Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 01:33 PM JST

PDB ID	:	7V25
Title	:	Crystal Structure of phthalate dioxygenase in complex with phthalate
Authors	:	Mahto, J.K.; Kumar, P.
Deposited on	:	2021-08-07
Resolution	:	2.74 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 (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:

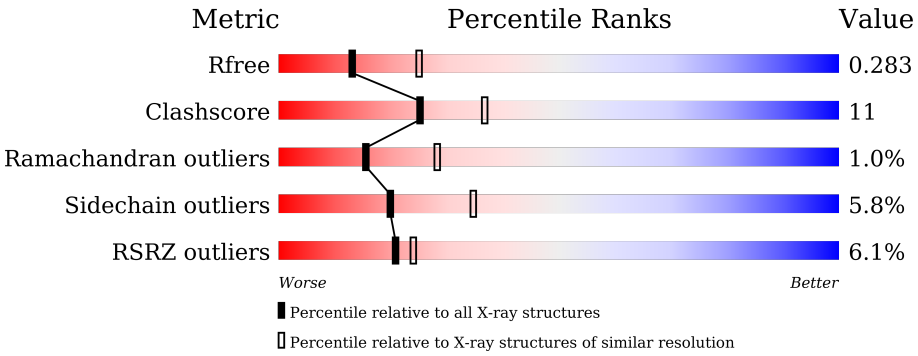
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	439	2% 74% 17% • 7%
1	B	439	5% 72% 22% • •
1	C	439	5% 73% 19% • 7%
1	D	439	3% 68% 22% • 8%
1	E	439	10% 69% 19% • 10%
1	F	439	9% 65% 26% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20542 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.

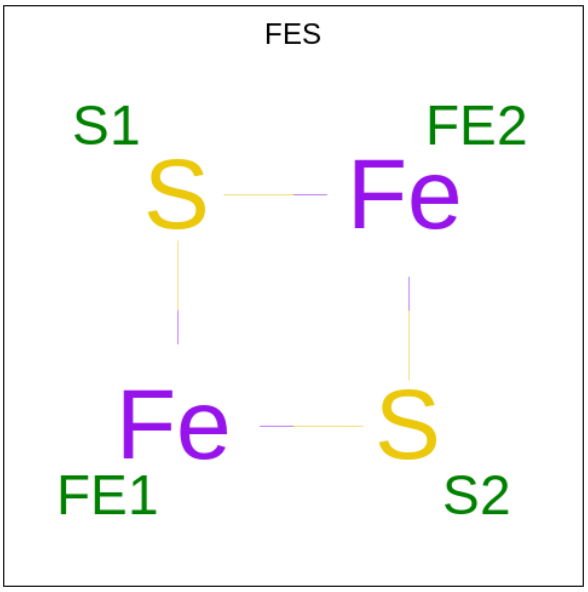
- Molecule 1 is a protein called Rieske (2Fe-2S) domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	423	Total	C	N	O	S	0	0	0
			3323	2094	588	617	24			
1	A	407	Total	C	N	O	S	0	0	0
			3213	2029	567	594	23			
1	C	407	Total	C	N	O	S	0	0	0
			3212	2029	567	593	23			
1	D	405	Total	C	N	O	S	0	0	0
			3203	2023	565	592	23			
1	E	395	Total	C	N	O	S	0	0	0
			3095	1952	545	574	24			
1	F	409	Total	C	N	O	S	0	0	0
			3228	2038	569	597	24			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

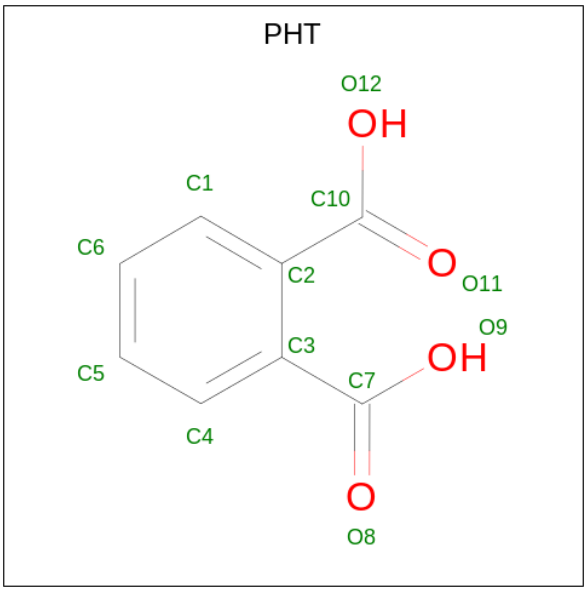
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 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
3	B	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	F	1	Total Fe S 4 2 2	0	0

- Molecule 4 is PHTHALIC ACID (three-letter code: PHT) (formula: $C_8H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 8 4	0	0

- Molecule 5 is water.

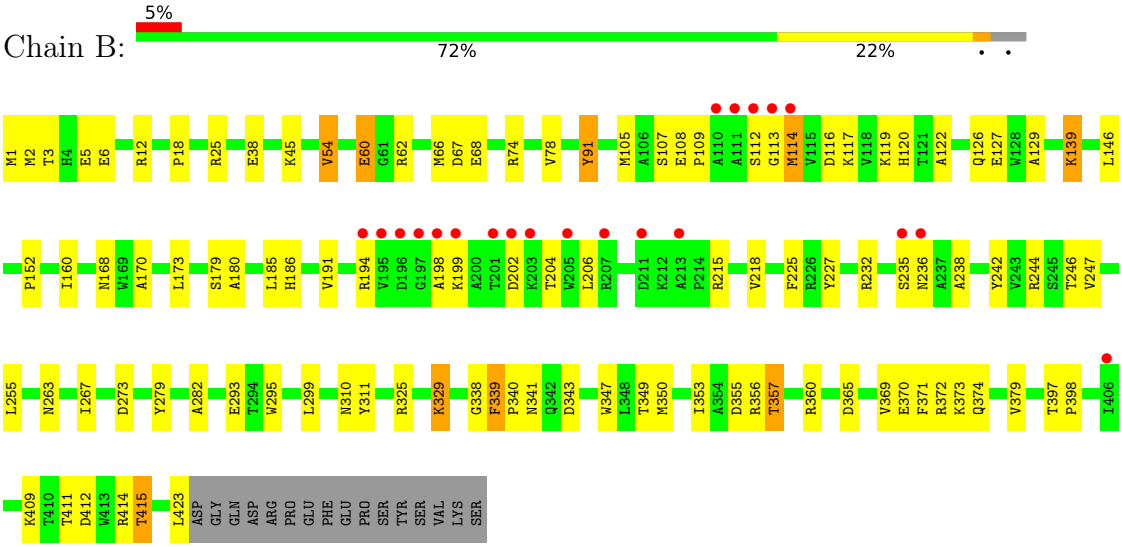
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	208	Total O 208 208	0	0
5	A	204	Total O 204 204	0	0
5	C	208	Total O 208 208	0	0
5	D	198	Total O 198 198	0	0
5	E	200	Total O 200 200	0	0
5	F	208	Total O 208 208	0	0

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.

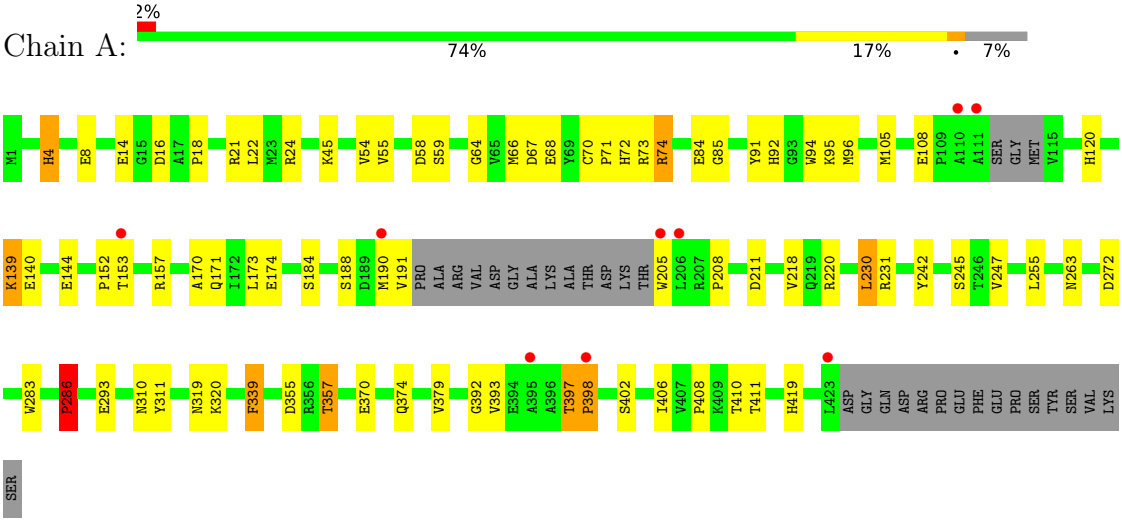
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain B:



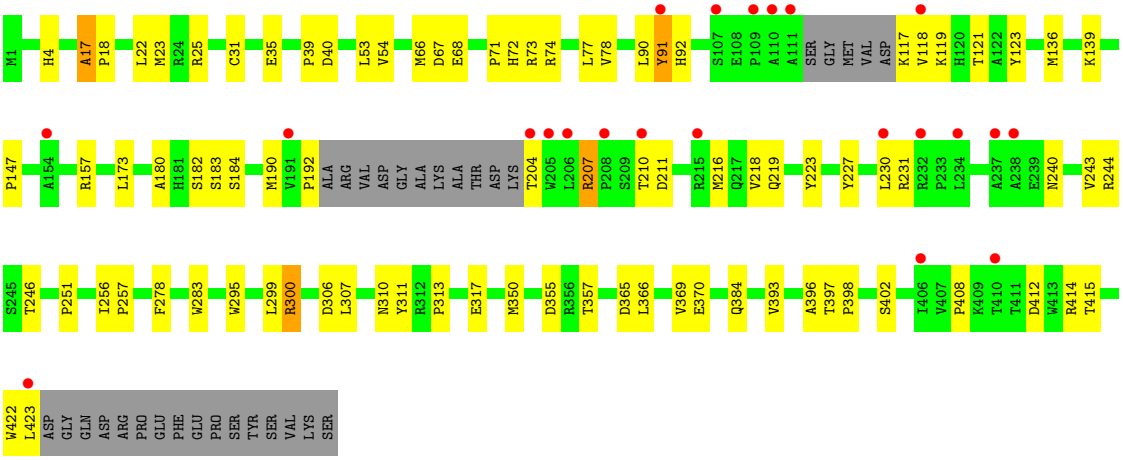
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain A:



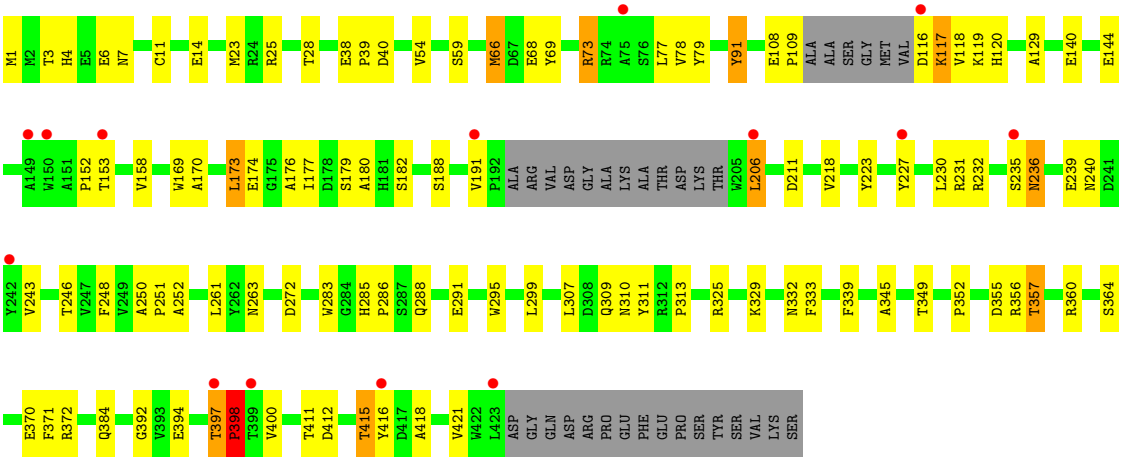
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain C:



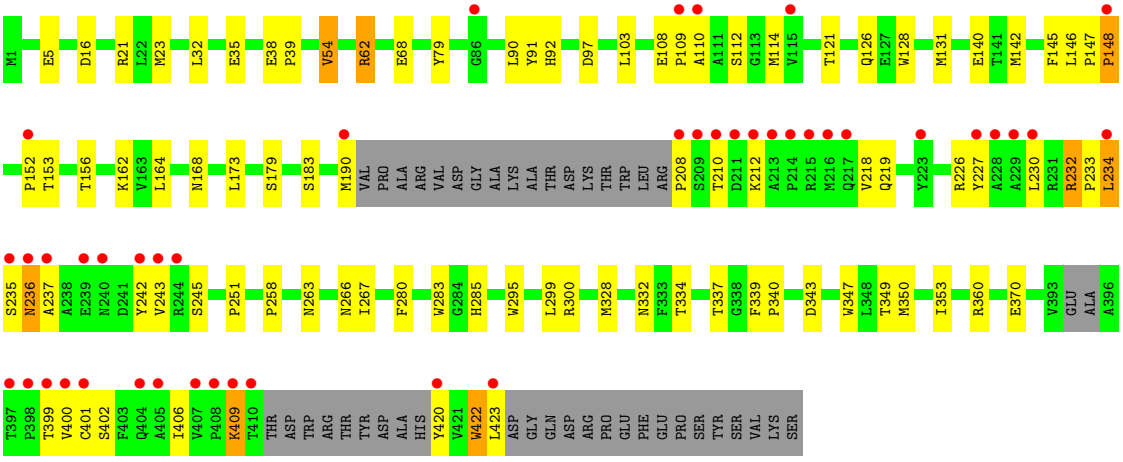
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain D:



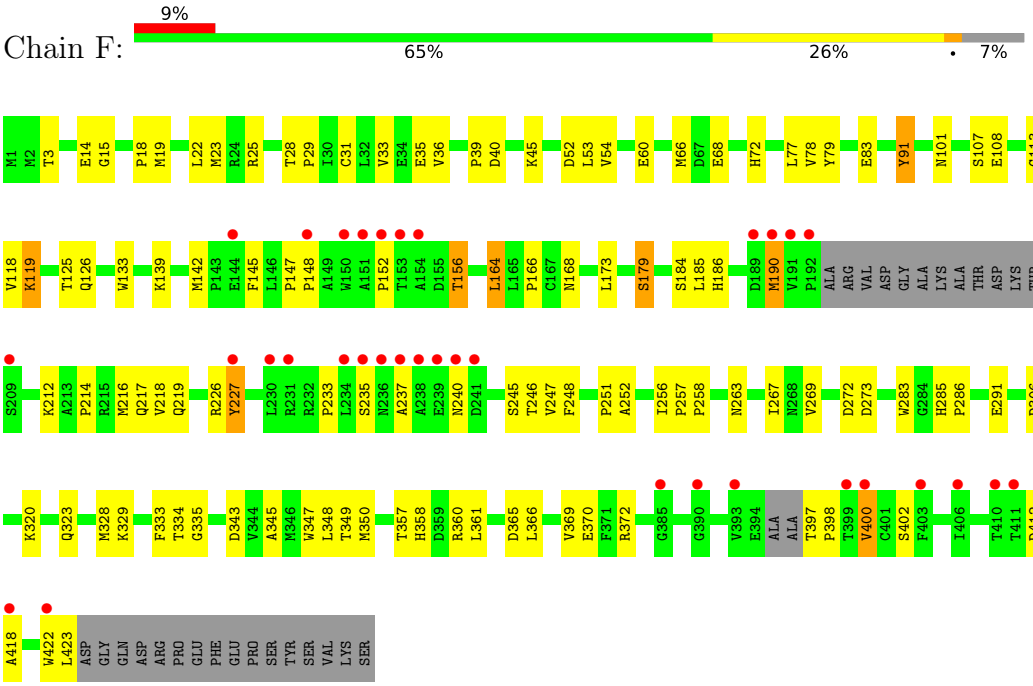
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain E:



• Molecule 1: Rieske (2Fe-2S) domain protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.03Å 122.18Å 162.94Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	159.88 – 2.74 159.88 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.0 (159.88-2.74) 98.0 (159.88-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.283 0.207 , 0.283	Depositor DCC
R_{free} test set	4388 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	20542	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: PHT, FE2, 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	0.35	0/3301	0.74	1/4497 (0.0%)
1	B	0.33	0/3414	0.75	1/4652 (0.0%)
1	C	0.33	0/3301	0.72	1/4498 (0.0%)
1	D	0.34	0/3292	0.72	0/4485
1	E	0.34	0/3176	0.73	0/4320
1	F	0.32	0/3317	0.72	0/4518
All	All	0.34	0/19801	0.73	3/26970 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	PHE	CB-CA-C	5.72	121.84	110.40
1	B	329	LYS	CB-CA-C	5.50	121.40	110.40
1	C	300	ARG	CG-CD-NE	-5.03	101.23	111.80

There are no chirality outliers.

