Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2024 – 09:39 AM JST

PDB ID	:	9JP5
Title	:	Phthalate 3,4-dioxygenase from Rhodococcus jostii RHA1
Authors	:	Kumar, K.A.; Kumar, P.
Deposited on	:	2024-09-25
Resolution	:	2.88 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:

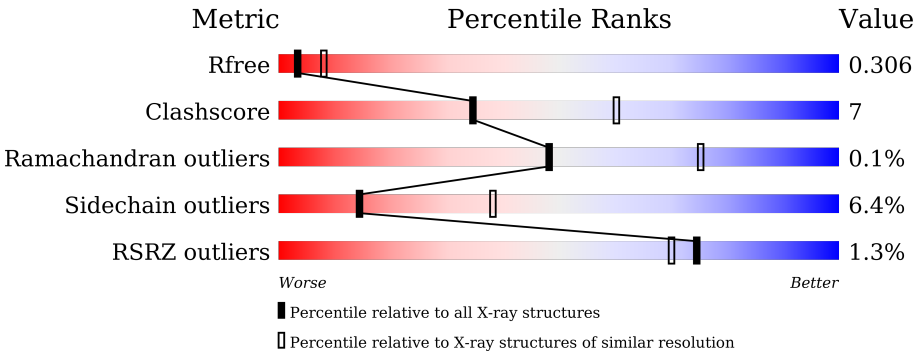
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.88 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}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	507	70% 18% • 11%
1	C	507	72% 12% •• 14%
1	E	507	71% 13% • 13%
1	G	507	72% 14% • 13%
2	B	208	73% 16% • 10%
2	D	208	73% 15% • 10%

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Mol	Chain	Length	Quality of chain
2	F	208	2% 72% 17% 8%
2	H	208	% 71% 17% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20893 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 Phthalate 3,4-dioxygenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	2	0
			3599	2275	619	684	21			
1	C	438	Total	C	N	O	S	0	0	0
			3504	2216	603	664	21			
1	E	441	Total	C	N	O	S	0	0	0
			3524	2226	606	671	21			
1	G	443	Total	C	N	O	S	0	0	0
			3539	2237	608	673	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP Q0RWD5
A	-29	GLY	-	expression tag	UNP Q0RWD5
A	-28	SER	-	expression tag	UNP Q0RWD5
A	-27	SER	-	expression tag	UNP Q0RWD5
A	-26	HIS	-	expression tag	UNP Q0RWD5
A	-25	HIS	-	expression tag	UNP Q0RWD5
A	-24	HIS	-	expression tag	UNP Q0RWD5
A	-23	HIS	-	expression tag	UNP Q0RWD5
A	-22	HIS	-	expression tag	UNP Q0RWD5
A	-21	HIS	-	expression tag	UNP Q0RWD5
A	-20	SER	-	expression tag	UNP Q0RWD5
A	-19	SER	-	expression tag	UNP Q0RWD5
A	-18	GLY	-	expression tag	UNP Q0RWD5
A	-17	LEU	-	expression tag	UNP Q0RWD5
A	-16	VAL	-	expression tag	UNP Q0RWD5
A	-15	PRO	-	expression tag	UNP Q0RWD5
A	-14	ARG	-	expression tag	UNP Q0RWD5
A	-13	GLY	-	expression tag	UNP Q0RWD5
A	-12	SER	-	expression tag	UNP Q0RWD5
A	-11	HIS	-	expression tag	UNP Q0RWD5
C	-30	MET	-	initiating methionine	UNP Q0RWD5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-29	GLY	-	expression tag	UNP Q0RWD5
C	-28	SER	-	expression tag	UNP Q0RWD5
C	-27	SER	-	expression tag	UNP Q0RWD5
C	-26	HIS	-	expression tag	UNP Q0RWD5
C	-25	HIS	-	expression tag	UNP Q0RWD5
C	-24	HIS	-	expression tag	UNP Q0RWD5
C	-23	HIS	-	expression tag	UNP Q0RWD5
C	-22	HIS	-	expression tag	UNP Q0RWD5
C	-21	HIS	-	expression tag	UNP Q0RWD5
C	-20	SER	-	expression tag	UNP Q0RWD5
C	-19	SER	-	expression tag	UNP Q0RWD5
C	-18	GLY	-	expression tag	UNP Q0RWD5
C	-17	LEU	-	expression tag	UNP Q0RWD5
C	-16	VAL	-	expression tag	UNP Q0RWD5
C	-15	PRO	-	expression tag	UNP Q0RWD5
C	-14	ARG	-	expression tag	UNP Q0RWD5
C	-13	GLY	-	expression tag	UNP Q0RWD5
C	-12	SER	-	expression tag	UNP Q0RWD5
C	-11	HIS	-	expression tag	UNP Q0RWD5
E	-30	MET	-	initiating methionine	UNP Q0RWD5
E	-29	GLY	-	expression tag	UNP Q0RWD5
E	-28	SER	-	expression tag	UNP Q0RWD5
E	-27	SER	-	expression tag	UNP Q0RWD5
E	-26	HIS	-	expression tag	UNP Q0RWD5
E	-25	HIS	-	expression tag	UNP Q0RWD5
E	-24	HIS	-	expression tag	UNP Q0RWD5
E	-23	HIS	-	expression tag	UNP Q0RWD5
E	-22	HIS	-	expression tag	UNP Q0RWD5
E	-21	HIS	-	expression tag	UNP Q0RWD5
E	-20	SER	-	expression tag	UNP Q0RWD5
E	-19	SER	-	expression tag	UNP Q0RWD5
E	-18	GLY	-	expression tag	UNP Q0RWD5
E	-17	LEU	-	expression tag	UNP Q0RWD5
E	-16	VAL	-	expression tag	UNP Q0RWD5
E	-15	PRO	-	expression tag	UNP Q0RWD5
E	-14	ARG	-	expression tag	UNP Q0RWD5
E	-13	GLY	-	expression tag	UNP Q0RWD5
E	-12	SER	-	expression tag	UNP Q0RWD5
E	-11	HIS	-	expression tag	UNP Q0RWD5
G	-30	MET	-	initiating methionine	UNP Q0RWD5
G	-29	GLY	-	expression tag	UNP Q0RWD5
G	-28	SER	-	expression tag	UNP Q0RWD5

