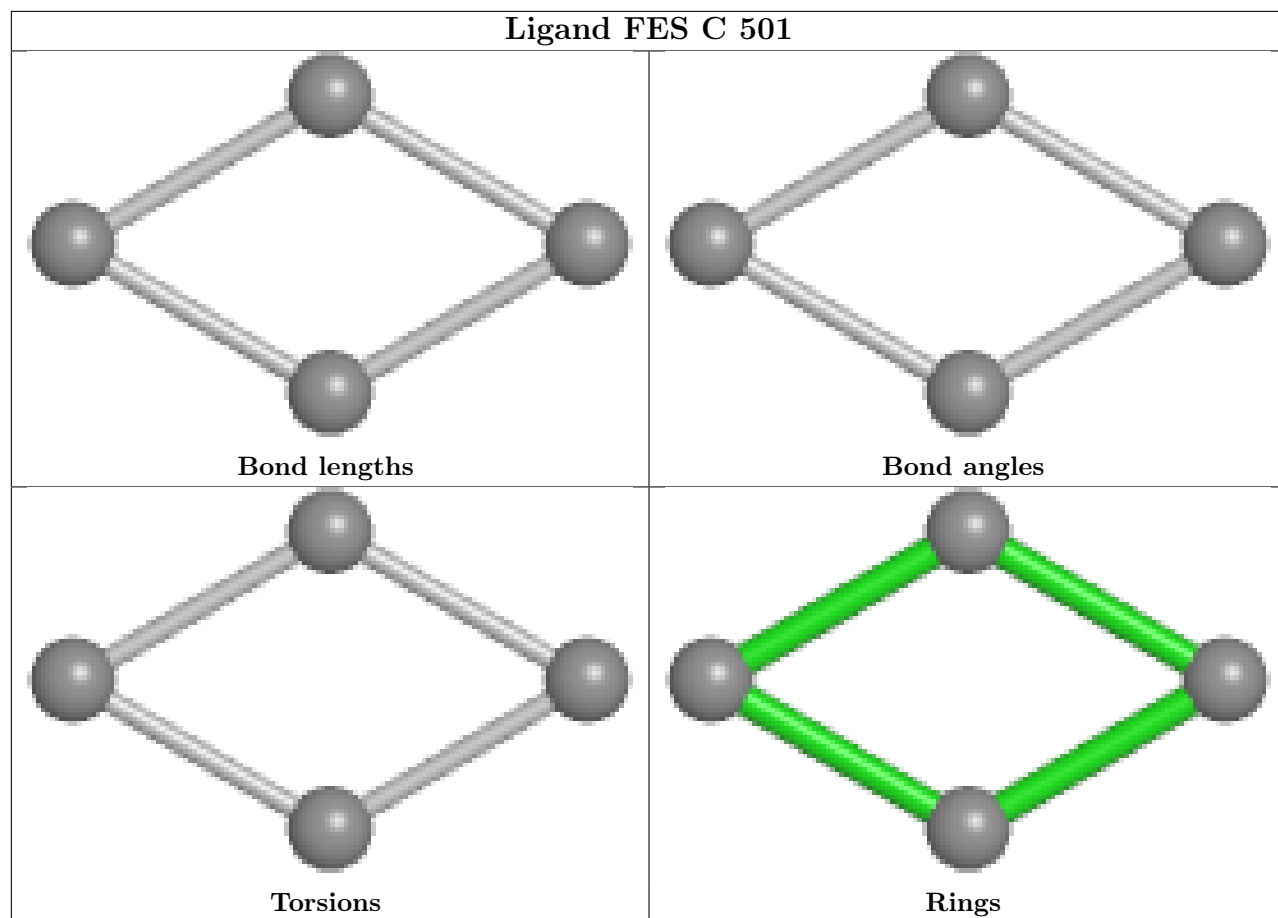
There are no ring outliers.