There are no planarity outliers.

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	3213	0	3096	47	0
1	B	3323	0	3210	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3212	0	3097	61	0
1	D	3203	0	3084	75	0
1	E	3095	0	2993	64	0
1	F	3228	0	3110	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
3	F	4	0	0	0	0
4	B	12	0	4	0	0
5	A	204	0	0	9	0
5	B	208	0	0	6	0
5	C	208	0	0	8	0
5	D	198	0	0	9	0
5	E	200	0	0	8	0
5	F	208	0	0	16	0
All	All	20542	0	18594	404	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 11.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:MET:HE1	1:B:372:ARG:HD3	1.22	1.16
1:F:397:THR:HB	1:F:398:PRO:HD3	1.31	1.08
1:B:66:MET:CE	1:B:120:HIS:HD2	1.70	1.03
1:B:66:MET:HE3	1:B:120:HIS:HD2	1.27	0.99
1:E:54:VAL:HG22	1:E:68:GLU:HA	1.45	0.98
1:E:218:VAL:HG11	1:E:370:GLU:HG2	1.46	0.97
1:F:397:THR:CB	1:F:398:PRO:HD3	1.97	0.93
1:C:216:MET:HE2	1:C:227:TYR:HE2	1.35	0.90
1:E:420:TYR:HE1	1:E:422:TRP:HE3	1.23	0.85
1:B:66:MET:CE	1:B:120:HIS:CD2	2.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:HB	1:B:398:PRO:HD2	1.59	0.84
1:D:230:LEU:CD2	1:D:243:VAL:HG22	2.08	0.83
1:C:218:VAL:HG11	1:C:370:GLU:HG2	1.59	0.83
1:A:211:ASP:HB3	1:A:231:ARG:HB3	1.61	0.82
1:D:397:THR:HB	1:D:398:PRO:HD2	1.62	0.81
1:B:218:VAL:HG11	1:B:370:GLU:HG2	1.62	0.81
1:D:230:LEU:HD23	1:D:243:VAL:HG22	1.62	0.80
1:C:4:HIS:HB3	5:C:672:HOH:O	1.82	0.79
1:B:360:ARG:NH2	1:F:118:VAL:HG13	1.98	0.78
1:F:173:LEU:HD21	1:F:248:PHE:HE1	1.48	0.78
1:B:66:MET:HE3	1:B:120:HIS:CD2	2.17	0.78
1:D:118:VAL:HG13	1:E:360:ARG:NH2	1.98	0.78
1:F:23:MET:CE	1:F:251:PRO:HB2	2.15	0.76
1:B:360:ARG:HH22	1:F:118:VAL:HG13	1.50	0.76
1:D:307:LEU:HD23	1:D:313:PRO:HA	1.68	0.76
1:C:216:MET:CE	1:C:227:TYR:HE2	1.99	0.75
1:F:212:LYS:O	1:F:214:PRO:HD3	1.87	0.75
1:E:54:VAL:CG2	1:E:68:GLU:HA	2.17	0.74
1:E:420:TYR:HE1	1:E:422:TRP:CE3	2.05	0.74
1:C:216:MET:HE2	1:C:227:TYR:CE2	2.20	0.74
1:B:235:SER:HB2	5:B:754:HOH:O	1.89	0.73
1:D:356:ARG:HG2	1:D:372:ARG:NH2	2.03	0.72
1:E:334:THR:HG23	5:E:643:HOH:O	1.89	0.72
1:F:397:THR:CB	1:F:398:PRO:CD	2.67	0.72
1:F:54:VAL:HG23	1:F:68:GLU:HA	1.72	0.72
1:B:54:VAL:HG22	1:B:68:GLU:HA	1.72	0.72
1:C:412:ASP:HB3	1:C:415:THR:HG22	1.73	0.71
1:D:4:HIS:HB3	5:D:735:HOH:O	1.91	0.71
1:B:412:ASP:O	1:B:415:THR:HG22	1.90	0.70
1:C:310:ASN:O	1:C:311:TYR:HB2	1.90	0.70
1:F:218:VAL:HG12	1:F:219:GLN:N	2.07	0.70
1:F:117:LYS:HA	5:F:684:HOH:O	1.91	0.70
1:E:263:ASN:HB2	1:E:283:TRP:CE2	2.27	0.69
1:F:173:LEU:HD21	1:F:248:PHE:CE1	2.27	0.69
1:F:412:ASP:O	1:F:415:THR:HG22	1.92	0.69
1:F:263:ASN:HB2	1:F:283:TRP:CE2	2.28	0.68
1:D:7:ASN:OD1	1:D:356:ARG:HD2	1.93	0.68
1:F:23:MET:HE1	1:F:251:PRO:HB2	1.75	0.68
1:B:2:MET:CE	1:B:372:ARG:HD3	2.14	0.67
1:E:328:MET:HA	1:E:332:ASN:O	1.95	0.67
1:F:416:TYR:CE2	1:F:418:ALA:HB2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:HB	1:B:255:LEU:HB2	1.77	0.66
1:A:16:ASP:HB3	5:A:705:HOH:O	1.94	0.66
1:D:416:TYR:CE2	1:D:418:ALA:HB2	2.31	0.66
1:F:101:ASN:HD22	1:F:119:LYS:HD2	1.60	0.65
1:A:393:VAL:HG12	5:A:723:HOH:O	1.97	0.65
1:F:101:ASN:ND2	1:F:119:LYS:HD2	2.11	0.65
1:C:54:VAL:CG2	1:C:68:GLU:HA	2.27	0.64
1:E:285:HIS:HD2	1:E:423:LEU:HB2	1.62	0.64
1:A:397:THR:HB	1:A:398:PRO:HD2	1.79	0.64
1:D:295:TRP:CE2	1:D:299:LEU:HD11	2.33	0.64
1:D:23:MET:CE	1:D:251:PRO:HB2	2.27	0.64
1:F:306:ASP:HB3	1:F:315:ARG:HH12	1.63	0.63
1:D:412:ASP:O	1:D:415:THR:HG22	1.99	0.63
1:D:416:TYR:HE2	1:D:418:ALA:HB2	1.63	0.63
1:E:233:PRO:HG3	1:E:242:TYR:HB2	1.81	0.63
1:F:179:SER:HB2	1:F:227:TYR:OH	1.99	0.63
1:F:54:VAL:CG2	1:F:68:GLU:HA	2.29	0.62
1:E:128:TRP:HH2	1:E:153:THR:HA	1.64	0.62
1:E:232:ARG:HD2	1:E:237:ALA:HB1	1.79	0.62
1:A:263:ASN:HB2	1:A:283:TRP:CE2	2.33	0.62
1:E:401:CYS:SG	1:E:420:TYR:HB3	2.40	0.62
1:E:230:LEU:HD23	1:E:243:VAL:HG22	1.82	0.62
1:D:310:ASN:O	1:D:311:TYR:HB2	1.99	0.62
1:B:185:LEU:HD23	1:B:186:HIS:CE1	2.34	0.62
1:C:216:MET:CE	1:C:227:TYR:CE2	2.79	0.61
1:F:23:MET:HE2	1:F:251:PRO:HB2	1.81	0.61
1:E:218:VAL:CG1	1:E:370:GLU:HG2	2.26	0.61
1:F:343:ASP:HB3	1:F:347:TRP:CZ2	2.36	0.61
1:A:16:ASP:HB2	5:A:626:HOH:O	2.00	0.60
1:D:285:HIS:CD2	1:D:286:PRO:HD2	2.36	0.60
1:B:139:LYS:HG3	5:B:767:HOH:O	2.01	0.60
1:E:97:ASP:HB3	1:E:103:LEU:HD21	1.83	0.60
1:B:107:SER:HB2	1:C:180:ALA:HB1	1.82	0.60
1:F:19:MET:O	1:F:23:MET:HG3	2.02	0.60
1:F:166:PRO:HD2	1:F:348:LEU:HD21	1.84	0.60
1:C:118:VAL:HG12	1:F:360:ARG:HH21	1.68	0.59
1:F:416:TYR:HE2	1:F:418:ALA:HB2	1.68	0.59
1:A:14:GLU:OE2	1:A:272:ASP:HB2	2.02	0.59
1:C:219:GLN:HE21	1:C:414:ARG:HD3	1.67	0.59
1:C:240:ASN:OD1	1:C:408:PRO:HA	2.01	0.59
1:F:218:VAL:HG11	1:F:370:GLU:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:VAL:CG1	1:F:219:GLN:N	2.64	0.59
1:D:397:THR:HB	1:D:398:PRO:CD	2.33	0.58
1:F:45:LYS:HE2	1:F:68:GLU:OE1	2.02	0.58
1:B:329:LYS:HG3	5:F:744:HOH:O	2.03	0.58
1:E:183:SER:HB3	1:E:212:LYS:HA	1.85	0.58
1:B:5:GLU:HG2	5:B:680:HOH:O	2.04	0.58
1:C:54:VAL:HG22	1:C:68:GLU:HA	1.86	0.58
1:C:365:ASP:O	1:C:369:VAL:HG23	2.04	0.57
1:B:397:THR:HB	1:B:398:PRO:CD	2.33	0.57
1:A:144:GLU:HB3	5:A:758:HOH:O	2.05	0.57
1:F:173:LEU:HD22	1:F:252:ALA:HA	1.86	0.57
1:D:23:MET:HE2	1:D:251:PRO:HB2	1.85	0.57
1:D:1:MET:CG	5:D:746:HOH:O	2.52	0.57
1:F:33:VAL:O	1:F:36:VAL:HG22	2.04	0.57
1:B:355:ASP:OD1	1:B:357:THR:HB	2.03	0.57
1:C:54:VAL:HG21	1:C:77:LEU:HB2	1.87	0.57
1:D:230:LEU:HD22	1:D:243:VAL:HG22	1.87	0.57
1:D:140:GLU:HB2	5:D:737:HOH:O	2.04	0.57
1:D:355:ASP:OD1	1:D:357:THR:HB	2.05	0.56
1:C:211:ASP:HB3	1:C:231:ARG:HG2	1.85	0.56
1:F:258:PRO:HB3	1:F:263:ASN:HA	1.88	0.56
1:D:39:PRO:O	1:D:40:ASP:HB2	2.05	0.56
1:F:139:LYS:HG3	5:F:774:HOH:O	2.04	0.56
1:F:156:THR:HG23	1:F:422:TRP:HZ3	1.71	0.56
1:D:384:GLN:HA	1:D:384:GLN:NE2	2.20	0.56
1:E:235:SER:O	1:E:236:ASN:HB2	2.05	0.56
1:F:115:VAL:HG11	5:F:786:HOH:O	2.06	0.56
1:B:114:MET:HA	1:B:117:LYS:HG2	1.88	0.55
1:B:60:GLU:HG3	1:B:62:ARG:NH1	2.21	0.55
1:C:397:THR:HB	1:C:398:PRO:HD2	1.88	0.55
1:B:236:ASN:C	1:B:238:ALA:H	2.09	0.55
5:B:710:HOH:O	1:C:317:GLU:HG2	2.07	0.55
1:D:1:MET:HG2	5:D:746:HOH:O	2.07	0.55
1:E:232:ARG:HD2	1:E:237:ALA:CB	2.36	0.55
1:E:263:ASN:HB2	1:E:283:TRP:NE1	2.22	0.55
1:F:54:VAL:HG21	1:F:77:LEU:HB2	1.88	0.55
1:F:218:VAL:CG1	1:F:219:GLN:H	2.20	0.55
1:F:237:ALA:HB3	5:F:751:HOH:O	2.05	0.55
1:A:18:PRO:HB2	1:A:379:VAL:HG22	1.89	0.55
1:D:356:ARG:HG2	1:D:372:ARG:CZ	2.36	0.55
1:F:218:VAL:HG23	1:F:366:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:MET:O	1:F:217:GLN:HG2	2.07	0.54
1:A:230:LEU:HD23	1:A:230:LEU:N	2.22	0.54
1:A:218:VAL:HG11	1:A:370:GLU:HG2	1.90	0.54
1:F:125:THR:HA	1:F:133:TRP:O	2.07	0.54
1:F:397:THR:HB	1:F:398:PRO:CD	2.19	0.54
1:B:152:PRO:HB3	1:B:398:PRO:HB3	1.89	0.54
1:A:211:ASP:CB	1:A:231:ARG:HB3	2.34	0.54
1:F:29:PRO:O	1:F:269:VAL:HG21	2.08	0.54
1:B:170:ALA:HB3	1:B:356:ARG:NH2	2.22	0.54
1:C:91:TYR:HE2	1:F:350:MET:CE	2.21	0.54
1:D:261:LEU:HA	1:D:288:GLN:HE21	1.72	0.54
1:E:295:TRP:CE2	1:E:299:LEU:HD11	2.43	0.54
1:D:173:LEU:HD13	1:D:252:ALA:HA	1.90	0.54
1:F:226:ARG:HG2	1:F:247:VAL:HG22	1.90	0.54
1:E:285:HIS:CD2	1:E:423:LEU:HB2	2.43	0.54
1:A:70:CYS:SG	1:A:71:PRO:HD2	2.47	0.53
1:E:235:SER:O	1:E:236:ASN:CB	2.56	0.53
1:B:105:MET:HB2	1:B:108:GLU:HB3	1.91	0.53
1:D:73:ARG:HH11	1:D:73:ARG:HG3	1.72	0.53
1:B:109:PRO:O	1:B:112:SER:HB2	2.09	0.53
1:B:116:ASP:O	1:B:119:LYS:NZ	2.41	0.53
1:F:400:VAL:HG21	5:F:617:HOH:O	2.09	0.53
1:A:73:ARG:O	1:A:74:ARG:HB2	2.09	0.52
1:A:45:LYS:HE2	1:A:68:GLU:OE1	2.09	0.52
1:C:39:PRO:O	1:C:40:ASP:HB2	2.09	0.52
1:D:177:ILE:HG13	1:D:177:ILE:O	2.10	0.52
1:C:92:HIS:HB2	3:C:502:FES:S1	2.50	0.52
1:D:129:ALA:HB1	1:D:158:VAL:HG11	1.91	0.52
1:D:263:ASN:HB2	1:D:283:TRP:CE2	2.44	0.52
1:B:199:LYS:HD2	1:B:202:ASP:OD2	2.10	0.52
1:A:92:HIS:HB2	3:A:502:FES:S2	2.50	0.52
1:C:355:ASP:OD1	1:C:357:THR:HB	2.09	0.52
1:D:69:TYR:O	1:D:120:HIS:HE1	1.92	0.52
1:B:227:TYR:CE1	1:B:246:THR:HB	2.45	0.52
1:D:23:MET:HE3	1:D:251:PRO:HB2	1.91	0.52
1:F:345:ALA:O	1:F:349:THR:HG23	2.10	0.52
1:A:247:VAL:HB	1:A:255:LEU:HD12	1.91	0.51
1:E:62:ARG:HG3	1:E:62:ARG:HH11	1.75	0.51
1:B:54:VAL:HG13	1:B:78:VAL:HG22	1.92	0.51
1:B:202:ASP:HB2	1:B:206:LEU:HD22	1.91	0.51
1:E:16:ASP:O	1:E:21:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:MET:CE	1:F:91:TYR:HE2	2.24	0.51
1:C:91:TYR:HE2	1:F:350:MET:HE1	1.75	0.51
1:A:16:ASP:O	1:A:21:ARG:NH1	2.44	0.51
1:E:179:SER:HB2	1:E:227:TYR:OH	2.11	0.51
1:C:227:TYR:CE1	1:C:246:THR:HB	2.46	0.50
1:B:113:GLY:O	1:B:117:LYS:HE3	2.11	0.50
1:D:345:ALA:O	1:D:349:THR:HG23	2.12	0.50
1:F:113:GLY:N	5:F:604:HOH:O	2.45	0.50
1:B:238:ALA:O	1:B:409:LYS:HE3	2.12	0.50
1:A:208:PRO:HD2	1:A:242:TYR:CZ	2.46	0.50
1:D:179:SER:OG	1:D:231:ARG:NH2	2.45	0.50
1:D:397:THR:CB	1:D:398:PRO:HD2	2.38	0.50
1:F:184:SER:O	1:F:333:PHE:CD2	2.65	0.50
1:A:24:ARG:HD2	5:A:628:HOH:O	2.12	0.50
1:C:90:LEU:HD13	1:F:334:THR:HG22	1.93	0.50
1:A:392:GLY:HA2	5:A:753:HOH:O	2.11	0.50
1:E:210:THR:HB	5:E:682:HOH:O	2.12	0.50
1:A:4:HIS:O	1:A:8:GLU:HG2	2.11	0.49
1:A:22:LEU:C	1:A:22:LEU:HD23	2.32	0.49
1:F:45:LYS:HE3	5:F:772:HOH:O	2.11	0.49