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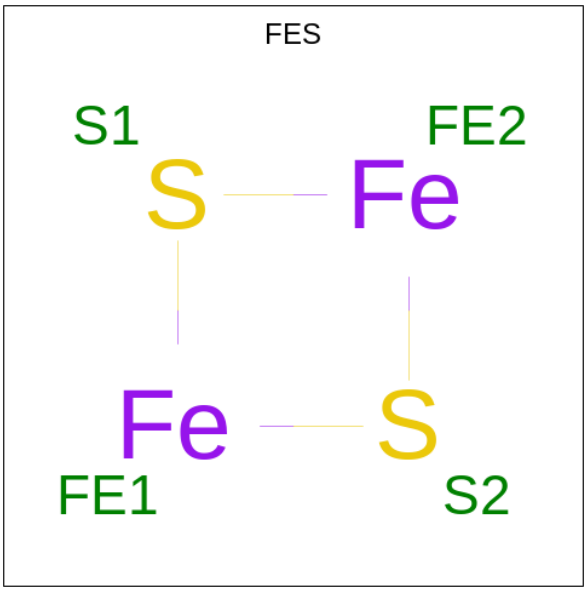
Chain	Residue	Modelled	Actual	Comment	Reference
G	-27	SER	-	expression tag	UNP Q0RWD5
G	-26	HIS	-	expression tag	UNP Q0RWD5
G	-25	HIS	-	expression tag	UNP Q0RWD5
G	-24	HIS	-	expression tag	UNP Q0RWD5
G	-23	HIS	-	expression tag	UNP Q0RWD5
G	-22	HIS	-	expression tag	UNP Q0RWD5
G	-21	HIS	-	expression tag	UNP Q0RWD5
G	-20	SER	-	expression tag	UNP Q0RWD5
G	-19	SER	-	expression tag	UNP Q0RWD5
G	-18	GLY	-	expression tag	UNP Q0RWD5
G	-17	LEU	-	expression tag	UNP Q0RWD5
G	-16	VAL	-	expression tag	UNP Q0RWD5
G	-15	PRO	-	expression tag	UNP Q0RWD5
G	-14	ARG	-	expression tag	UNP Q0RWD5
G	-13	GLY	-	expression tag	UNP Q0RWD5
G	-12	SER	-	expression tag	UNP Q0RWD5
G	-11	HIS	-	expression tag	UNP Q0RWD5