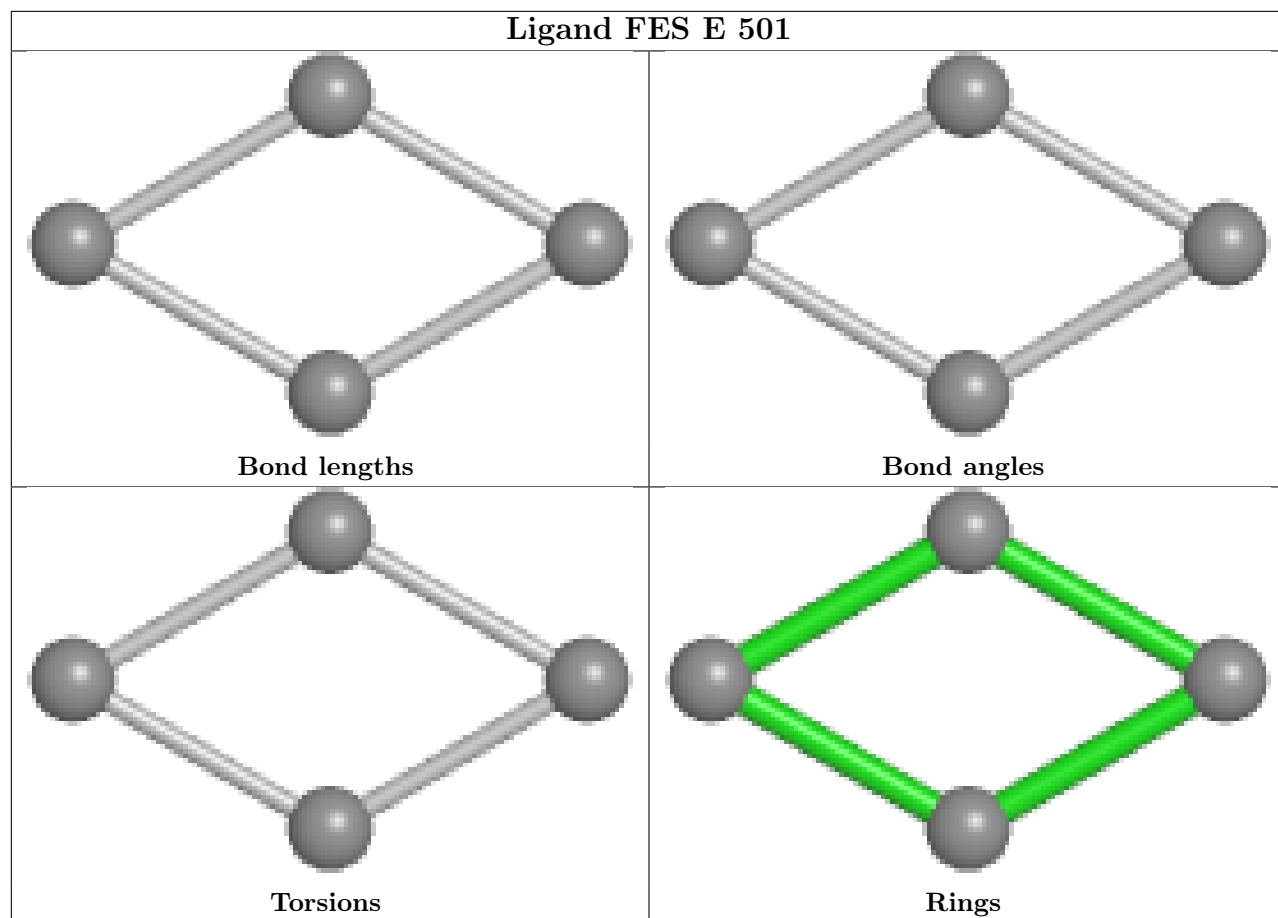
1 monomer is involved in 1 short contact:

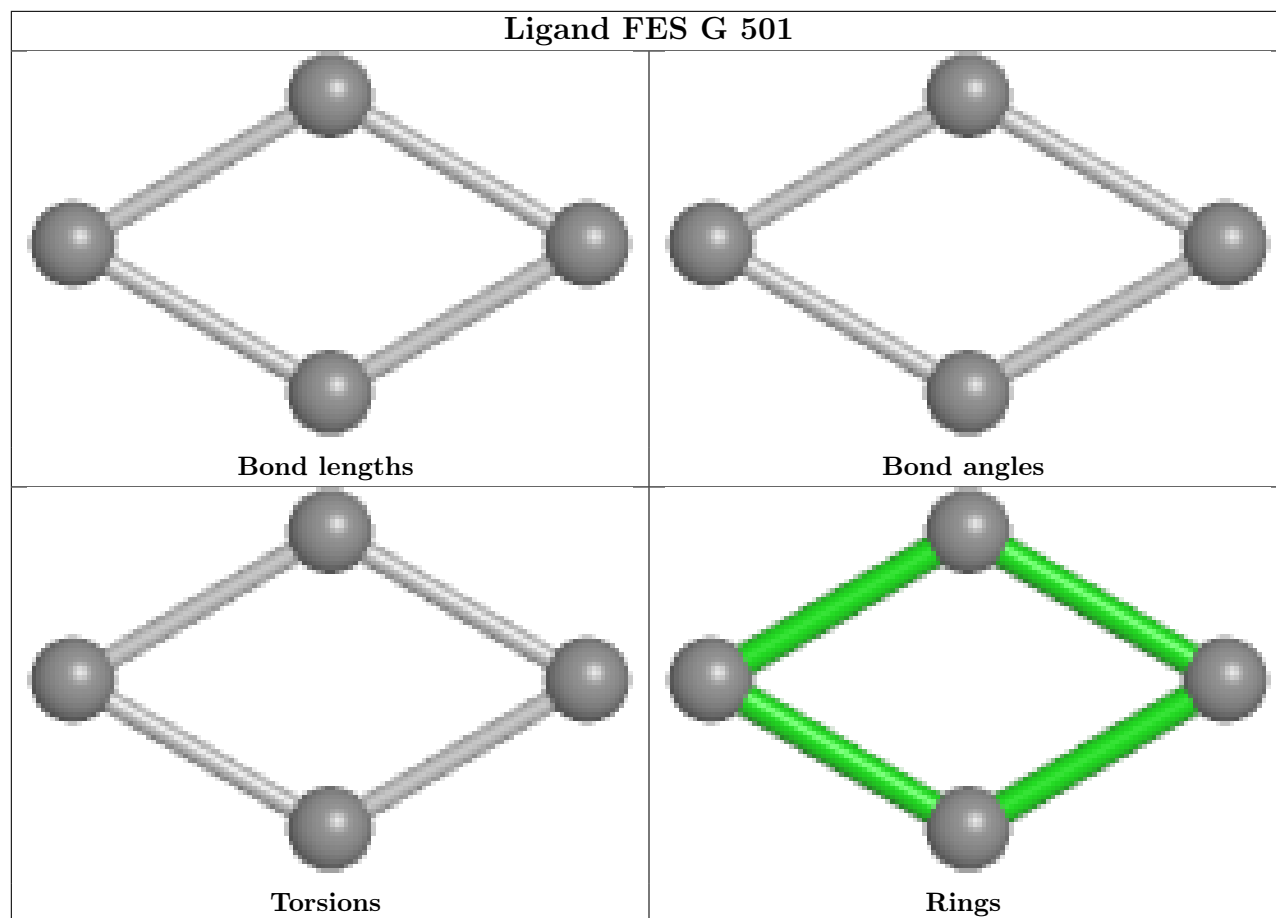
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	FES	1	0

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	383/442 (86%)	-0.05	8 (2%) 63 58	29, 50, 73, 100	0
1	C	383/442 (86%)	0.06	14 (3%) 41 34	35, 57, 82, 126	0
1	E	383/442 (86%)	0.08	19 (4%) 28 23	28, 53, 84, 140	0
1	G	383/442 (86%)	0.21	19 (4%) 28 23	35, 61, 89, 134	0
2	B	161/161 (100%)	-0.23	0 100 100	21, 33, 58, 76	0