1:F:256:ILE:HD13	1:F:256:ILE:N	2.27	0.49
1:C:397:THR:HB	1:C:398:PRO:CD	2.41	0.49
1:F:60:GLU:HG3	5:F:674:HOH:O	2.12	0.49
1:A:157:ARG:NH1	1:A:286:PRO:O	2.45	0.49
1:E:360:ARG:HG3	1:E:360:ARG:NH1	2.27	0.49
1:C:54:VAL:HG23	1:C:68:GLU:HA	1.95	0.49
1:D:38:GLU:HB2	5:D:742:HOH:O	2.13	0.49
1:F:152:PRO:HA	1:F:398:PRO:CG	2.43	0.49
1:F:400:VAL:HB	5:F:671:HOH:O	2.12	0.49
1:B:12:ARG:HD3	1:B:273:ASP:OD2	2.12	0.49
1:D:360:ARG:NH2	5:D:606:HOH:O	2.46	0.49
1:B:91:TYR:HE2	1:C:350:MET:HE1	1.78	0.48
1:B:126:GLN:HG3	1:B:127:GLU:N	2.28	0.48
1:E:162:LYS:HE3	1:E:164:LEU:CD1	2.43	0.48
1:C:412:ASP:HB3	1:C:415:THR:CG2	2.43	0.48
1:F:323:GLN:NE2	1:F:328:MET:SD	2.87	0.48
1:B:60:GLU:HG3	1:B:62:ARG:HH11	1.78	0.48
1:B:365:ASP:O	1:B:369:VAL:HG23	2.14	0.48
1:E:156:THR:HG1	1:E:422:TRP:HH2	1.60	0.48
1:B:38:GLU:HB2	5:B:678:HOH:O	2.14	0.48
1:B:369:VAL:HG12	1:B:373:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:MET:HG2	1:C:251:PRO:HG3	1.95	0.48
1:D:227:TYR:CE1	1:D:246:THR:HB	2.49	0.48
1:E:162:LYS:HE3	1:E:164:LEU:HD11	1.96	0.48
1:C:192:PRO:HG3	1:C:210:THR:HG22	1.95	0.48
1:C:256:ILE:CG2	1:C:257:PRO:HD2	2.44	0.48
1:F:227:TYR:CE2	1:F:246:THR:HB	2.49	0.48
1:F:18:PRO:HD2	5:F:612:HOH:O	2.13	0.47
1:F:328:MET:HG3	1:F:335:GLY:HA3	1.95	0.47
1:A:55:VAL:HA	1:A:64:GLY:O	2.13	0.47
1:A:374:GLN:NE2	5:A:608:HOH:O	2.47	0.47
1:D:66:MET:HB2	1:D:66:MET:HE3	1.75	0.47
1:D:261:LEU:HB3	1:D:288:GLN:HG2	1.96	0.47
1:F:365:ASP:O	1:F:369:VAL:HG23	2.14	0.47
1:B:339:PHE:N	1:B:340:PRO:CD	2.78	0.47
1:E:168:ASN:HB2	1:E:353:ILE:HG12	1.96	0.47
1:E:218:VAL:HG11	1:E:370:GLU:CG	2.31	0.47
1:D:117:LYS:HB2	1:D:117:LYS:NZ	2.30	0.47
1:E:360:ARG:HG3	1:E:360:ARG:HH11	1.79	0.47
1:F:258:PRO:HD3	1:F:402:SER:OG	2.15	0.47
1:A:355:ASP:OD1	1:A:357:THR:HB	2.14	0.47
1:A:397:THR:CB	1:A:398:PRO:HD2	2.44	0.47
1:E:343:ASP:HB3	1:E:347:TRP:CZ2	2.50	0.47
1:D:291:GLU:OE1	1:F:291:GLU:HG3	2.14	0.47
1:E:126:GLN:HG2	1:E:145:PHE:CG	2.49	0.47
1:F:343:ASP:HB3	1:F:347:TRP:CE2	2.50	0.47
1:B:3:THR:HG23	1:B:6:GLU:OE2	2.15	0.47
1:B:91:TYR:HE2	1:C:350:MET:CE	2.27	0.47
1:D:69:TYR:O	1:D:120:HIS:CE1	2.68	0.47
1:D:173:LEU:HD22	1:D:371:PHE:CE1	2.50	0.47
1:F:101:ASN:HD22	1:F:119:LYS:CD	2.26	0.47
1:F:156:THR:HG23	1:F:422:TRP:CZ3	2.50	0.47
1:B:202:ASP:O	1:B:204:THR:N	2.45	0.47
1:D:170:ALA:O	1:D:174:GLU:HG3	2.15	0.47
1:E:400:VAL:HG13	5:E:694:HOH:O	2.15	0.47
1:D:191:VAL:O	1:D:206:LEU:HA	2.15	0.46
1:A:139:LYS:HG2	1:A:140:GLU:N	2.31	0.46
1:E:242:TYR:HD1	1:E:406:ILE:HG12	1.80	0.46
1:C:295:TRP:CE2	1:C:299:LEU:HD11	2.51	0.46
1:C:31:CYS:HB2	1:C:35:GLU:OE2	2.15	0.46
1:A:84:GLU:HB2	1:A:95:LYS:NZ	2.30	0.46
1:C:118:VAL:CG1	1:F:360:ARG:NH2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TRP:CD1	1:A:105:MET:HG2	2.51	0.46
1:A:157:ARG:O	1:A:283:TRP:HA	2.15	0.45
1:C:123:TYR:CD1	1:C:136:MET:HA	2.50	0.45
1:B:180:ALA:HB1	1:F:107:SER:OG	2.16	0.45
1:D:11:CYS:SG	1:D:356:ARG:NH1	2.89	0.45
1:D:14:GLU:OE2	1:D:272:ASP:HB2	2.16	0.45
1:D:236:ASN:HB3	1:D:240:ASN:HD22	1.81	0.45
1:F:52:ASP:HB3	1:F:68:GLU:OE1	2.17	0.45
1:F:263:ASN:HB2	1:F:283:TRP:NE1	2.31	0.45
1:B:25:ARG:HA	1:B:25:ARG:HD3	1.69	0.45
1:B:350:MET:HE1	1:F:91:TYR:HE2	1.82	0.45
1:D:116:ASP:HA	1:D:119:LYS:NZ	2.32	0.45
1:F:256:ILE:CG2	1:F:257:PRO:HD2	2.47	0.45
1:D:79:TYR:HE2	1:E:349:THR:HG21	1.81	0.45
1:D:291:GLU:HG3	1:F:291:GLU:OE1	2.16	0.45
1:E:300:ARG:HD2	5:E:604:HOH:O	2.16	0.45
1:E:62:ARG:HG3	1:E:62:ARG:NH1	2.32	0.45
1:F:168:ASN:HB2	1:F:273:ASP:O	2.17	0.45
1:D:332:ASN:OD1	1:D:333:PHE:N	2.49	0.45
1:B:170:ALA:HB3	1:B:356:ARG:HH22	1.80	0.45
1:A:319:ASN:O	1:A:320:LYS:HB2	2.16	0.45
1:C:300:ARG:HD2	5:C:629:HOH:O	2.15	0.45
1:D:309:GLN:HB2	5:D:780:HOH:O	2.16	0.45
1:E:32:LEU:HB2	1:E:35:GLU:HG3	1.99	0.45
1:B:295:TRP:CE2	1:B:299:LEU:HD11	2.52	0.45
1:A:170:ALA:O	1:A:174:GLU:HG3	2.17	0.45
1:F:39:PRO:O	1:F:40:ASP:HB2	2.16	0.45
1:D:54:VAL:HG13	1:D:78:VAL:HG22	1.98	0.44
1:D:91:TYR:HE2	1:E:350:MET:CE	2.31	0.44
1:B:225:PHE:HD2	1:B:374:GLN:OE1	1.99	0.44
1:E:128:TRP:NE1	1:E:148:PRO:HD2	2.32	0.44
1:C:25:ARG:NH1	5:C:603:HOH:O	2.37	0.44
1:D:169:TRP:N	5:D:609:HOH:O	2.51	0.44
1:F:357:THR:HG22	1:F:358:HIS:CD2	2.52	0.44
1:A:58:ASP:HB2	1:A:85:GLY:HA2	1.99	0.44
1:A:220:ARG:HD3	1:A:370:GLU:OE2	2.17	0.44
1:A:310:ASN:O	1:A:311:TYR:HB2	2.17	0.44
1:A:408:PRO:C	1:A:410:THR:H	2.21	0.44
1:D:117:LYS:NZ	1:D:117:LYS:CB	2.81	0.44
1:A:74:ARG:HA	1:A:74:ARG:HD2	1.68	0.44
1:D:248:PHE:CZ	1:D:250:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:HA	1:F:25:ARG:HD3	1.72	0.44
1:B:66:MET:HG2	1:B:122:ALA:HB2	2.00	0.43
1:C:25:ARG:HD3	1:C:25:ARG:HA	1.79	0.43
1:D:211:ASP:HB3	1:D:231:ARG:HB3	1.99	0.43
1:E:92:HIS:HB2	3:E:502:FES:S2	2.58	0.43
1:B:329:LYS:HD2	5:F:744:HOH:O	2.18	0.43
1:C:53:LEU:HA	1:C:66:MET:O	2.18	0.43
1:D:54:VAL:CG2	1:D:68:GLU:HA	2.48	0.43
1:E:108:GLU:O	1:E:110:ALA:N	2.52	0.43
1:F:256:ILE:HG22	1:F:257:PRO:HD2	2.00	0.43
1:C:23:MET:C	1:C:25:ARG:H	2.20	0.43
1:C:230:LEU:HD22	1:C:243:VAL:HG22	2.00	0.43
1:F:164:LEU:HD22	1:F:310:ASN:O	2.18	0.43
1:F:218:VAL:HG12	1:F:219:GLN:H	1.79	0.43
1:E:266:ASN:HB2	1:E:280:PHE:HD1	1.83	0.43
1:C:118:VAL:HG12	1:F:360:ARG:NH2	2.31	0.43
1:D:73:ARG:HG3	1:D:73:ARG:NH1	2.33	0.43
1:E:146:LEU:HD13	5:E:785:HOH:O	2.18	0.43
1:F:400:VAL:HG12	5:F:622:HOH:O	2.18	0.43
1:B:66:MET:HE2	1:B:120:HIS:CD2	2.48	0.43
1:A:72:HIS:CD2	1:A:94:TRP:CZ2	3.06	0.43
1:B:173:LEU:CD2	1:B:371:PHE:CE1	3.01	0.43
1:B:267:ILE:HG23	1:B:279:TYR:HB2	2.00	0.43
1:E:23:MET:HG2	1:E:251:PRO:HG3	1.99	0.43
1:F:14:GLU:OE2	1:F:272:ASP:HB2	2.19	0.43
1:B:129:ALA:O	1:B:160:ILE:HD11	2.19	0.43
1:B:242:TYR:CE2	1:B:244:ARG:HD2	2.54	0.43
1:C:23:MET:HG2	1:C:251:PRO:CG	2.48	0.43
1:C:190:MET:HB2	5:C:601:HOH:O	2.18	0.43
1:F:53:LEU:HA	1:F:66:MET:O	2.19	0.43
1:F:147:PRO:O	1:F:397:THR:CG2	2.67	0.43
1:B:168:ASN:HB2	1:B:353:ILE:HG12	2.01	0.43
1:D:3:THR:N	1:D:6:GLU:OE2	2.48	0.43
1:A:16:ASP:CB	5:A:705:HOH:O	2.60	0.43
1:C:67:ASP:HB2	5:C:651:HOH:O	2.18	0.43
1:C:223:TYR:CG	1:C:396:ALA:HB2	2.53	0.43
1:F:68:GLU:HG3	1:F:78:VAL:HG23	2.01	0.43
1:B:18:PRO:HB2	1:B:379:VAL:CG2	2.49	0.42
1:B:282:ALA:HB2	1:B:295:TRP:CZ2	2.54	0.42
1:B:310:ASN:O	1:B:311:TYR:HB2	2.18	0.42
1:B:343:ASP:HB3	1:B:347:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:HIS:HB3	5:A:677:HOH:O	2.18	0.42
1:C:22:LEU:C	1:C:22:LEU:HD23	2.40	0.42
1:C:68:GLU:HG3	1:C:78:VAL:HG23	2.00	0.42
1:C:91:TYR:CE2	1:F:350:MET:CE	3.02	0.42
1:D:180:ALA:HB2	1:D:364:SER:HB2	2.01	0.42
1:A:67:ASP:HB3	1:A:120:HIS:CE1	2.54	0.42
1:D:54:VAL:HG21	1:D:77:LEU:HB2	2.01	0.42
1:D:392:GLY:C	1:D:394:GLU:H	2.22	0.42
1:F:22:LEU:O	1:F:22:LEU:HD23	2.18	0.42
1:E:140:GLU:C	1:E:142:MET:H	2.23	0.42
1:F:142:MET:HE2	5:F:774:HOH:O	2.17	0.42
1:A:245:SER:O	1:A:402:SER:HB2	2.19	0.42
1:F:166:PRO:HD2	1:F:348:LEU:CD2	2.48	0.42
1:B:293:GLU:HB3	1:A:293:GLU:HB3	2.01	0.42
1:F:22:LEU:HD23	1:F:22:LEU:C	2.39	0.42
1:B:2:MET:HE1	1:B:372:ARG:CD	2.16	0.42
1:E:337:THR:HG21	5:E:669:HOH:O	2.19	0.42
1:C:4:HIS:CE1	5:C:633:HOH:O	2.73	0.42
1:C:139:LYS:HE2	5:C:731:HOH:O	2.20	0.42
1:B:173:LEU:HD23	1:B:371:PHE:CE1	2.55	0.42
1:D:352:PRO:HD2	5:D:674:HOH:O	2.19	0.42
1:F:233:PRO:C	1:F:235:SER:H	2.23	0.41
1:A:66:MET:HB2	1:A:66:MET:HE3	1.71	0.41
1:A:72:HIS:HB2	1:A:94:TRP:CD2	2.54	0.41
1:E:339:PHE:CG	1:E:340:PRO:HD3	2.55	0.41
1:F:3:THR:HB	5:F:685:HOH:O	2.19	0.41
1:C:25:ARG:HD2	5:C:603:HOH:O	2.18	0.41
1:C:73:ARG:O	1:C:74:ARG:HB2	2.20	0.41
1:F:190:MET:HE1	5:F:760:HOH:O	2.20	0.41
1:B:45:LYS:HE3	1:B:68:GLU:OE1	2.20	0.41
1:C:157:ARG:O	1:C:283:TRP:HA	2.21	0.41
1:B:338:GLY:O	1:B:341:ASN:HB2	2.20	0.41
1:C:17:ALA:HA	1:C:18:PRO:HD3	1.95	0.41
1:D:23:MET:C	1:D:25:ARG:H	2.24	0.41
1:E:79:TYR:O	1:E:90:LEU:HD11	2.20	0.41
1:F:397:THR:OG1	1:F:398:PRO:CD	2.69	0.41
1:C:71:PRO:O	1:F:360:ARG:HD3	2.21	0.41
1:D:108:GLU:HG3	1:D:109:PRO:HD2	2.02	0.41
1:E:128:TRP:CH2	1:E:153:THR:HA	2.51	0.41
1:E:233:PRO:O	1:E:234:LEU:C	2.59	0.41
1:B:325:ARG:HD3	1:B:325:ARG:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:THR:HG21	1:F:79:TYR:CE2	2.55	0.41
1:D:218:VAL:HG11	1:D:370:GLU:HG2	2.03	0.41
1:D:232:ARG:HB3	1:D:232:ARG:CZ	2.51	0.41
1:E:23:MET:HG2	1:E:251:PRO:CG	2.51	0.41
1:E:232:ARG:NH1	5:E:609:HOH:O	2.54	0.41
1:F:31:CYS:HB2	1:F:35:GLU:OE2	2.21	0.41
1:F:185:LEU:HD23	1:F:186:HIS:CE1	2.56	0.41
1:F:361:LEU:HD11	1:F:372:ARG:NH1	2.36	0.41
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.86	0.41
1:B:199:LYS:HG3	5:B:747:HOH:O	2.21	0.40
1:D:25:ARG:HA	1:D:25:ARG:HD3	1.70	0.40
1:D:173:LEU:O	1:D:176:ALA:N	2.47	0.40
1:E:332:ASN:HB2	5:E:739:HOH:O	2.21	0.40
1:F:126:GLN:HG2	1:F:145:PHE:CD2	2.56	0.40
1:F:416:TYR:CD2	1:F:418:ALA:HB2	2.57	0.40
1:E:110:ALA:C	1:E:112:SER:H	2.23	0.40
1:E:258:PRO:HD3	1:E:402:SER:OG	2.21	0.40
1:C:207:ARG:NH1	1:C:244:ARG:HH12	2.19	0.40
1:C:307:LEU:HD23	1:C:313:PRO:HA	2.04	0.40
1:D:223:TYR:CE2	1:D:400:VAL:HG21	2.57	0.40
1:E:420:TYR:CE1	1:E:422:TRP:HE3	2.16	0.40
1:B:236:ASN:C	1:B:238:ALA:N	2.73	0.40
1:E:38:GLU:HB3	1:E:39:PRO:HD2	2.03	0.40
1:E:227:TYR:O	1:E:245:SER:HA	2.22	0.40
1:F:285:HIS:CE1	1:F:423:LEU:HD11	2.57	0.40