- Molecule 2 is a protein called Phthalate 3,4-dioxygenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1541	962	280	294	5			
2	D	188	Total	C	N	O	S	0	0	0
			1541	962	280	294	5			
2	F	191	Total	C	N	O	S	0	0	0
			1559	972	283	299	5			
2	H	188	Total	C	N	O	S	0	0	0
			1541	962	280	294	5			

- 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	A	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 97 97	0	0

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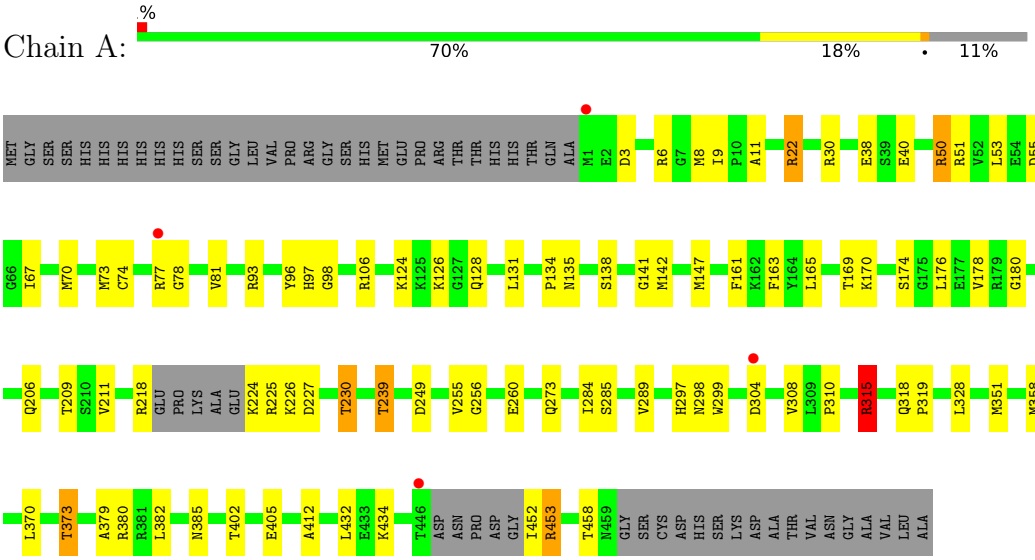
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	53	Total O 53 53	0	0
5	C	97	Total O 97 97	0	0
5	D	37	Total O 37 37	0	0
5	E	88	Total O 88 88	0	0
5	F	38	Total O 38 38	0	0
5	G	81	Total O 81 81	0	0
5	H	34	Total O 34 34	0	0

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.

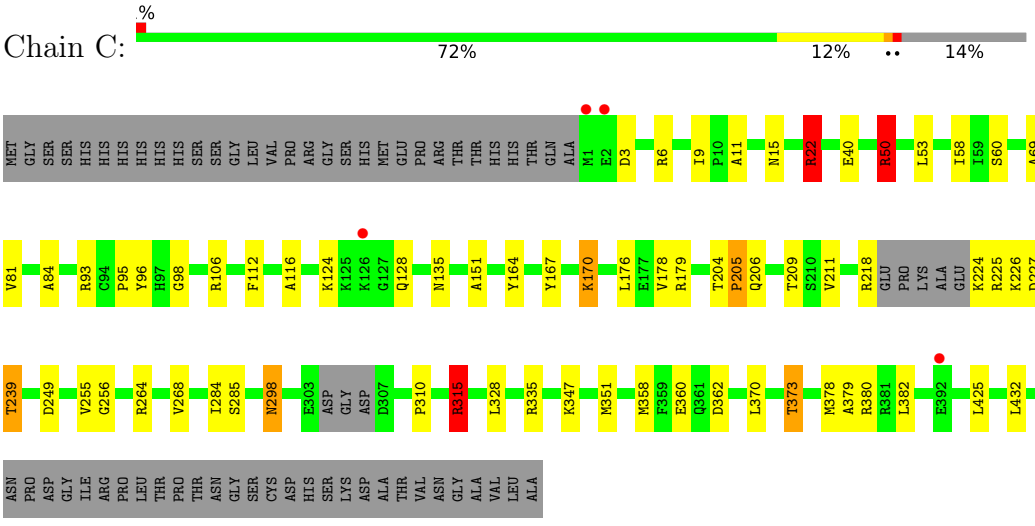
• Molecule 1: Phthalate 3,4-dioxygenase alpha subunit