2	D	161/161 (100%)	-0.22	1 (0%) 89 88	22, 34, 55, 102	0
2	F	161/161 (100%)	-0.25	1 (0%) 89 88	20, 33, 53, 100	0
2	H	161/161 (100%)	-0.24	0 100 100	21, 33, 55, 87	0
All	All	2176/2412 (90%)	-0.02	62 (2%) 53 46	20, 50, 80, 140	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	5.4
1	E	136	ASP	4.9
1	A	288	LEU	4.8
1	G	136	ASP	4.5
1	C	19	GLY	3.8
1	G	13	GLN	3.6
1	G	134	LYS	3.6
1	G	137	GLY	3.6
1	C	18	PRO	3.5
1	G	133	VAL	3.5
1	A	286	PRO	3.5
1	E	13	GLN	3.5
1	G	289	LEU	3.4
1	E	288	LEU	3.4
1	C	136	ASP	3.3
1	G	298	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	GLN	3.2
1	E	135	GLN	3.1
2	D	99	ASP	3.0
1	C	13	GLN	2.9
1	G	16	LYS	2.9
1	G	404	MET	2.8
1	G	147	PHE	2.8
2	F	99	ASP	2.7
1	C	397	GLU	2.7
1	E	131	ARG	2.7
1	C	289	LEU	2.7
1	C	20	GLU	2.6
1	C	288	LEU	2.6
1	E	127	VAL	2.6
1	E	147	PHE	2.6
1	E	284	ASN	2.5
1	E	286	PRO	2.5
1	E	19	GLY	2.5
1	G	139	VAL	2.3
1	A	13	GLN	2.3
1	E	145	LYS	2.3
1	E	146	ASP	2.3
1	C	287	ARG	2.3
1	E	343	GLU	2.3
1	G	129	PHE	2.2
1	G	19	GLY	2.2
1	C	134	LYS	2.2
1	A	344	ASP	2.2
1	A	135	GLN	2.2
1	C	422	GLY	2.2
1	G	395	GLY	2.2