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	401/439 (91%)	368 (92%)	29 (7%)	4 (1%)	15 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	421/439 (96%)	386 (92%)	33 (8%)	2 (0%)	29 48
1	C	401/439 (91%)	369 (92%)	29 (7%)	3 (1%)	22 40
1	D	399/439 (91%)	367 (92%)	29 (7%)	3 (1%)	19 36
1	E	387/439 (88%)	350 (90%)	30 (8%)	7 (2%)	8 15
1	F	403/439 (92%)	368 (91%)	31 (8%)	4 (1%)	15 28
All	All	2412/2634 (92%)	2208 (92%)	181 (8%)	23 (1%)	15 28

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	236	ASN
1	F	15	GLY
1	A	74	ARG
1	E	409	LYS
1	B	198	ALA
1	C	72	HIS
1	D	236	ASN
1	E	109	PRO
1	E	422	TRP
1	F	72	HIS
1	B	74	ARG
1	A	286	PRO
1	C	17	ALA
1	C	422	TRP
1	D	152	PRO
1	D	398	PRO
1	F	148	PRO
1	E	147	PRO
1	E	152	PRO
1	A	152	PRO
1	F	286	PRO
1	A	398	PRO
1	E	148	PRO

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	337/363 (93%)	315 (94%)	22 (6%)	17	30
1	B	348/363 (96%)	329 (94%)	19 (6%)	21	37
1	C	337/363 (93%)	319 (95%)	18 (5%)	22	39
1	D	337/363 (93%)	314 (93%)	23 (7%)	16	28
1	E	326/363 (90%)	309 (95%)	17 (5%)	23	39
1	F	340/363 (94%)	322 (95%)	18 (5%)	22	39
All	All	2025/2178 (93%)	1908 (94%)	117 (6%)	20	35

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	54	VAL
1	B	60	GLU
1	B	67	ASP
1	B	91	TYR
1	B	114	MET
1	B	139	LYS
1	B	146	LEU
1	B	179	SER
1	B	191	VAL
1	B	194	ARG
1	B	232	ARG
1	B	263	ASN
1	B	339	PHE
1	B	357	THR
1	B	411	THR
1	B	414	ARG
1	B	415	THR
1	B	423	LEU
1	A	4	HIS
1	A	54	VAL
1	A	59	SER
1	A	91	TYR
1	A	96	MET
1	A	108	GLU
1	A	139	LYS
1	A	153	THR

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	173	LEU
1	A	184	SER
1	A	188	SER
1	A	190	MET
1	A	191	VAL
1	A	205	TRP
1	A	230	LEU
1	A	286	PRO
1	A	339	PHE
1	A	357	THR
1	A	397	THR
1	A	406	ILE
1	A	411	THR
1	C	91	TYR
1	C	117	LYS
1	C	119	LYS
1	C	121	THR
1	C	147	PRO
1	C	173	LEU
1	C	182	SER
1	C	183	SER
1	C	184	SER
1	C	204	THR
1	C	207	ARG
1	C	278	PHE
1	C	306	ASP
1	C	366	LEU
1	C	384	GLN
1	C	393	VAL
1	C	402	SER
1	C	423	LEU
1	D	28	THR
1	D	59	SER
1	D	66	MET
1	D	73	ARG
1	D	91	TYR
1	D	117	LYS
1	D	144	GLU
1	D	153	THR
1	D	173	LEU
1	D	182	SER

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Mol	Chain	Res	Type
1	D	188	SER
1	D	206	LEU
1	D	235	SER
1	D	239	GLU
1	D	325	ARG
1	D	329	LYS
1	D	339	PHE
1	D	357	THR
1	D	397	THR
1	D	398	PRO
1	D	411	THR
1	D	415	THR
1	D	421	VAL
1	E	5	GLU
1	E	54	VAL
1	E	62	ARG
1	E	91	TYR
1	E	114	MET
1	E	121	THR
1	E	131	MET
1	E	173	LEU
1	E	190	MET
1	E	208	PRO
1	E	219	GLN
1	E	226	ARG
1	E	232	ARG
1	E	234	LEU
1	E	267	ILE
1	E	399	THR
1	E	409	LYS
1	F	28	THR
1	F	83	GLU
1	F	91	TYR
1	F	108	GLU
1	F	114	MET
1	F	119	LYS
1	F	156	THR
1	F	164	LEU
1	F	179	SER
1	F	190	MET
1	F	227	TYR
1	F	240	ASN

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Mol	Chain	Res	Type
1	F	245	SER
1	F	267	ILE
1	F	320	LYS
1	F	329	LYS
1	F	400	VAL
1	F	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	HIS
1	B	288	GLN
1	A	288	GLN
1	C	168	ASN
1	C	219	GLN
1	D	120	HIS
1	D	240	ASN
1	D	263	ASN
1	D	288	GLN
1	D	384	GLN
1	E	219	GLN
1	E	342	GLN
1	F	101	ASN
1	F	260	ASN
1	F	358	HIS

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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	E	502	1	0,4,4	-	-	-		
3	FES	D	502	1	0,4,4	-	-	-		
3	FES	C	502	1	0,4,4	-	-	-		
3	FES	B	502	1	0,4,4	-	-	-		
4	PHT	B	503	-	12,12,12	1.09	1 (8%)	16,16,16	1.02	0
3	FES	F	502	1	0,4,4	-	-	-		
3	FES	A	502	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	E	502	1	-	-	0/1/1/1
3	FES	D	502	1	-	-	0/1/1/1
3	FES	C	502	1	-	-	0/1/1/1
3	FES	B	502	1	-	-	0/1/1/1
4	PHT	B	503	-	-	2/8/8/8	0/1/1/1
3	FES	F	502	1	-	-	0/1/1/1
3	FES	A	502	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	PHT	O9-C7	-2.03	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	PHT	C4-C3-C7-O9
4	B	503	PHT	C4-C3-C7-O8

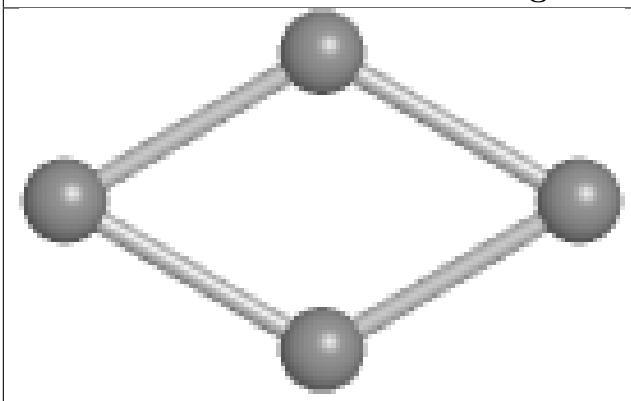
There are no ring outliers.

3 monomers are involved in 3 short contacts:

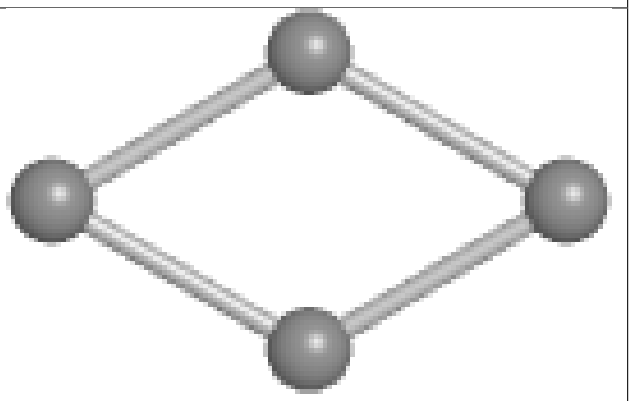
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	FES	1	0
3	C	502	FES	1	0
3	A	502	FES	1	0

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 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.