Chain A:



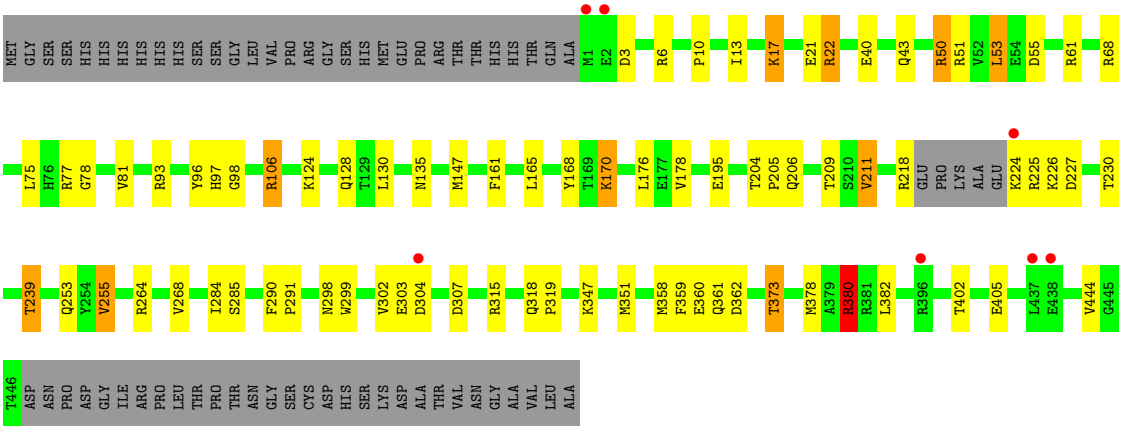
• Molecule 1: Phthalate 3,4-dioxygenase alpha subunit

Chain C:



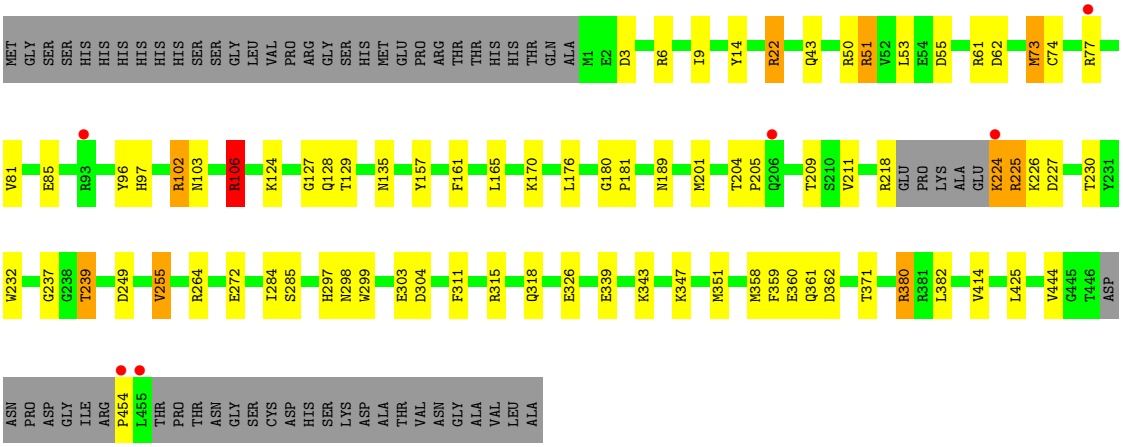
• Molecule 1: Phthalate 3,4-dioxygenase alpha subunit