1	C	23	SER	2.2
1	E	149	LEU	2.2
1	A	131	ARG	2.2
1	E	137	GLY	2.1
1	G	21	GLY	2.1
1	G	138	LYS	2.1
1	E	285	ASP	2.1
1	E	150	GLU	2.1
1	C	286	PRO	2.1
1	G	145	LYS	2.1
1	A	14	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	134	LYS	2.0
1	G	18	PRO	2.0
1	E	347	GLU	2.0
1	G	110	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

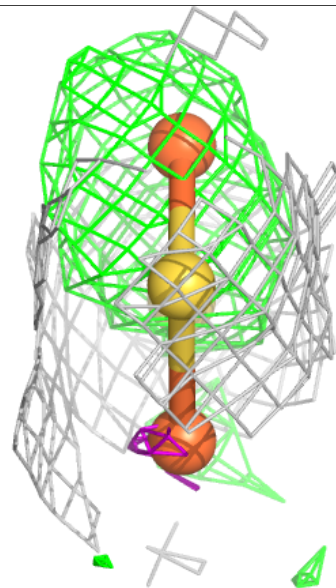
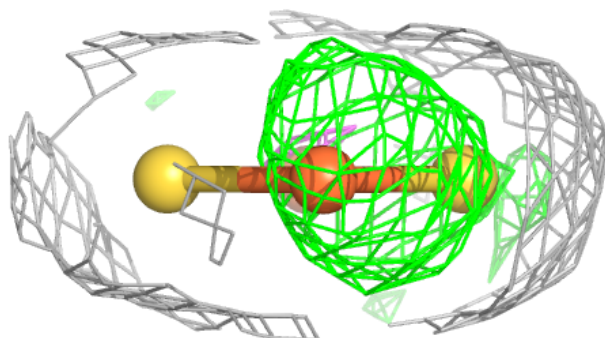
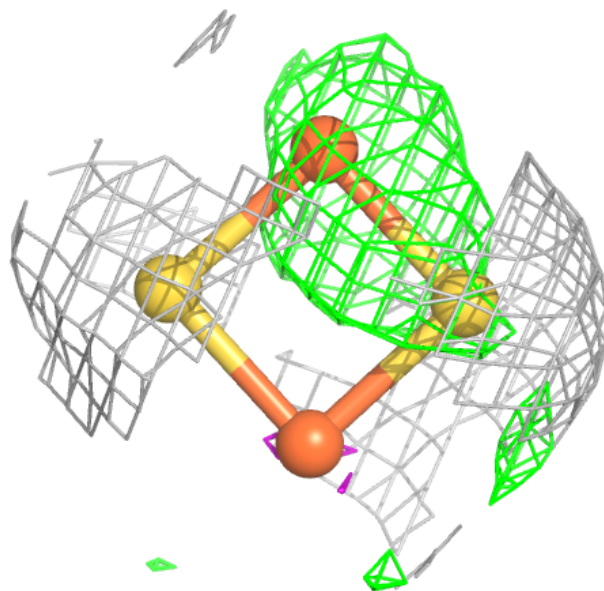
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FES	A	501	4/4	0.93	0.18	37,39,41,73	0