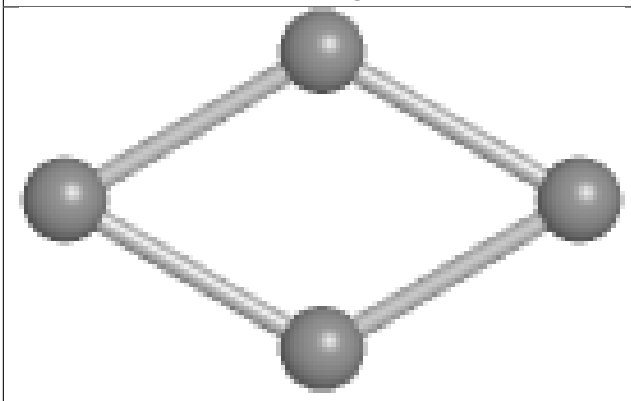
Ligand FES E 502



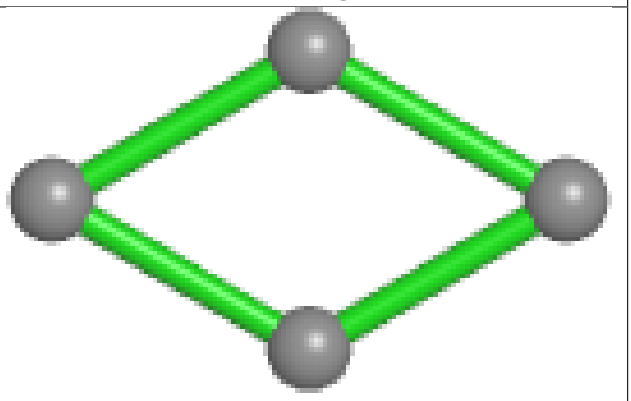
Bond lengths



Bond angles

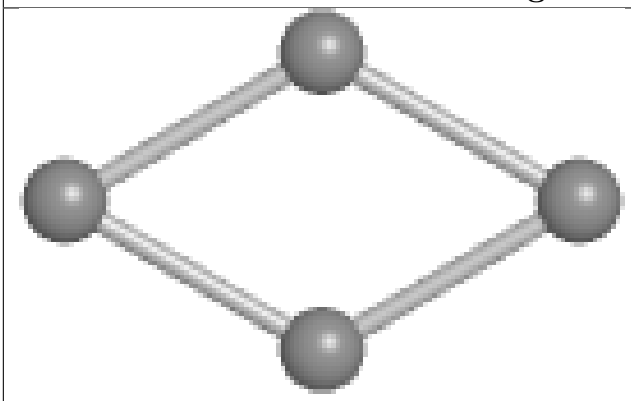


Torsions

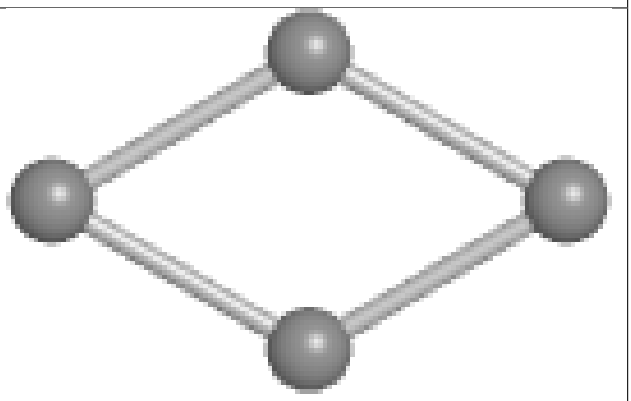


Rings

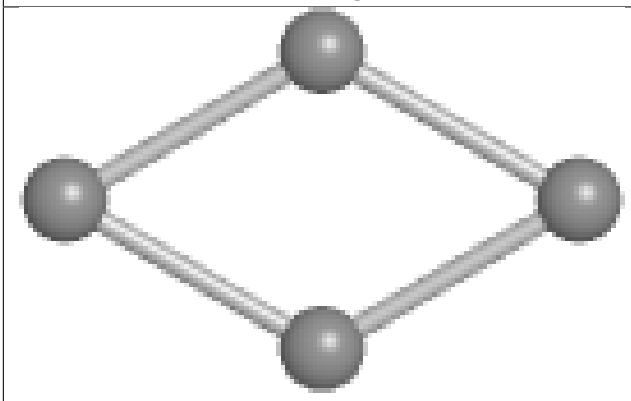
Ligand FES D 502



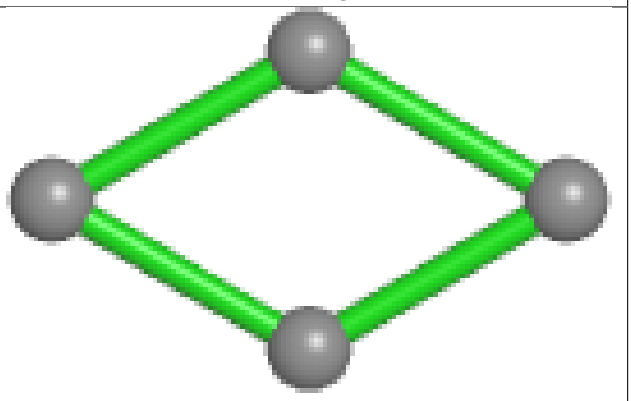
Bond lengths



Bond angles

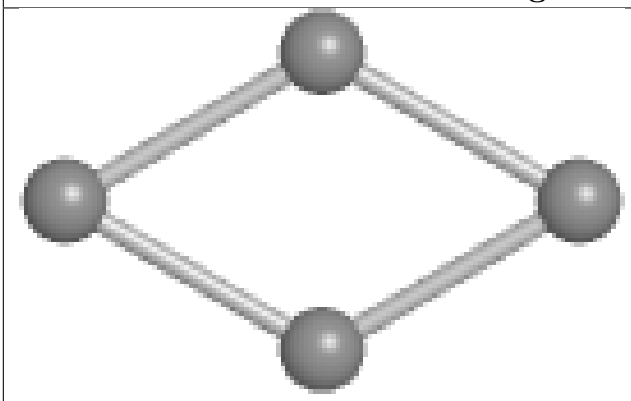


Torsions

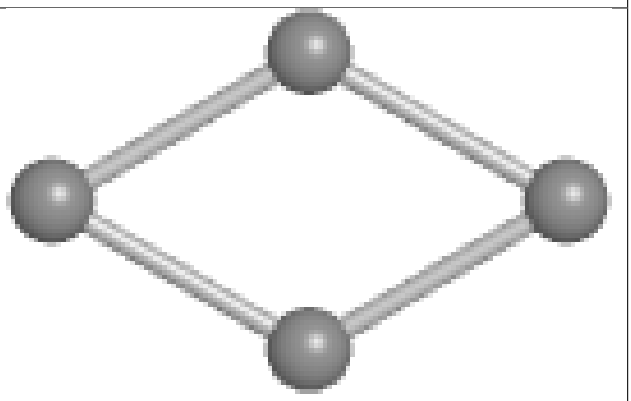


Rings

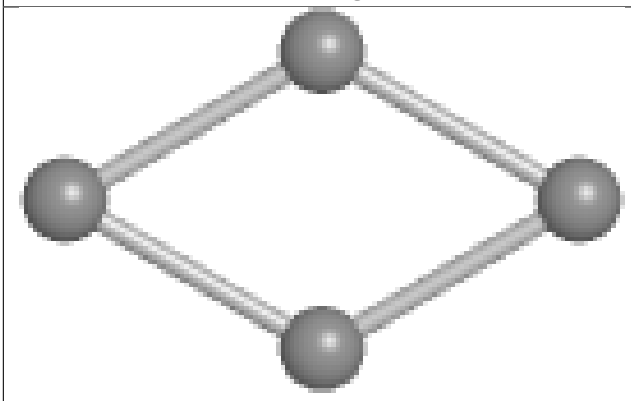
Ligand FES C 502



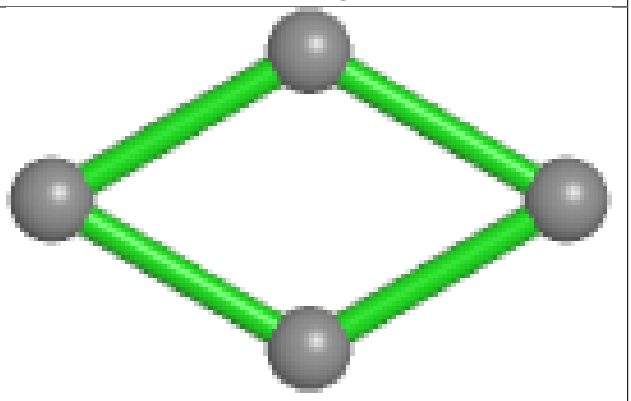
Bond lengths



Bond angles

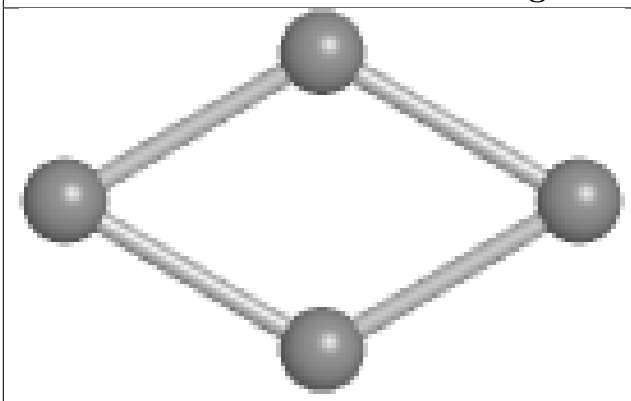


Torsions

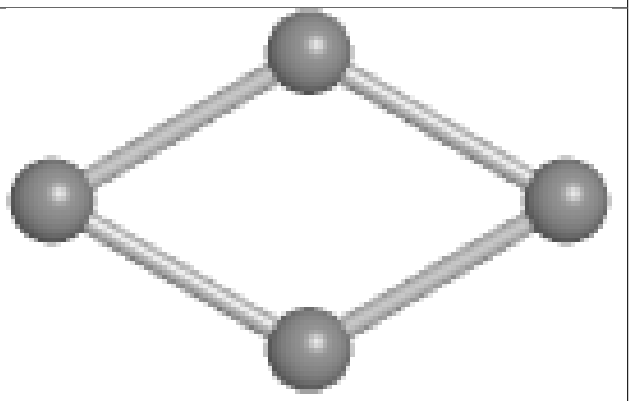


Rings

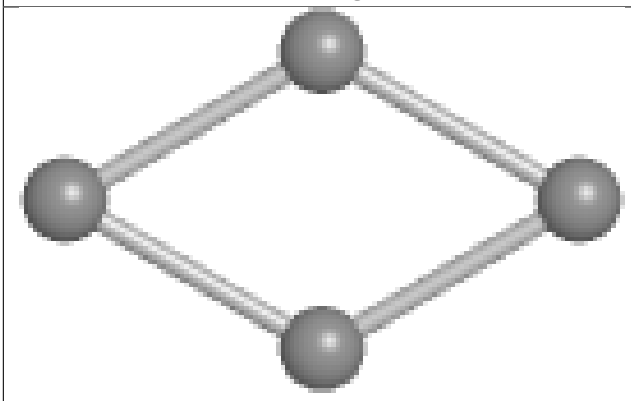
Ligand FES B 502



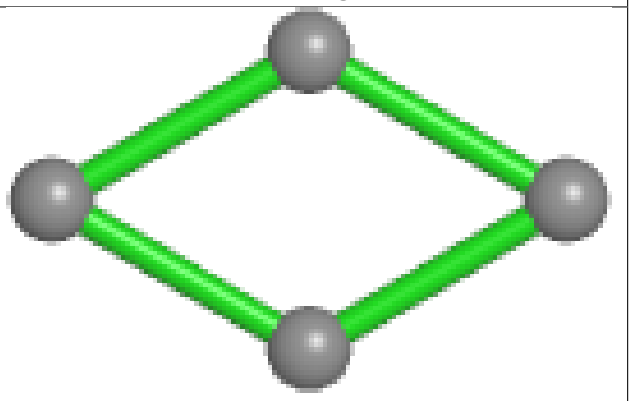
Bond lengths



Bond angles

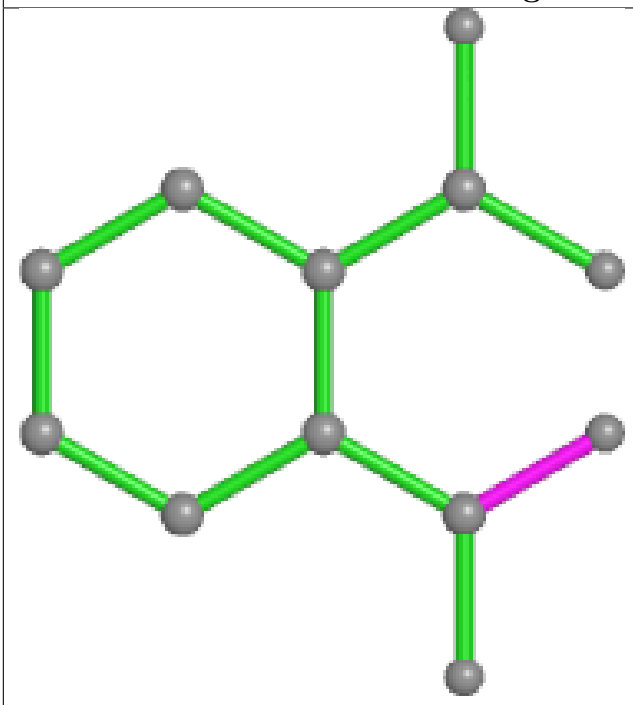


Torsions

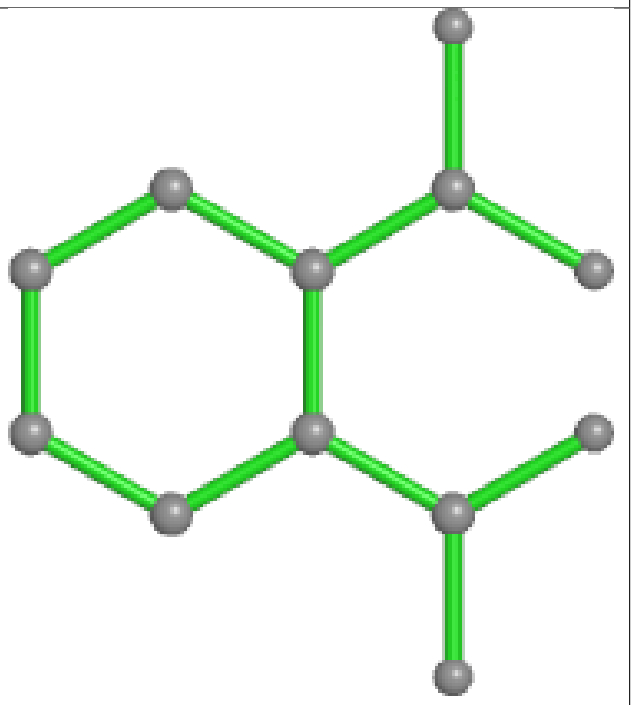


Rings

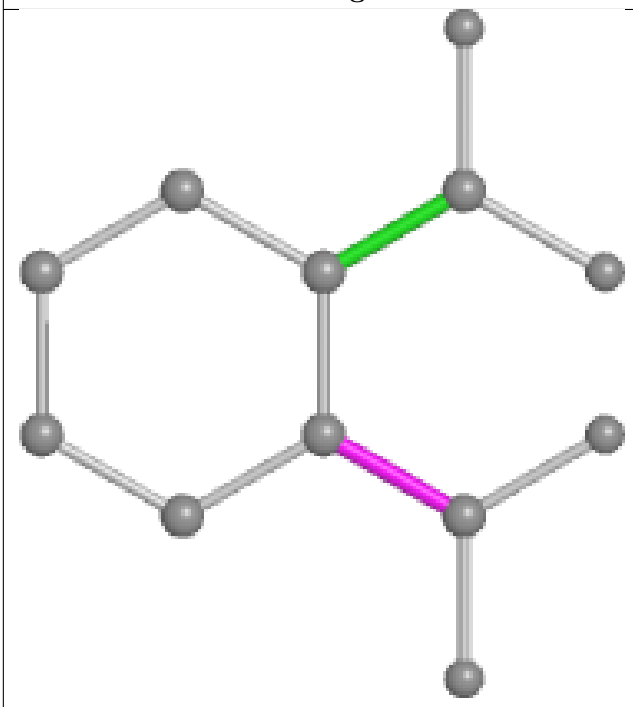
Ligand PHT B 503



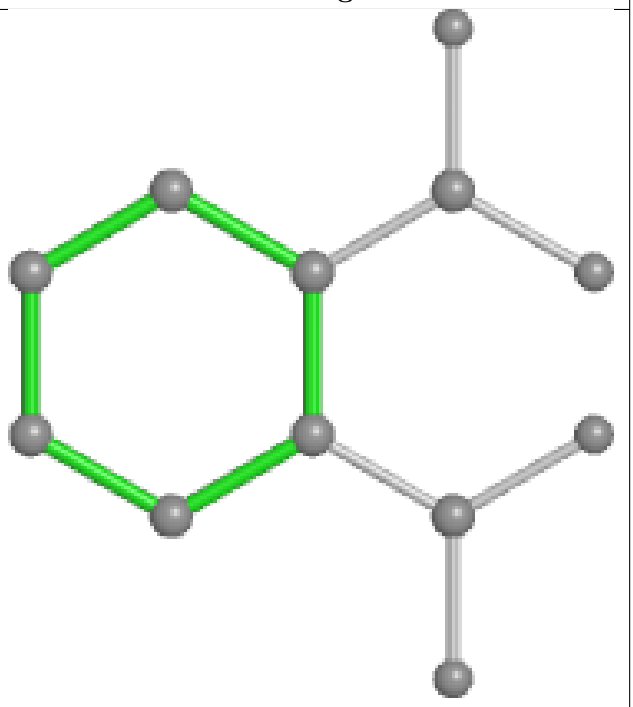
Bond lengths



Bond angles

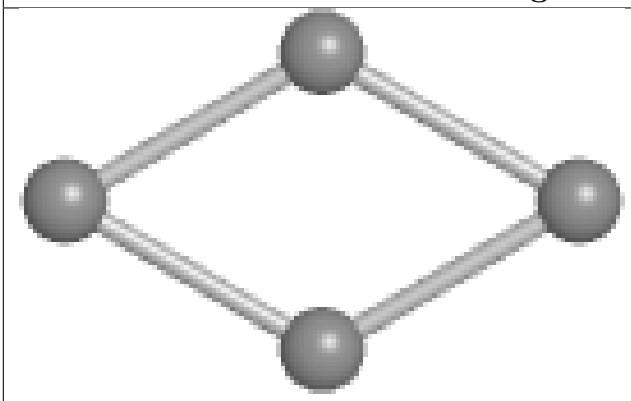


Torsions

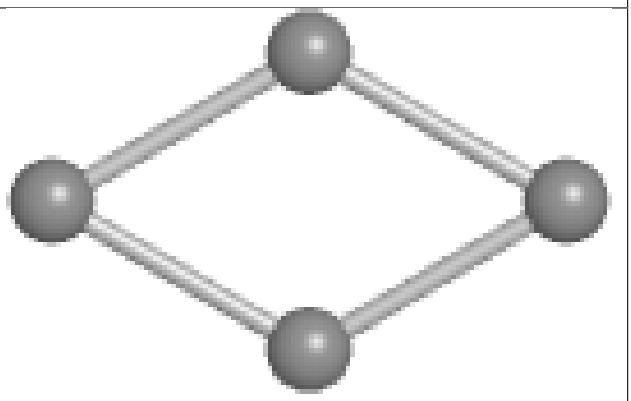


Rings

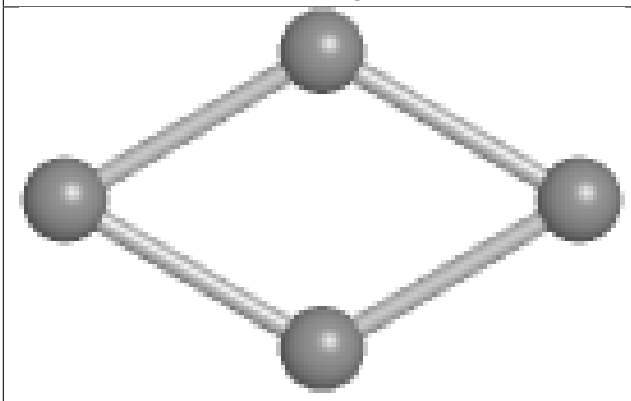
Ligand FES F 502



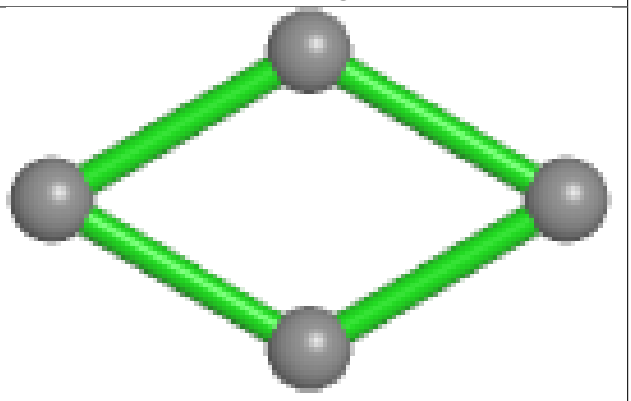
Bond lengths



Bond angles

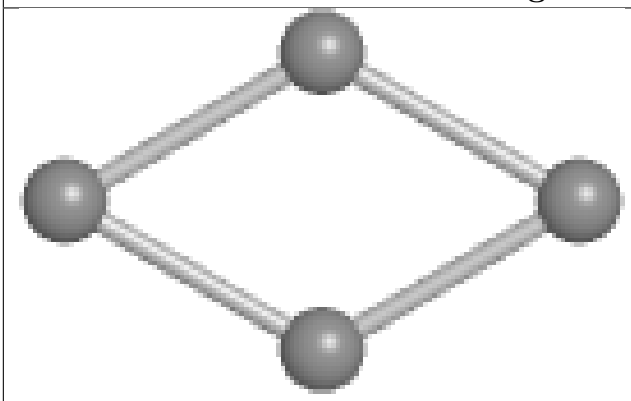


Torsions

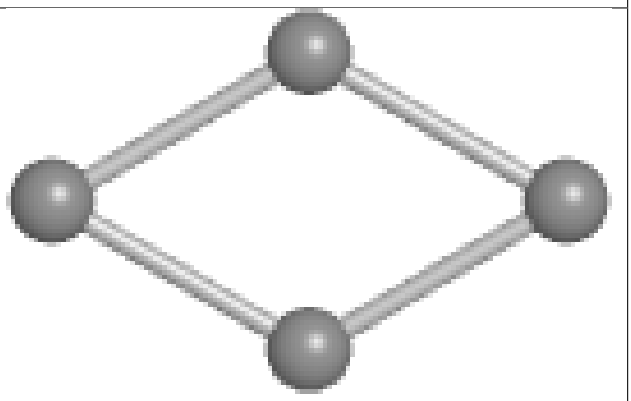


Rings

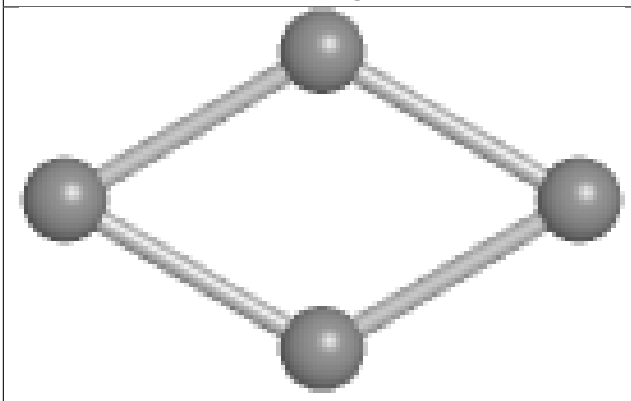
Ligand FES A 502



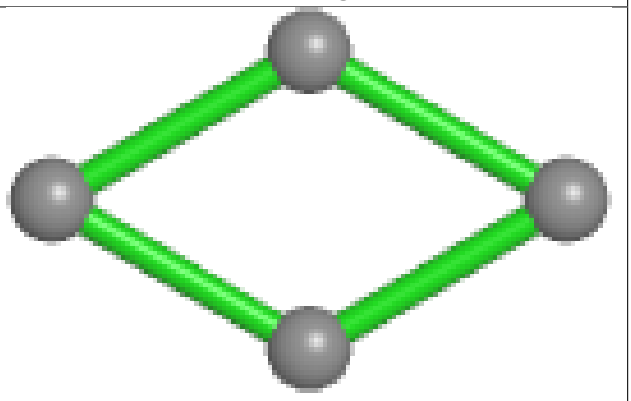
Bond lengths



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	407/439 (92%)	0.24	9 (2%) 62 69	22, 40, 75, 116	0
1	B	423/439 (96%)	0.45	21 (4%) 28 32	21, 40, 104, 159	0
1	C	407/439 (92%)	0.39	22 (5%) 25 29	23, 40, 98, 136	0
1	D	405/439 (92%)	0.37	14 (3%) 44 49	25, 44, 91, 128	0
1	E	395/439 (89%)	0.59	44 (11%) 5 5	24, 43, 132, 187	0
1	F	409/439 (93%)	0.68	40 (9%) 7 7	28, 49, 114, 132	0
All	All	2446/2634 (92%)	0.45	150 (6%) 21 24	21, 43, 107, 187	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	399	THR	9.5
1	C	111	ALA	8.4
1	E	400	VAL	7.4
1	B	201	THR	6.4
1	E	234	LEU	6.4
1	B	110	ALA	5.8
1	E	213	ALA	5.7
1	B	202	ASP	5.6
1	E	405	ALA	5.6
1	F	192	PRO	5.6
1	E	110	ALA	5.3
1	A	205	TRP	5.0
1	F	151	ALA	4.9
1	F	415	THR	4.8
1	F	206	LEU	4.8
1	E	215	ARG	4.7
1	F	230	LEU	4.5
1	C	238	ALA	4.4
1	E	239	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	4.3
1	B	111	ALA	4.3
1	E	423	LEU	4.3
1	E	398	PRO	4.3
1	E	148	PRO	4.3
1	F	238	ALA	4.3
1	F	237	ALA	4.2
1	E	208	PRO	4.2
1	E	235	SER	4.1
1	E	210	THR	4.0
1	F	191	VAL	4.0
1	E	229	ALA	3.9
1	E	397	THR	3.7
1	F	208	PRO	3.7
1	F	406	ILE	3.7
1	C	215	ARG	3.6
1	F	411	THR	3.6
1	D	423	LEU	3.6
1	C	234	LEU	3.6
1	E	216	MET	3.6
1	C	110	ALA	3.6
1	A	153	THR	3.5
1	F	234	LEU	3.5