Chain E:



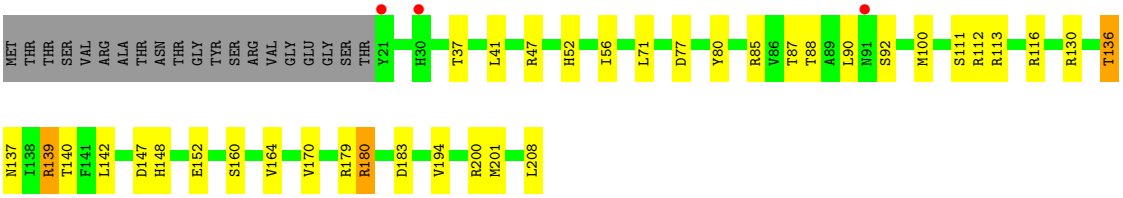
• Molecule 1: Phthalate 3,4-dioxygenase alpha subunit

Chain G:



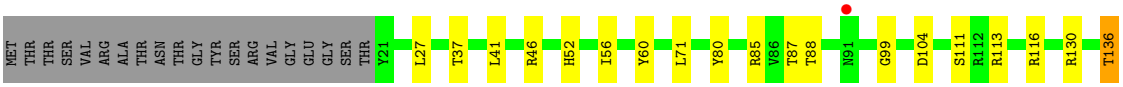
• Molecule 2: Phthalate 3,4-dioxygenase beta subunit

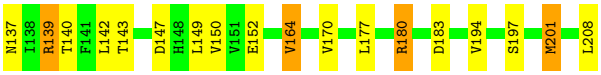
Chain B:



• Molecule 2: Phthalate 3,4-dioxygenase beta subunit

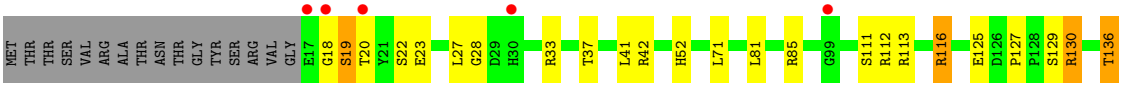
Chain D:

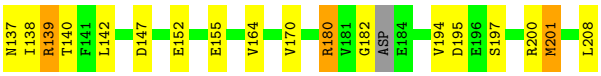




• Molecule 2: Phthalate 3,4-dioxygenase beta subunit

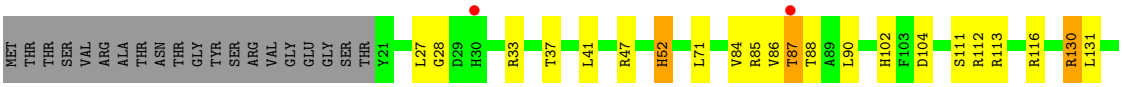
Chain F:

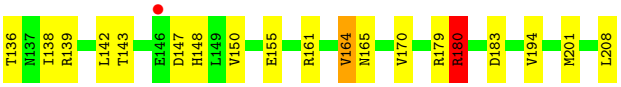




• Molecule 2: Phthalate 3,4-dioxygenase beta subunit

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	194.60Å 194.60Å 157.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.46 – 2.88 27.46 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (27.46-2.88) 99.2 (27.46-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.247 , 0.306 0.247 , 0.306	Depositor DCC
R_{free} test set	3833 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	20893	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: 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	0.45	0/3695	0.80	1/4991 (0.0%)
1	C	0.44	0/3592	0.77	2/4850 (0.0%)
1	E	0.43	0/3613	0.76	1/4880 (0.0%)
1	G	0.50	2/3628 (0.1%)	0.84	3/4899 (0.1%)
2	B	0.41	0/1574	0.78	0/2134
2	D	0.38	0/1574	0.75	0/2134
2	F	0.41	0/1591	0.79	1/2155 (0.0%)
2	H	0.42	0/1574	0.81	3/2134 (0.1%)
All	All	0.44	2/20841 (0.0%)	0.79	11/28177 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	2
1	E	0	4
1	G	0	3
2	B	0	1
2	F	0	2
2	H	0	1
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	326	GLU	CD-OE2	-6.33	1.18	1.25
1	G	326	GLU	CD-OE1	-5.83	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	77	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	G	380	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	G	106	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	315	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	F	116	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	380	ARG	CG-CD-NE	-5.51	100.23	111.80
1	C	22	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	H	180	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	H	180	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	50	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	H	139	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ARG	Sidechain
1	A	315	ARG	Sidechain
1	A	50	ARG	Sidechain
2	B	200	ARG	Sidechain
1	C	315	ARG	Sidechain
1	C	50	ARG	Sidechain
1	E	380	ARG	Sidechain
1	E	50	ARG	Sidechain
1	E	61	ARG	Sidechain
1	E	77	ARG	Sidechain
2	F	130	ARG	Sidechain
2	F	19	SER	Peptide
1	G	50	ARG	Sidechain
1	G	51	ARG	Sidechain
1	G	61	ARG	Sidechain
2	H	130	ARG	Sidechain

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	3599	0	3443	72	0
1	C	3504	0	3344	50	0
1	E	3524	0	3356	56	0
1	G	3539	0	3374	56	0
2	B	1541	0	1480	29	0
2	D	1541	0	1480	29	0
2	F	1559	0	1496	34	0
2	H	1541	0	1480	33	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0
3	E	4	0	0	1	0
3	G	4	0	0	1	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	97	0	0	4	0
5	B	53	0	0	2	0
5	C	97	0	0	7	0
5	D	37	0	0	1	0
5	E	88	0	0	5	0
5	F	38	0	0	3	0
5	G	81	0	0	11	0
5	H	34	0	0	1	0
All	All	20893	0	19453	295	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 7.