4	FE	C	502	1/1	0.97	0.14	67,67,67,67	0
4	FE	G	502	1/1	0.97	0.13	62,62,62,62	0
3	FES	C	501	4/4	0.98	0.15	34,37,51,52	0
4	FE	E	502	1/1	0.98	0.18	55,55,55,55	0
3	FES	E	501	4/4	0.98	0.15	51,51,52,53	0
3	FES	G	501	4/4	0.99	0.13	32,44,53,54	0
4	FE	A	502	1/1	1.00	0.08	59,59,59,59	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.

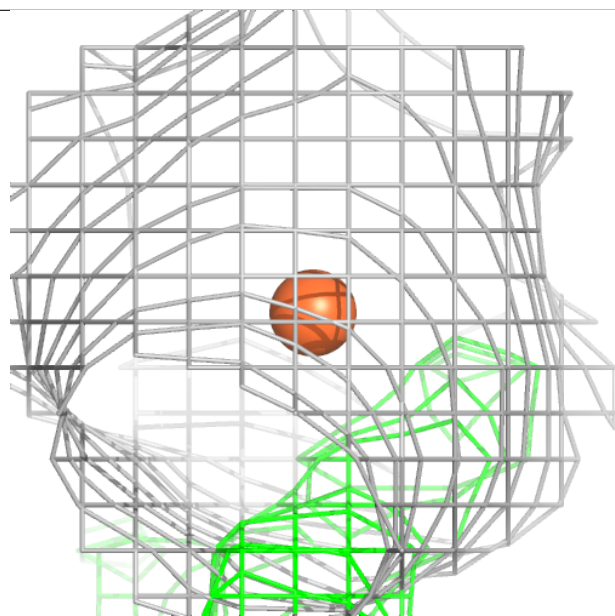
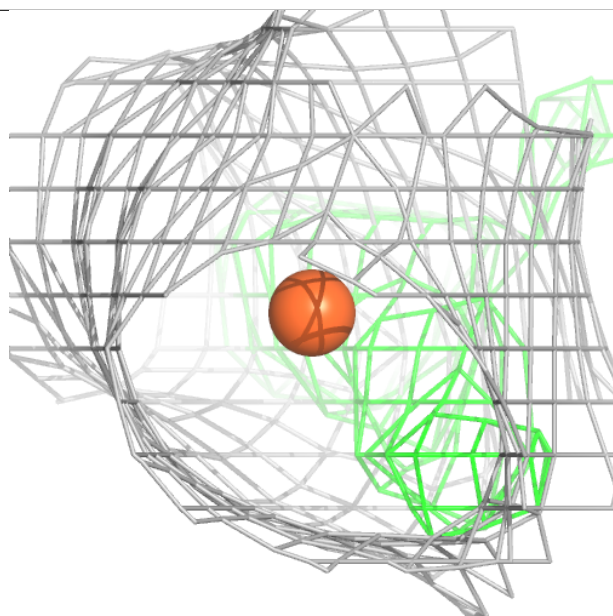
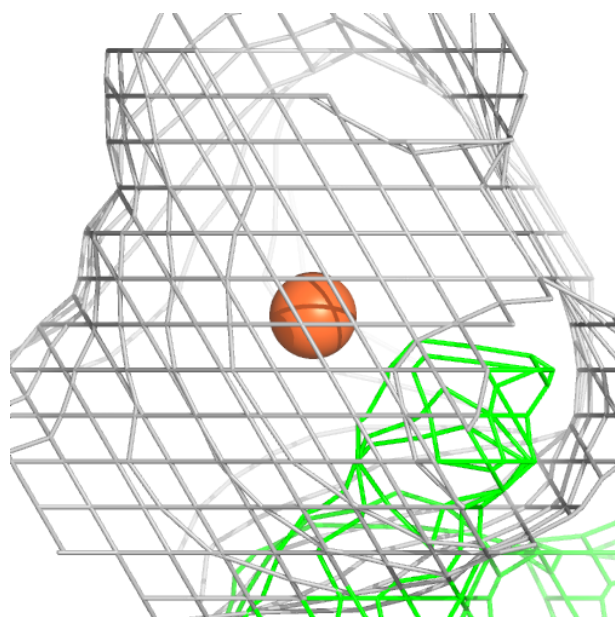
Electron density around FES A 501:

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



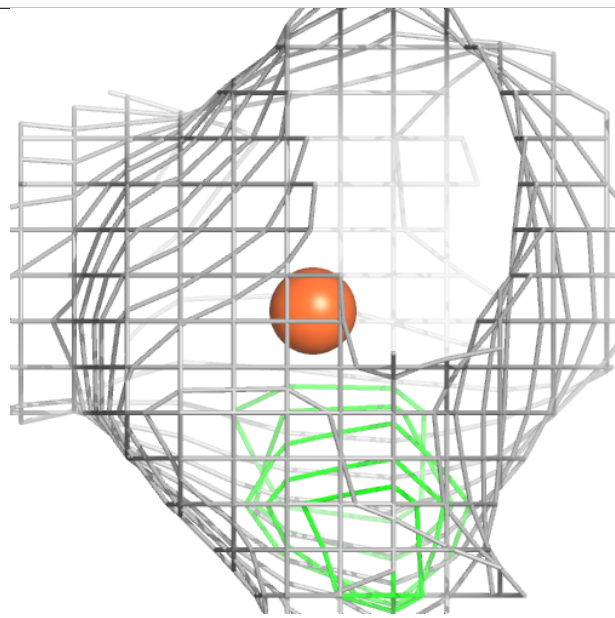
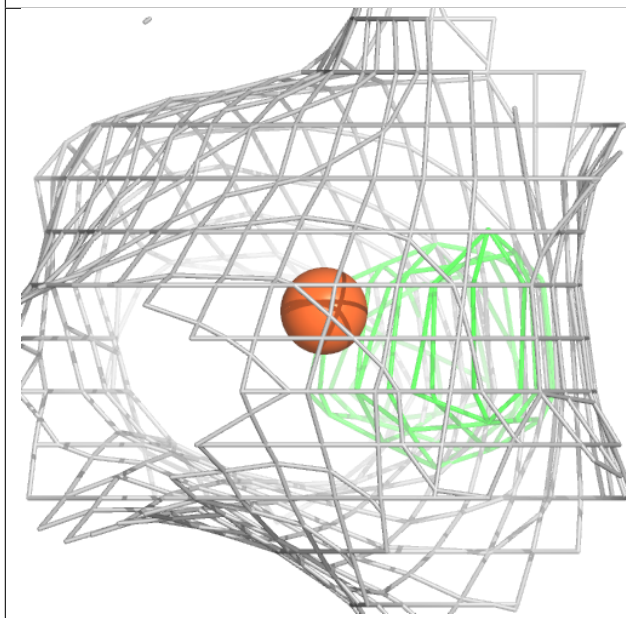
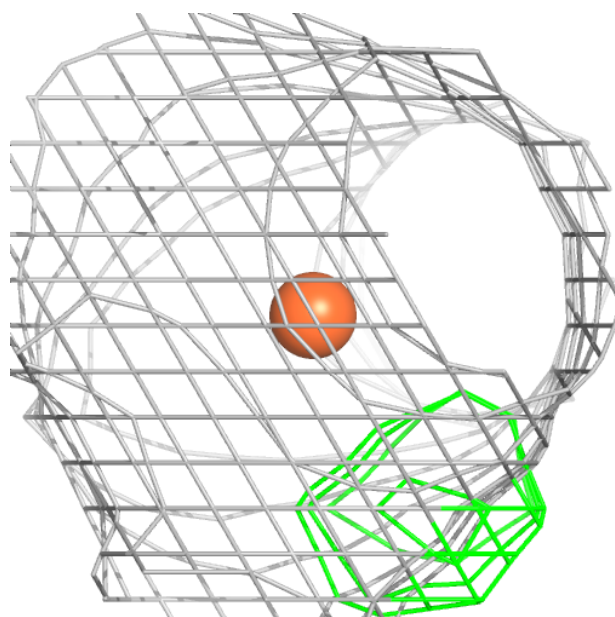
Electron density around FE C 502:

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



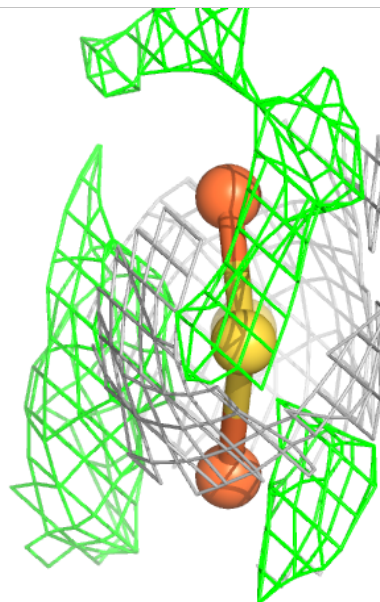
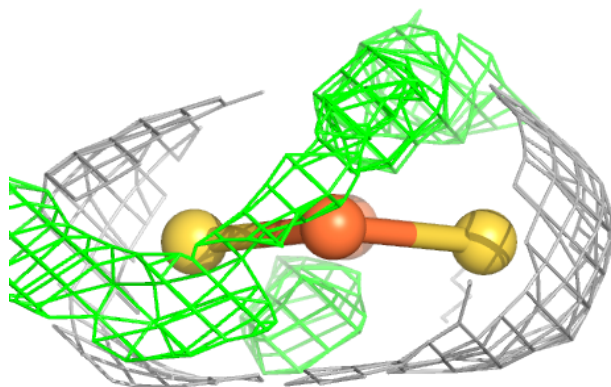
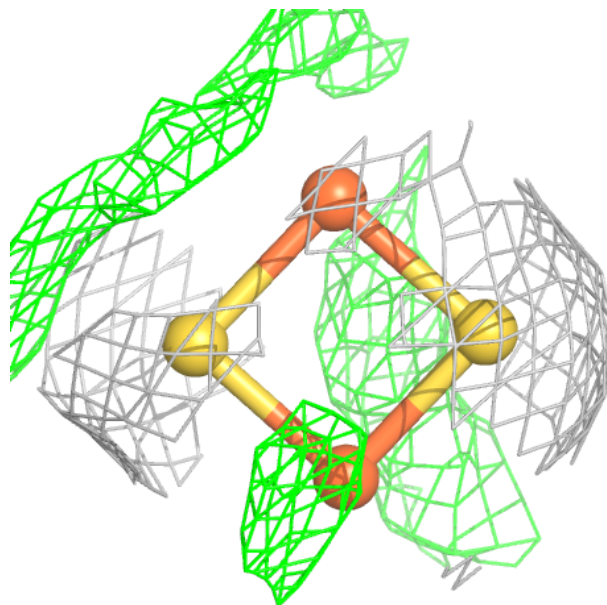
Electron density around FE G 502:

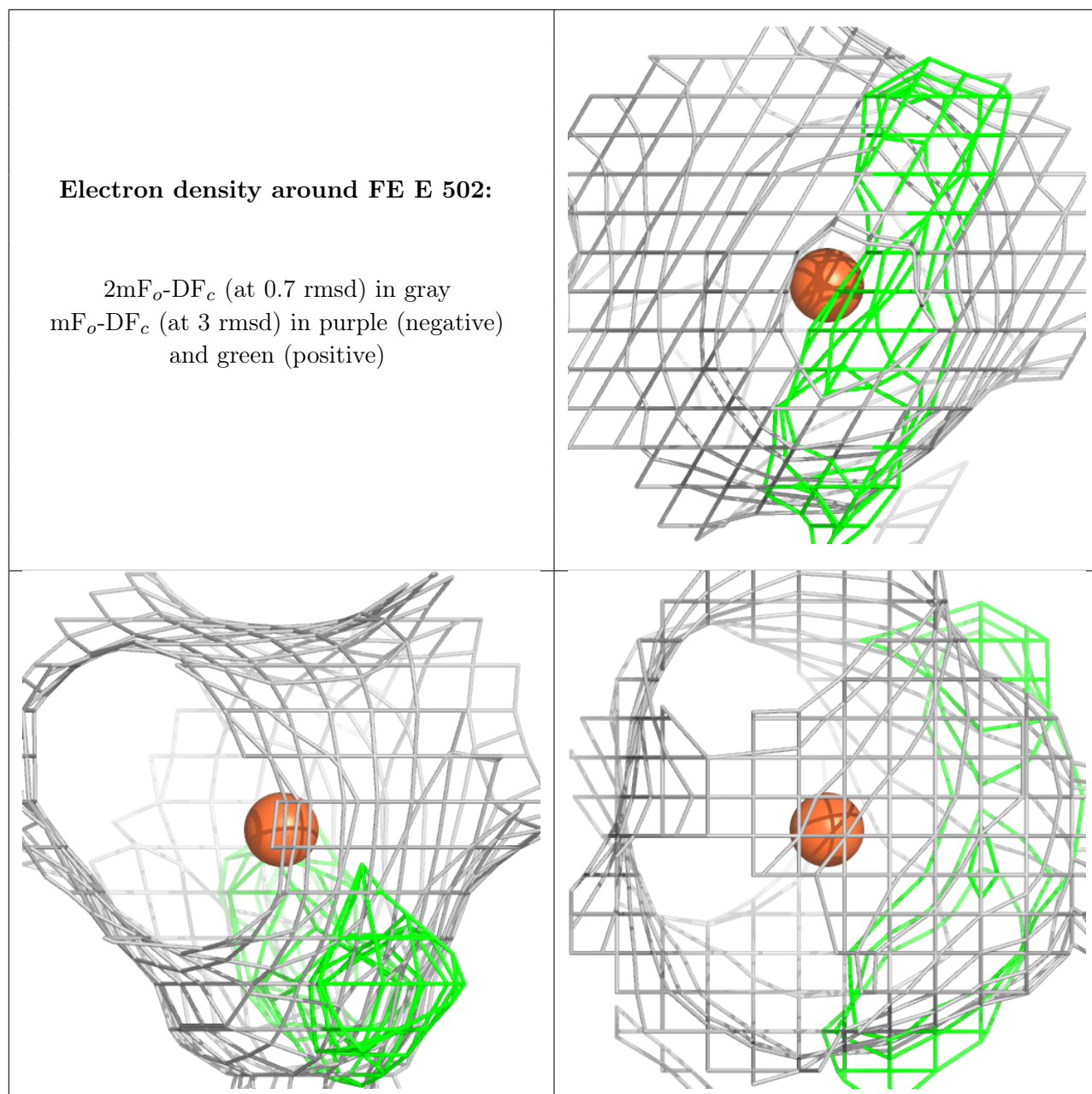
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FES C 501:

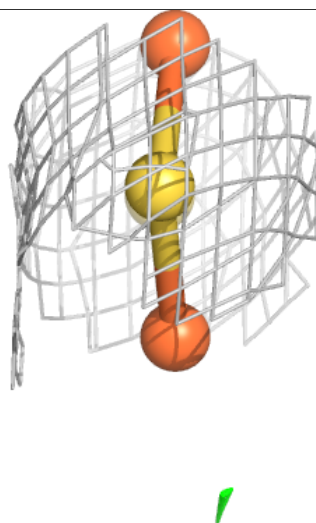
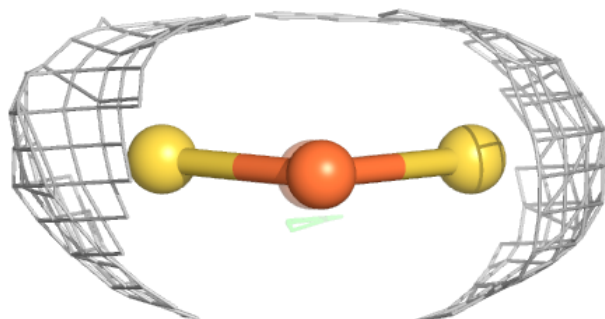
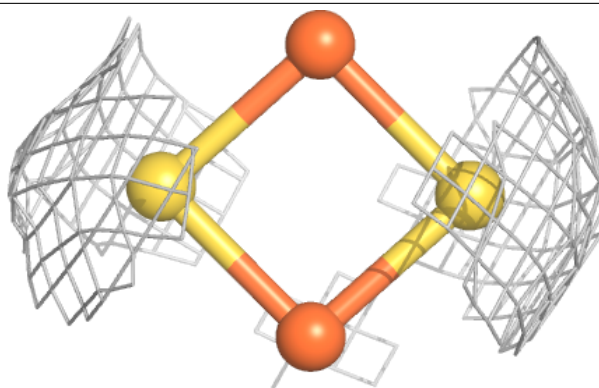
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





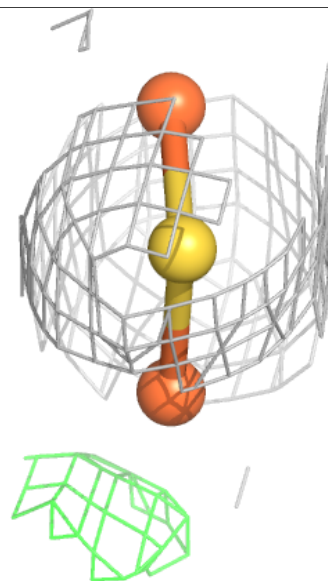
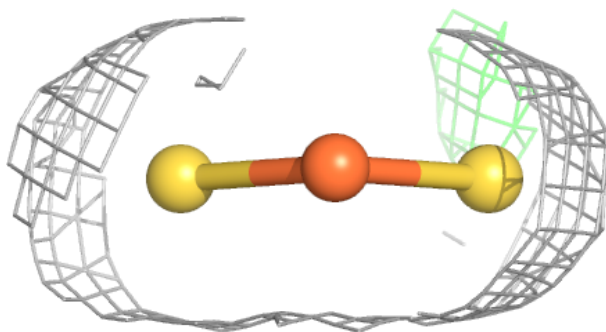
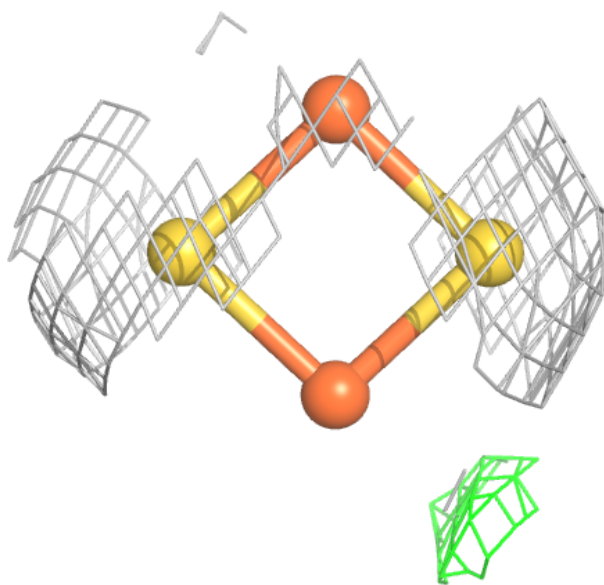
Electron density around FES E 501:

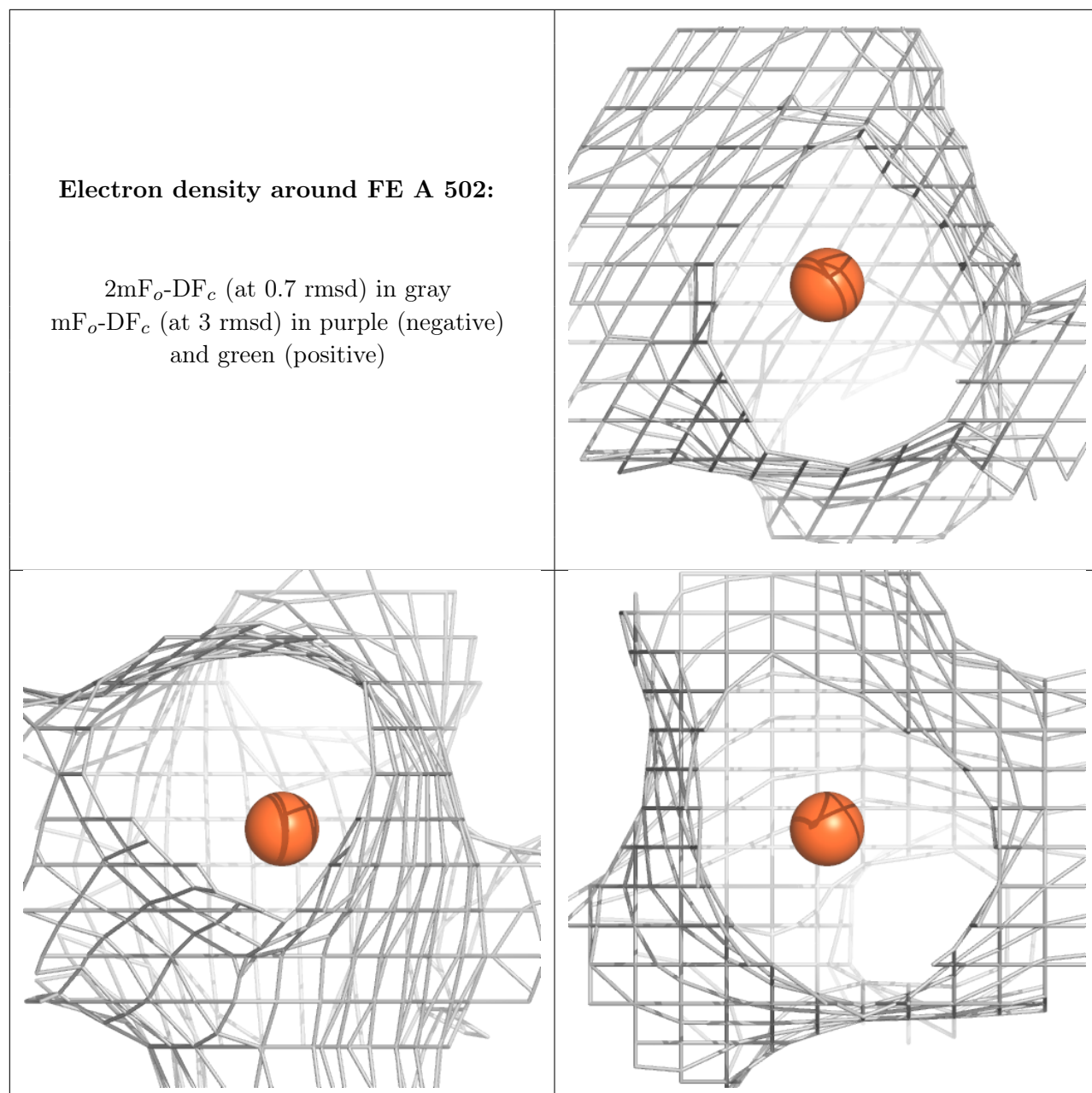
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FES G 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.