1	E	214	PRO	3.5
1	C	204	THR	3.4
1	F	190	MET	3.4
1	C	210	THR	3.3
1	F	410	THR	3.3
1	E	209	SER	3.3
1	F	150	TRP	3.3
1	B	198	ALA	3.3
1	B	203	LYS	3.3
1	E	230	LEU	3.3
1	B	113	GLY	3.3
1	E	227	TYR	3.2
1	C	205	TRP	3.2
1	F	418	ALA	3.2
1	B	199	LYS	3.2
1	C	423	LEU	3.2
1	F	393	VAL	3.1
1	E	243	VAL	3.1
1	B	196	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	404	GLN	3.1
1	E	420	TYR	3.1
1	C	191	VAL	3.0
1	A	111	ALA	3.0
1	B	194	ARG	3.0
1	D	242	TYR	3.0
1	F	205	TRP	3.0
1	B	406	ILE	3.0
1	E	401	CYS	3.0
1	D	206	LEU	3.0
1	F	209	SER	3.0
1	F	416	TYR	2.9
1	F	235	SER	2.9
1	A	110	ALA	2.9
1	A	398	PRO	2.9
1	A	206	LEU	2.8
1	E	236	ASN	2.8
1	F	422	TRP	2.8
1	E	408	PRO	2.8
1	B	213	ALA	2.8
1	E	242	TYR	2.8
1	E	228	ALA	2.8
1	E	212	LYS	2.8
1	F	114	MET	2.8
1	F	153	THR	2.8
1	C	154	ALA	2.7
1	E	240	ASN	2.7
1	D	150	TRP	2.7
1	F	403	PHE	2.6
1	D	116	ASP	2.6
1	F	385	GLY	2.6
1	F	241	ASP	2.6
1	B	235	SER	2.6
1	B	205	TRP	2.5
1	D	416	TYR	2.5
1	C	206	LEU	2.5
1	A	395	ALA	2.5
1	C	91	TYR	2.5
1	E	409	LYS	2.5
1	F	154	ALA	2.5
1	E	190	MET	2.5
1	F	399	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	397	THR	2.4
1	C	208	PRO	2.4
1	F	152	PRO	2.4
1	E	211	ASP	2.4
1	B	197	GLY	2.4
1	B	114	MET	2.4
1	D	149	ALA	2.4
1	F	144	GLU	2.4
1	C	118	VAL	2.3
1	C	107	SER	2.3
1	E	109	PRO	2.3
1	B	112	SER	2.3
1	E	217	GLN	2.3
1	F	400	VAL	2.3
1	B	236	ASN	2.2
1	F	227	TYR	2.2
1	E	115	VAL	2.2
1	E	407	VAL	2.2
1	F	231	ARG	2.2
1	F	189	ASP	2.2
1	E	152	PRO	2.2
1	C	232	ARG	2.2
1	C	406	ILE	2.2
1	F	236	ASN	2.2
1	C	230	LEU	2.2
1	F	148	PRO	2.2
1	E	410	THR	2.2
1	E	244	ARG	2.2
1	E	223	TYR	2.1
1	F	390	GLY	2.1
1	D	399	THR	2.1
1	F	240	ASN	2.1
1	B	211	ASP	2.1
1	D	75	ALA	2.1
1	A	423	LEU	2.1
1	D	153	THR	2.1
1	C	410	THR	2.1
1	F	239	GLU	2.1
1	E	237	ALA	2.1
1	A	190	MET	2.1
1	D	191	VAL	2.0
1	D	227	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	207	ARG	2.0
1	C	237	ALA	2.0
1	D	235	SER	2.0
1	E	86	GLY	2.0
1	C	109	PRO	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)

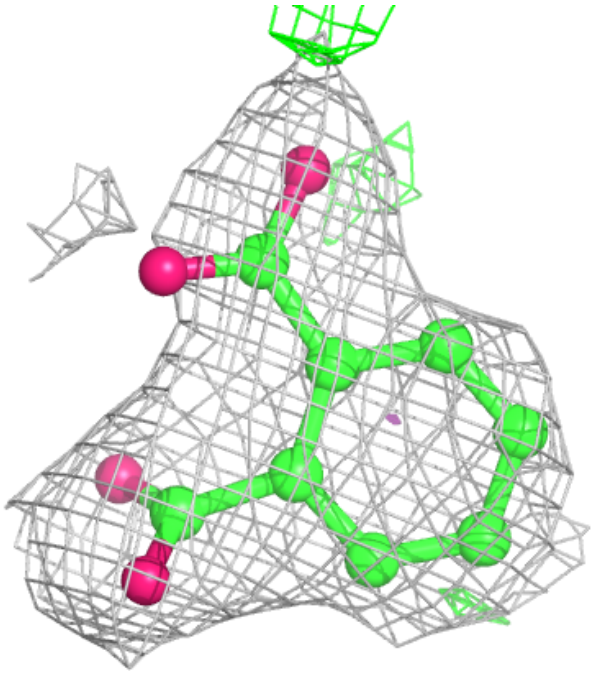
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

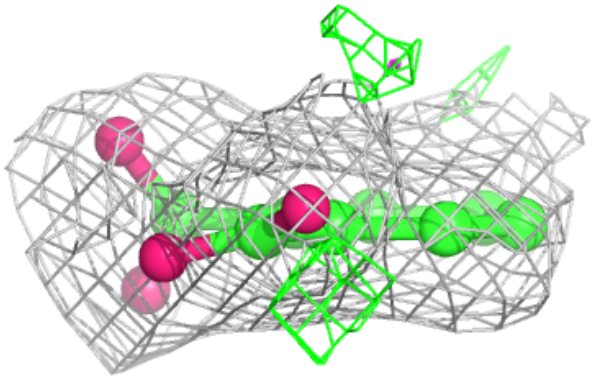
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PHT	B	503	12/12	0.84	0.26	62,75,84,88	0
2	FE2	F	501	1/1	0.96	0.12	45,45,45,45	0
2	FE2	E	501	1/1	0.96	0.16	40,40,40,40	0
3	FES	C	502	4/4	0.98	0.11	39,41,41,50	0
2	FE2	D	501	1/1	0.98	0.12	34,34,34,34	0
2	FE2	C	501	1/1	0.99	0.14	30,30,30,30	0
3	FES	A	502	4/4	0.99	0.12	30,33,36,40	0
2	FE2	B	501	1/1	0.99	0.12	36,36,36,36	0
3	FES	D	502	4/4	0.99	0.14	35,38,40,44	0
3	FES	E	502	4/4	0.99	0.14	25,27,30,32	0
3	FES	F	502	4/4	0.99	0.12	33,35,36,45	0
2	FE2	A	501	1/1	0.99	0.17	27,27,27,27	0
3	FES	B	502	4/4	1.00	0.12	29,29,33,35	0

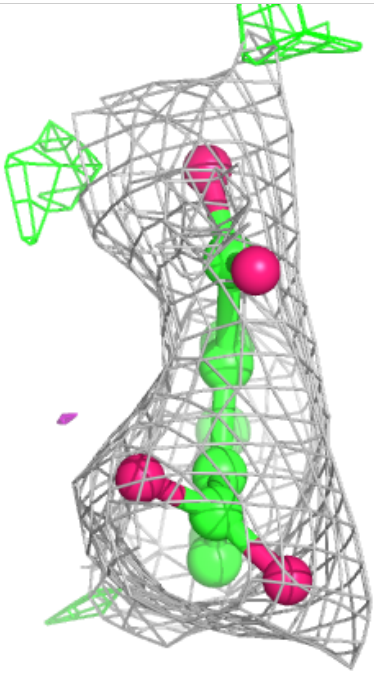
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PHT B 503:

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

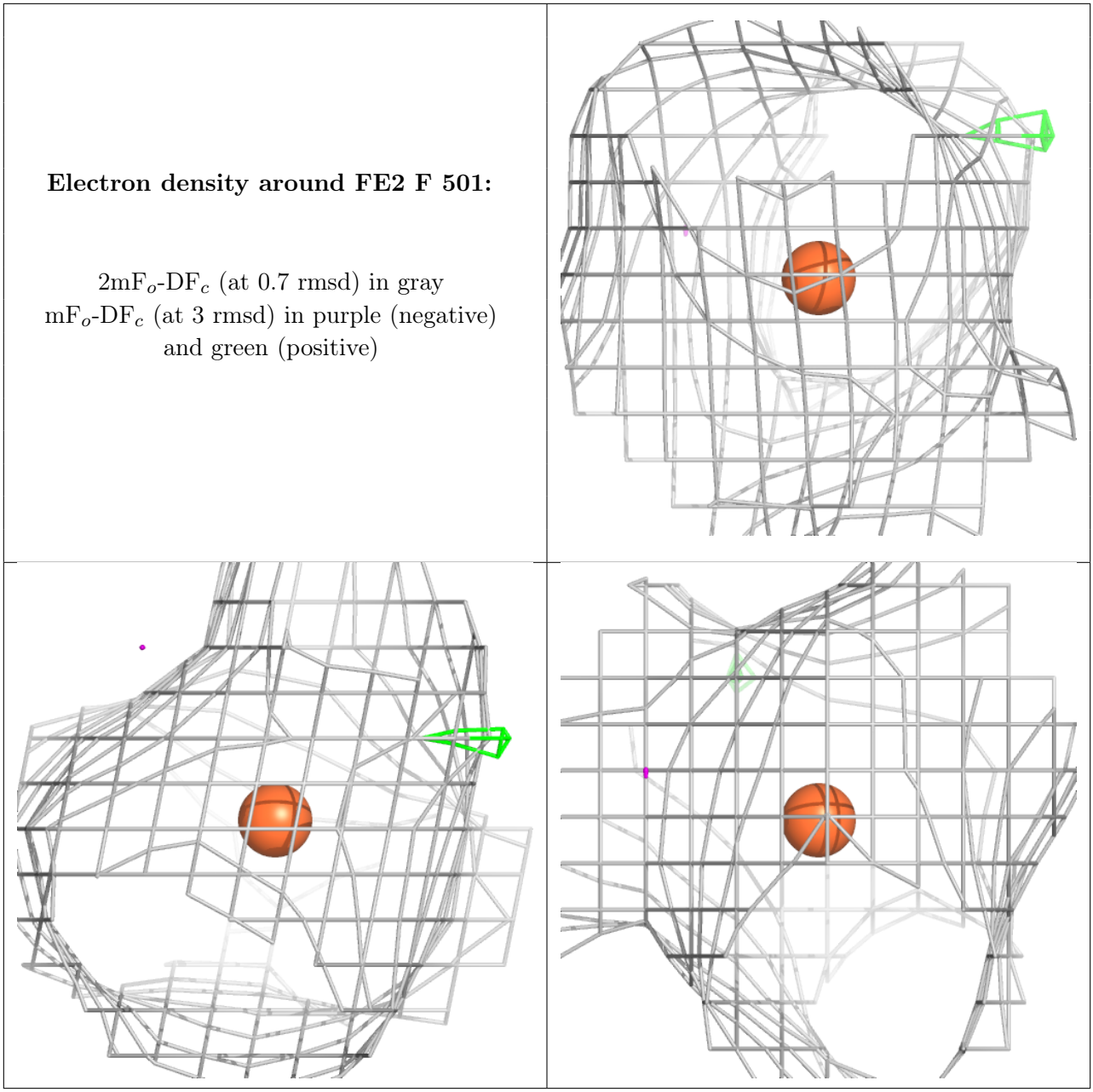






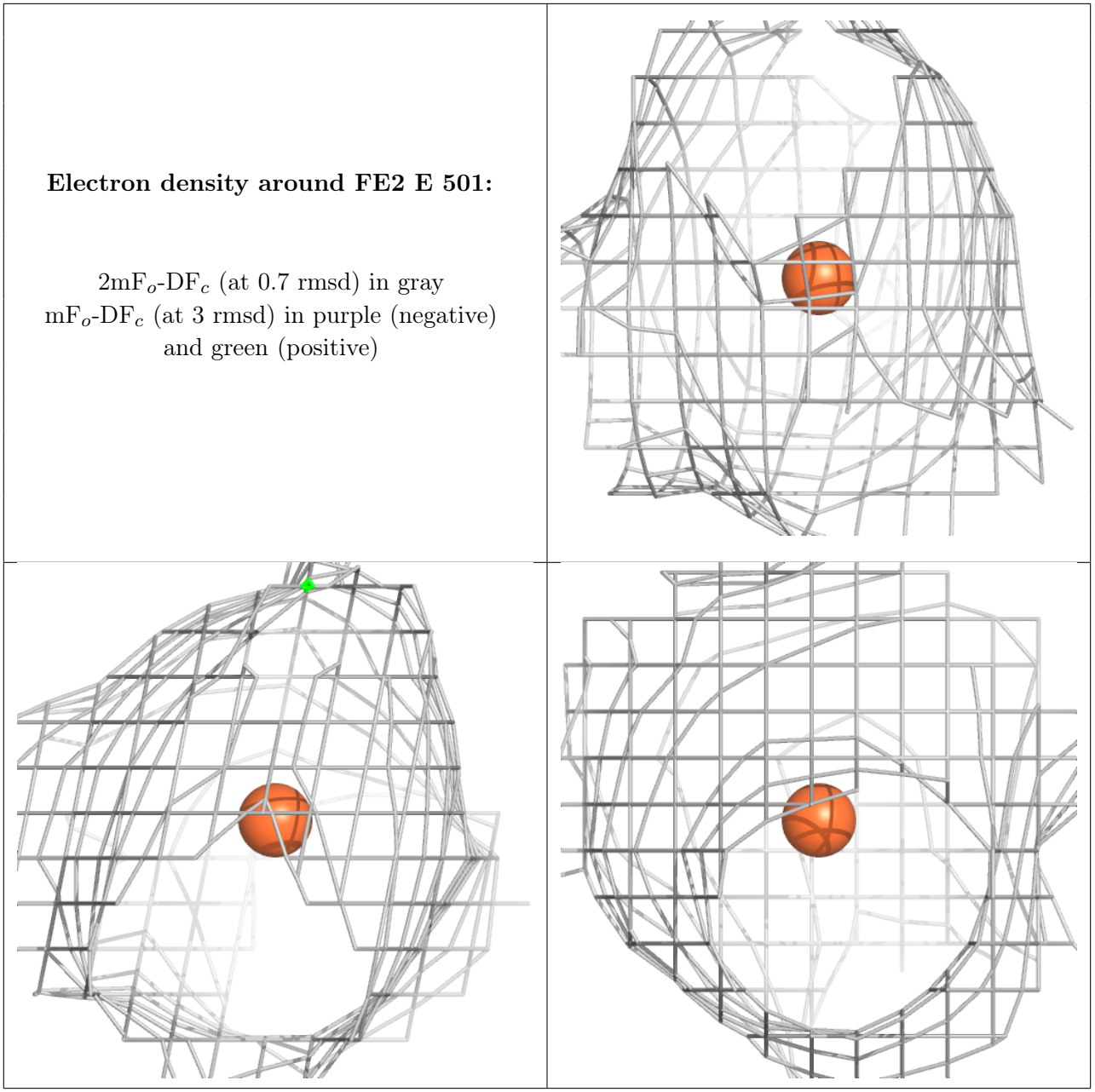
Electron density around FE2 F 501:

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



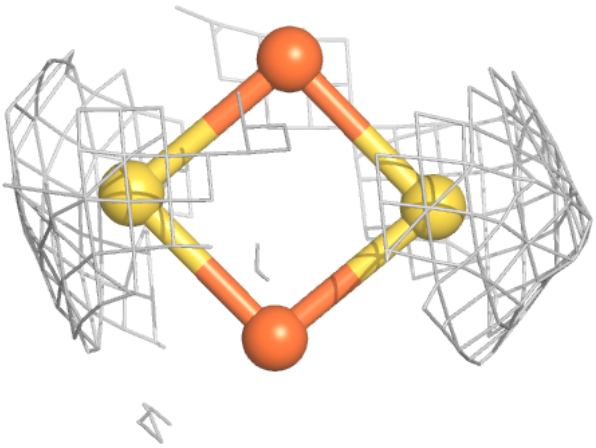
Electron density around FE2 E 501:

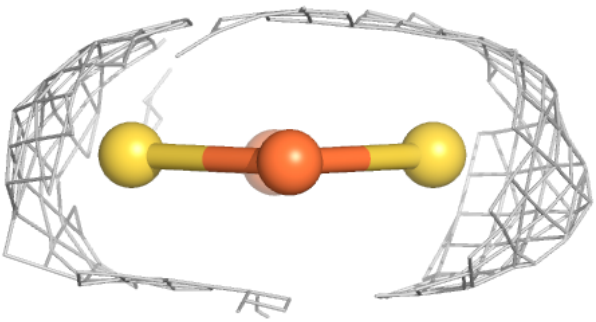
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

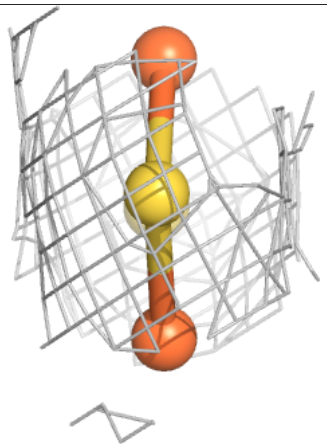


Electron density around FES C 502:

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

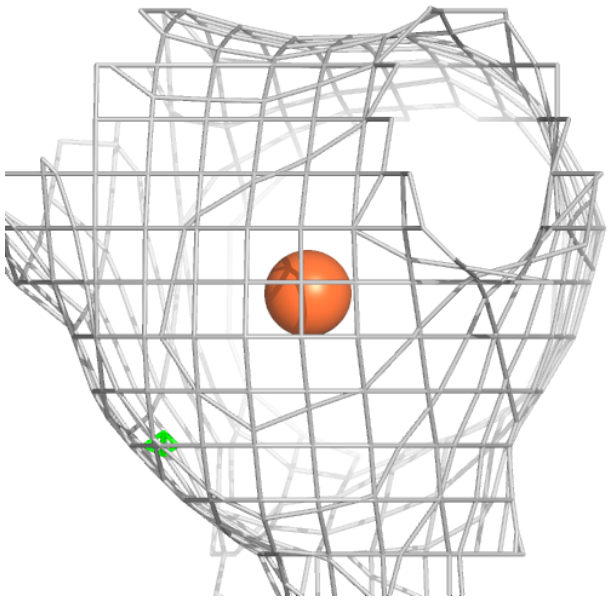


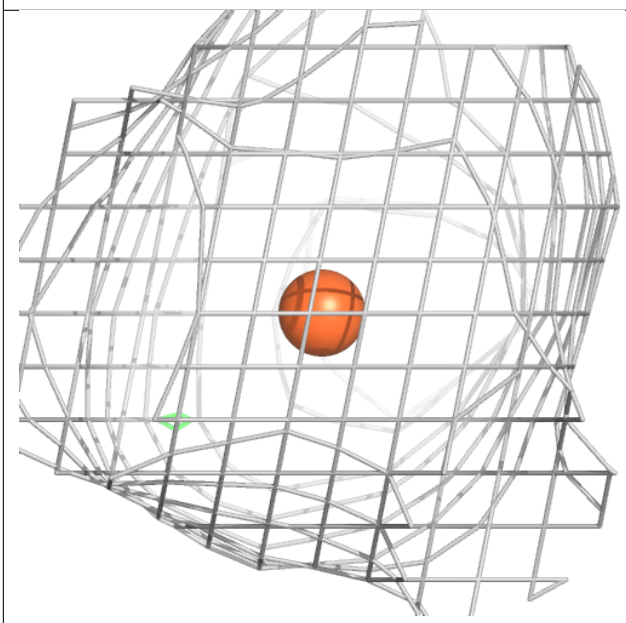


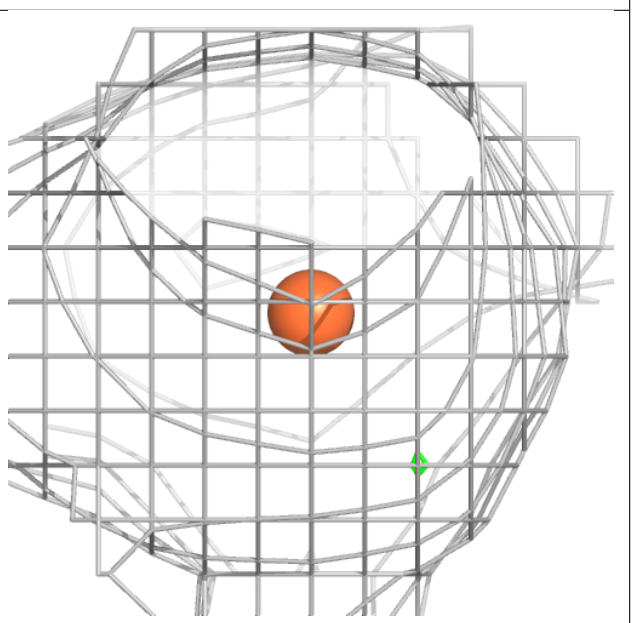


Electron density around FE2 D 501:

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

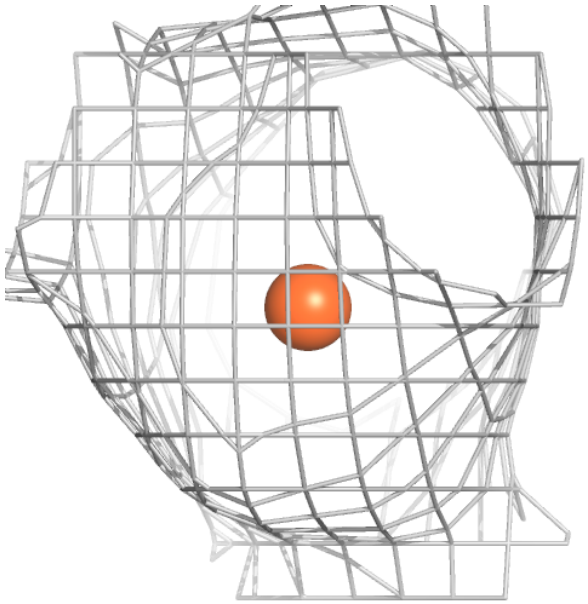


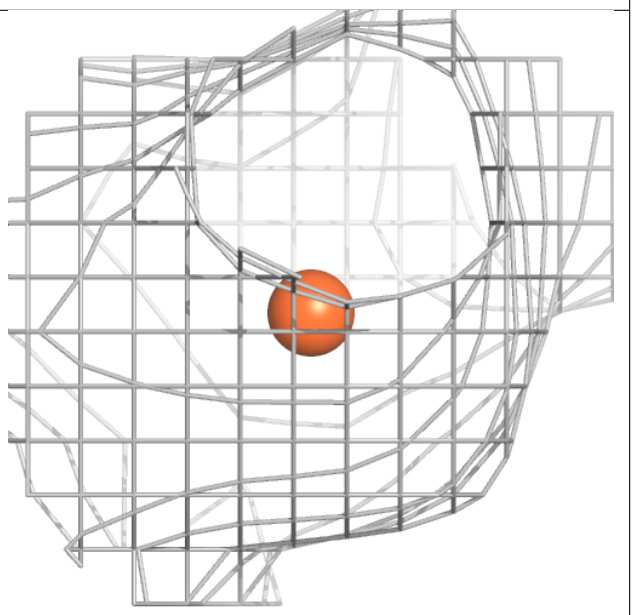




Electron density around FE2 C 501:

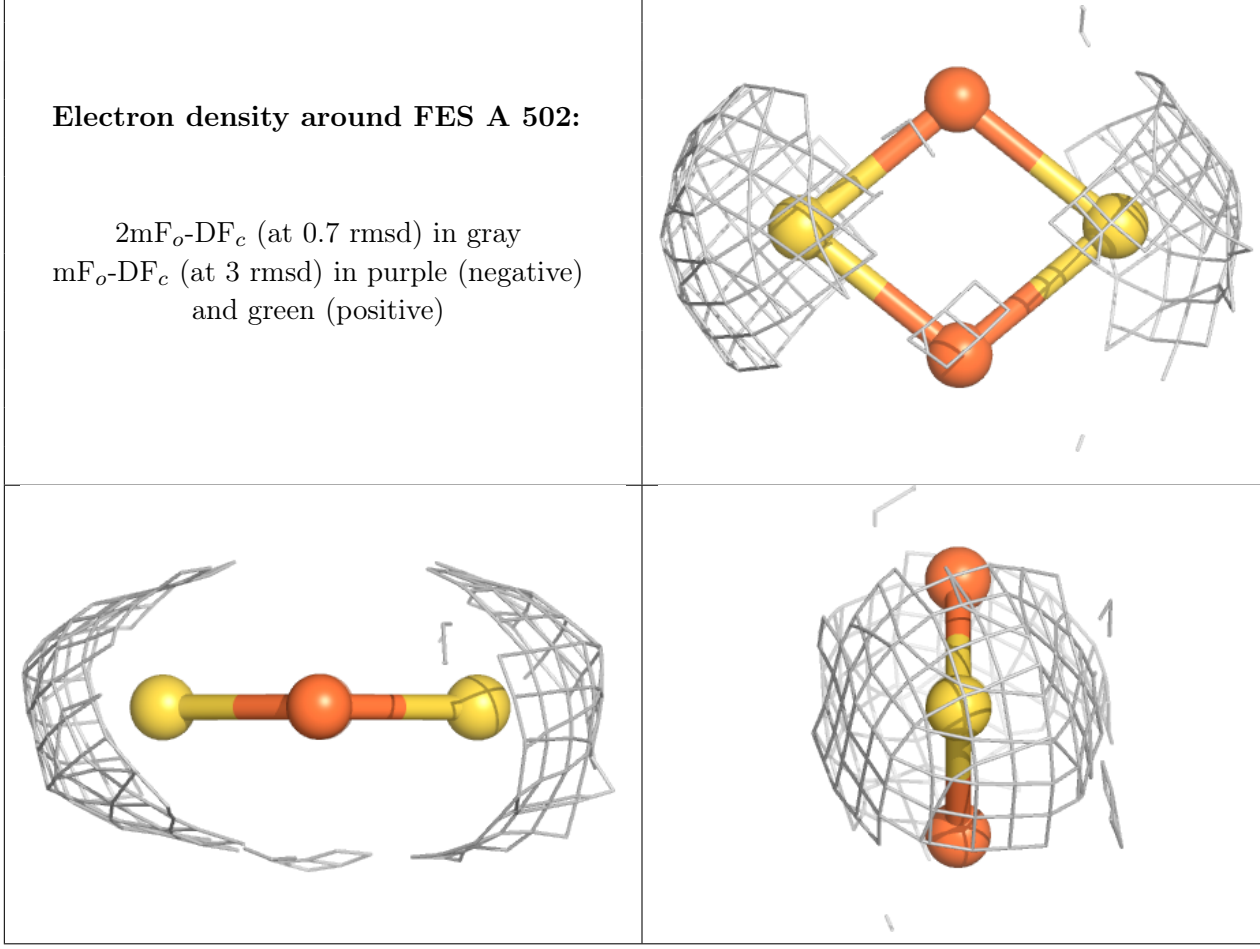
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