All (295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HG3	1:A:22:ARG:HH11	1.12	1.06
1:G:102:ARG:HD3	5:G:636:HOH:O	1.57	1.01
1:A:358:MET:HE2	2:B:116:ARG:HD2	1.46	0.98
1:C:22:ARG:HG3	1:C:22:ARG:HH11	1.29	0.96
1:C:239:THR:HG22	1:C:285:SER:HB3	1.48	0.94
1:A:22:ARG:HG3	1:A:22:ARG:NH1	1.82	0.92
1:G:454:PRO:HG3	5:G:676:HOH:O	1.70	0.90
1:E:22:ARG:HH11	1:E:22:ARG:CG	1.84	0.89
1:A:22:ARG:HH11	1:A:22:ARG:CG	1.86	0.89
1:C:22:ARG:HH11	1:C:22:ARG:CG	1.84	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:MET:HE2	2:F:116:ARG:HD2	1.54	0.89
1:C:351:MET:O	1:C:358:MET:HG3	1.74	0.87
2:F:19:SER:HB2	5:F:336:HOH:O	1.75	0.86
1:G:22:ARG:HH11	1:G:22:ARG:CG	1.88	0.85
1:G:102:ARG:HG2	5:G:611:HOH:O	1.77	0.84
1:C:358:MET:HE1	2:D:113:ARG:HA	1.59	0.84
1:E:239:THR:HG22	1:E:285:SER:HB3	1.60	0.83
1:C:358:MET:HE2	2:D:116:ARG:HD2	1.60	0.82
1:G:358:MET:HE2	2:H:116:ARG:HD2	1.61	0.82
1:E:22:ARG:HH11	1:E:22:ARG:HG3	1.46	0.81
1:G:239:THR:HG22	1:G:285:SER:HB3	1.63	0.80
1:C:22:ARG:HG3	1:C:22:ARG:NH1	1.90	0.77
1:G:3:ASP:OD1	1:G:6:ARG:NH2	2.18	0.77
1:G:454:PRO:CG	5:G:676:HOH:O	2.30	0.76
1:A:239:THR:HG22	1:A:285:SER:HB3	1.67	0.75
2:D:139:ARG:NH1	2:D:152:GLU:OE2	2.18	0.75
1:A:206:GLN:HG3	1:C:93:ARG:HH12	1.52	0.75
1:G:85:GLU:HG3	2:H:87:THR:HG22	1.69	0.74
1:E:358:MET:CE	2:F:113:ARG:HA	2.18	0.74
1:G:22:ARG:HH11	1:G:22:ARG:HG2	1.52	0.74
2:H:147:ASP:HB3	2:H:180:ARG:HB3	1.71	0.73
1:A:358:MET:HE1	2:B:113:ARG:HA	1.71	0.72
1:E:22:ARG:HG3	1:E:22:ARG:NH1	2.02	0.72
1:E:3:ASP:OD1	1:E:6:ARG:NH2	2.23	0.72
1:G:351:MET:O	1:G:358:MET:HG3	1.90	0.72
1:A:351:MET:O	1:A:358:MET:HG3	1.89	0.72
1:A:138:SER:OG	1:A:458:THR:HG21	1.90	0.71
1:G:272:GLU:HB2	5:G:656:HOH:O	1.88	0.71
1:G:358:MET:CE	2:H:116:ARG:HD2	2.20	0.71
1:C:93:ARG:HB2	5:C:691:HOH:O	1.91	0.71
1:E:351:MET:O	1:E:358:MET:HG3	1.92	0.70
1:G:361:GLN:OE1	2:H:116:ARG:NH1	2.24	0.70
1:A:224:LYS:HA	1:A:227:ASP:OD2	1.91	0.70
1:A:38:GLU:OE1	1:A:458:THR:HG22	1.93	0.69
1:C:335:ARG:HD2	5:C:641:HOH:O	1.92	0.69
1:E:97:HIS:HB2	3:E:501:FES:S1	2.32	0.68
1:E:358:MET:HE1	2:F:113:ARG:HA	1.74	0.68
2:F:18:GLY:HA3	2:F:23:GLU:HB3	1.75	0.68
1:G:22:ARG:NH1	1:G:22:ARG:HG3	2.09	0.68
1:G:157:TYR:CD1	5:G:677:HOH:O	2.48	0.67
1:G:22:ARG:CG	1:G:22:ARG:NH1	2.51	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:MET:HE3	2:H:113:ARG:HA	1.77	0.66
1:E:17:LYS:HE2	1:E:21:GLU:OE1	1.96	0.66
2:H:47:ARG:NH1	2:H:142:LEU:HD21	2.11	0.66
1:C:151:ALA:HA	5:C:612:HOH:O	1.96	0.65
1:A:358:MET:HE2	2:B:116:ARG:CD	2.25	0.65
1:E:362:ASP:CG	2:F:116:ARG:HH22	1.99	0.65
2:B:92:SER:HB2	5:B:349:HOH:O	1.97	0.64
2:F:112:ARG:HG2	2:F:112:ARG:HH11	1.63	0.64