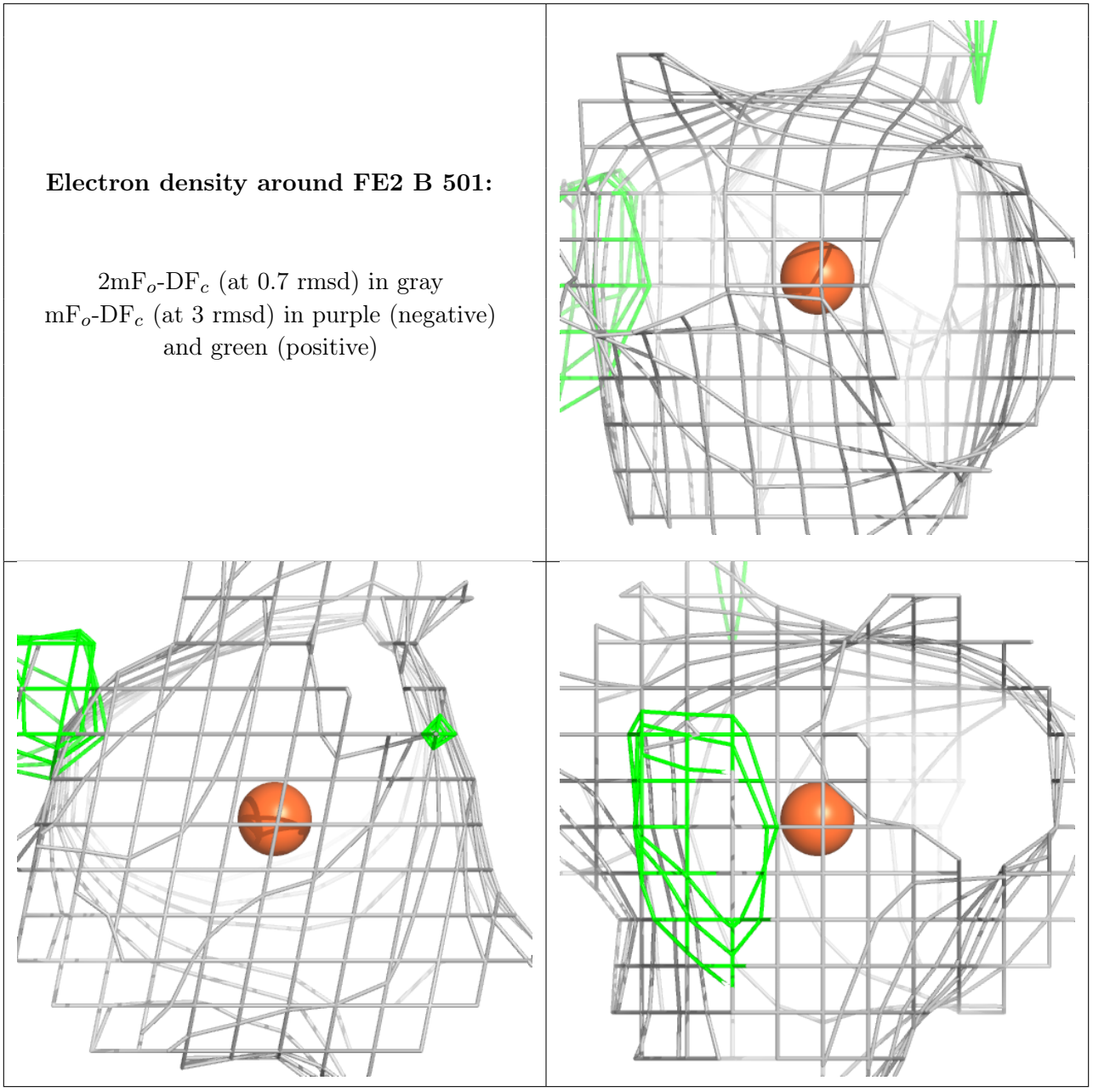
Electron density around FES A 502:

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



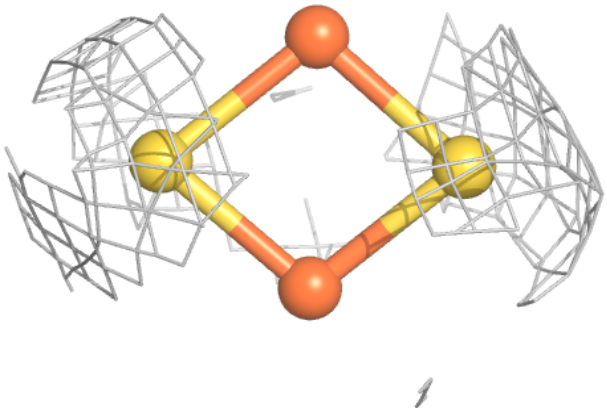
Electron density around FE2 B 501:

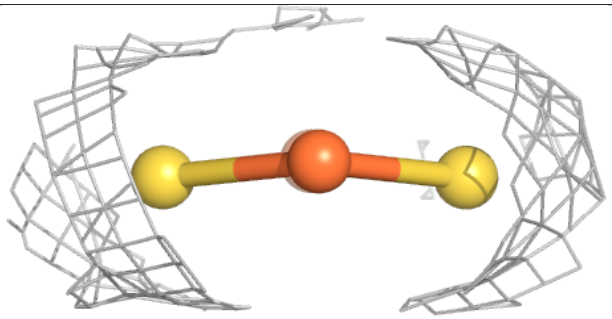
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

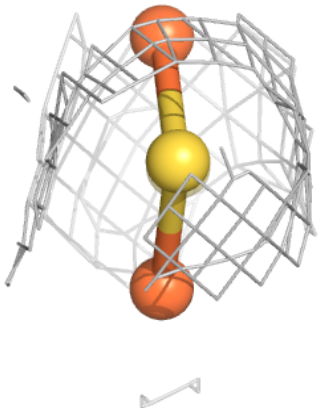


Electron density around FES D 502:

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

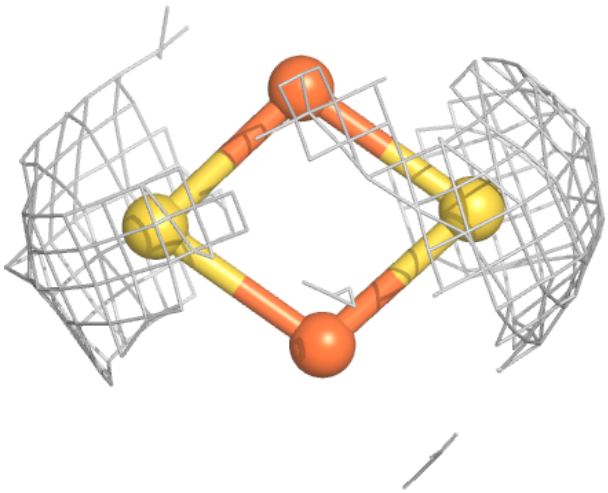


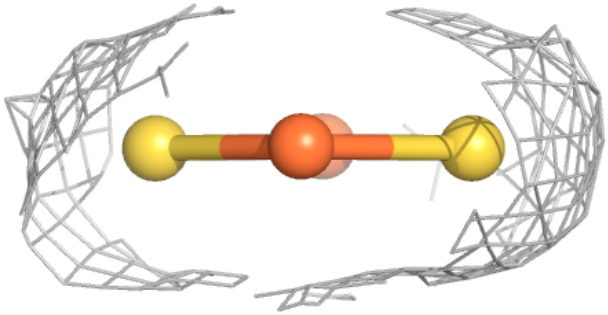


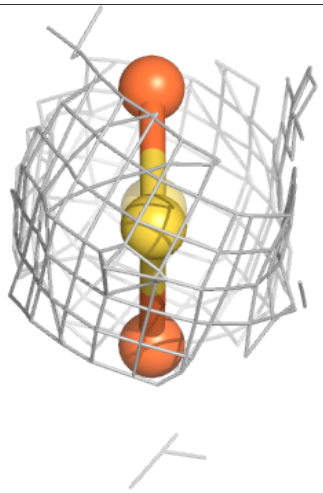


Electron density around FES E 502:

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

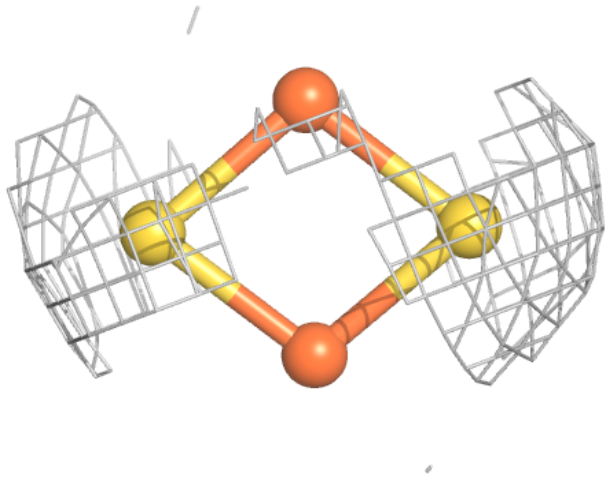


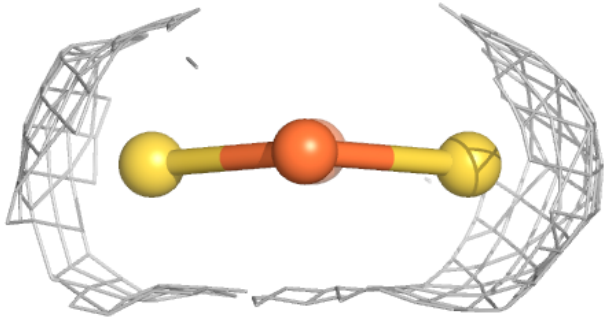


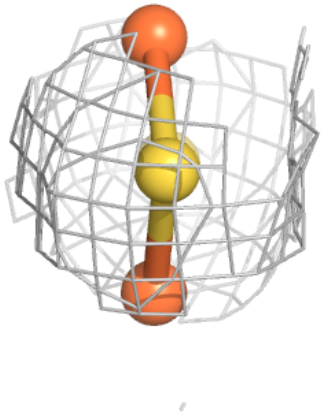


Electron density around FES F 502:

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

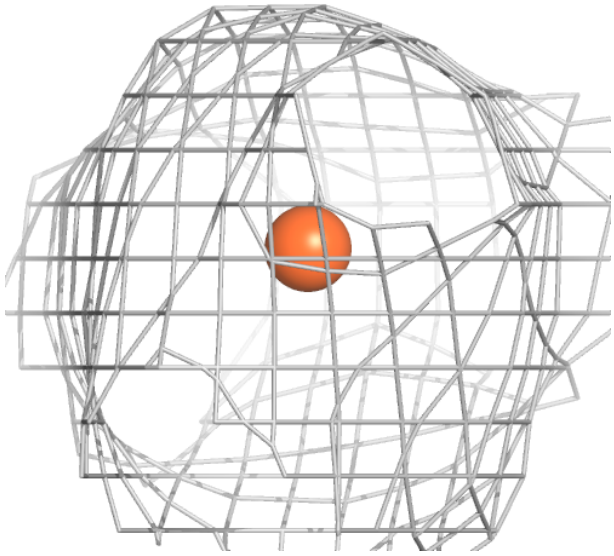


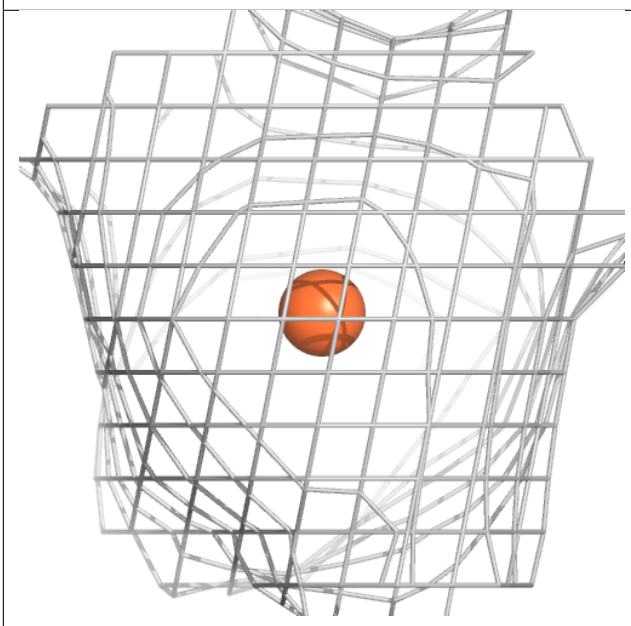


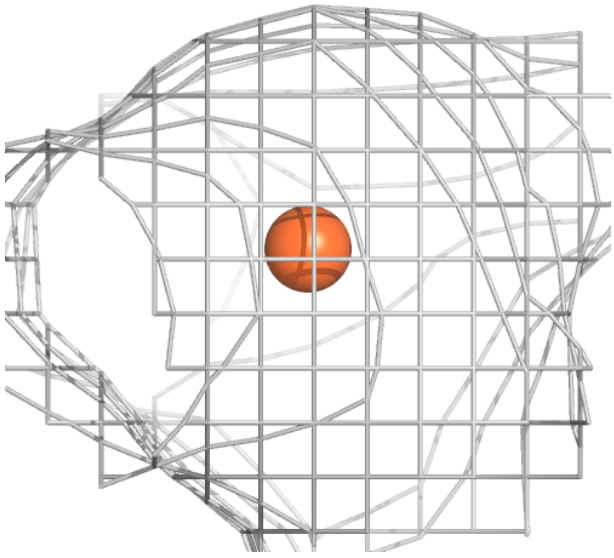


Electron density around FE2 A 501:

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

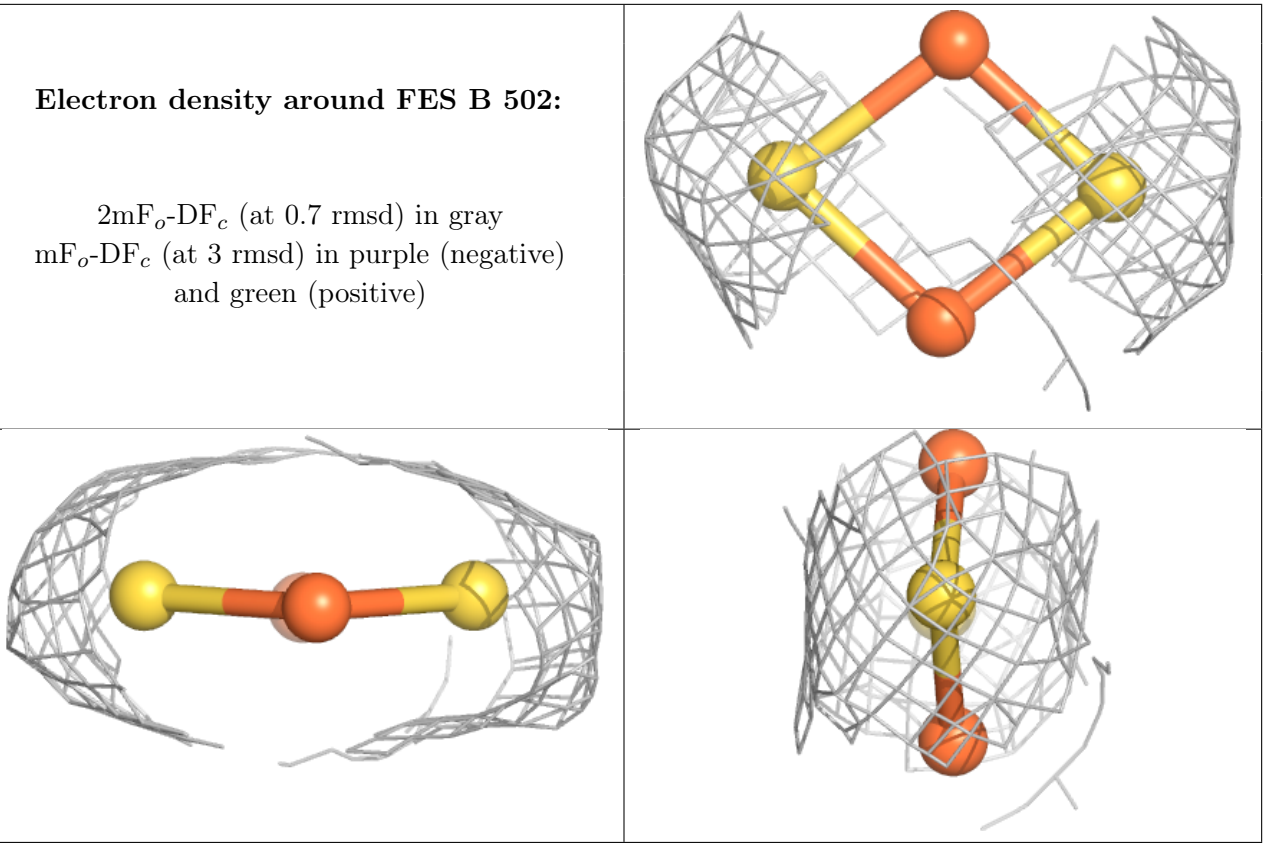






Electron density around FES B 502:

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



6.5 Other polymers

There are no such residues in this entry.