1:C:264:ARG:NH1	5:C:602:HOH:O	2.26	0.64
1:E:224:LYS:HA	1:E:227:ASP:OD2	1.98	0.63
1:E:22:ARG:HH11	1:E:22:ARG:HG2	1.59	0.63
1:G:362:ASP:CG	2:H:116:ARG:HH22	2.01	0.63
1:E:106:ARG:CG	5:E:637:HOH:O	2.46	0.63
1:G:22:ARG:HH11	1:G:22:ARG:HG3	1.61	0.63
1:E:106:ARG:HG2	5:E:637:HOH:O	1.97	0.63
1:C:362:ASP:CG	2:D:116:ARG:HH22	2.02	0.63
1:G:102:ARG:CD	5:G:636:HOH:O	2.31	0.63
1:C:358:MET:CE	2:D:113:ARG:HA	2.28	0.62
1:A:206:GLN:HG2	1:C:98:GLY:HA3	1.79	0.62
2:F:200:ARG:HD3	5:F:320:HOH:O	1.98	0.62
1:C:206:GLN:HG3	1:E:93:ARG:HH12	1.64	0.62
1:G:362:ASP:OD2	2:H:116:ARG:NH2	2.32	0.62
1:G:43:GLN:OE1	1:G:43:GLN:HA	2.01	0.60
1:G:204:THR:HB	1:G:205:PRO:HD3	1.83	0.60
2:D:147:ASP:HB3	2:D:180:ARG:HB3	1.83	0.60
1:A:358:MET:CE	2:B:113:ARG:HA	2.32	0.60
2:B:136:THR:HG23	2:B:137:ASN:OD1	2.02	0.59
2:B:85:ARG:HG3	2:B:194:VAL:O	2.02	0.58
2:B:170:VAL:HG23	2:B:201:MET:HE3	1.85	0.58
1:A:141:GLY:H	1:A:458:THR:HG23	1.68	0.58
1:A:3:ASP:OD1	1:A:6:ARG:NH2	2.36	0.58
1:C:370:LEU:HD13	1:E:78:GLY:HA3	1.84	0.58
1:A:61:ARG:NH1	1:A:65:GLY:O	2.36	0.58
2:F:155:GLU:OE2	2:F:208:LEU:OXT	2.22	0.58
1:G:358:MET:HE1	2:H:116:ARG:HB2	1.85	0.57
1:C:373:THR:HG22	5:E:623:HOH:O	2.04	0.57
1:A:361:GLN:OE1	2:B:116:ARG:NH1	2.37	0.57
1:C:362:ASP:OD2	2:D:116:ARG:NH2	2.38	0.57
1:A:134:PRO:HG3	1:E:378:MET:HE3	1.86	0.56
1:G:358:MET:CE	2:H:113:ARG:HA	2.36	0.56
1:G:362:ASP:CG	2:H:116:ARG:NH2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HH12	1:A:360:GLU:CD	2.09	0.56
1:C:362:ASP:CG	2:D:116:ARG:NH2	2.59	0.56
1:E:362:ASP:CG	2:F:116:ARG:NH2	2.60	0.55
2:B:147:ASP:HB3	2:B:180:ARG:HB2	1.87	0.55
2:B:112:ARG:HG2	2:B:112:ARG:HH11	1.71	0.55
1:C:124:LYS:O	1:C:128:GLN:HG3	2.06	0.55
1:A:77:ARG:NH1	1:E:195:GLU:OE2	2.39	0.55
2:F:139:ARG:NH1	2:F:152:GLU:OE2	2.37	0.55
1:C:206:GLN:HG2	1:E:98:GLY:HA3	1.88	0.55
1:E:43:GLN:HA	1:E:43:GLN:OE1	2.07	0.54
2:B:148:HIS:NE2	2:B:179:ARG:HD3	2.22	0.54
2:B:139:ARG:NH1	2:B:152:GLU:OE2	2.37	0.54
1:E:204:THR:HB	1:E:205:PRO:HD3	1.89	0.54
2:D:170:VAL:HG23	2:D:201:MET:HE3	1.90	0.53
2:F:180:ARG:NH1	2:F:182:GLY:O	2.40	0.53
1:A:30:ARG:HD2	1:A:434:LYS:HD2	1.90	0.53
2:B:77:ASP:OD1	2:B:179:ARG:NH2	2.42	0.53
1:G:284:ILE:HG13	1:G:297:HIS:HD1	1.74	0.53
1:E:124:LYS:O	1:E:128:GLN:HG3	2.08	0.52
2:F:85:ARG:HG3	2:F:194:VAL:O	2.07	0.52
2:D:41:LEU:HD21	2:D:142:LEU:HG	1.89	0.52
1:A:370:LEU:HD12	1:A:370:LEU:O	2.09	0.52
2:B:47:ARG:NH1	2:B:142:LEU:HD21	2.25	0.52
2:H:84:VAL:HG22	2:H:102:HIS:CE1	2.44	0.52
1:E:362:ASP:OD2	2:F:116:ARG:NH2	2.42	0.52
1:A:453:ARG:HA	1:A:453:ARG:NE	2.25	0.52
1:G:358:MET:HE1	2:H:116:ARG:CB	2.40	0.52
1:G:255:VAL:HG22	1:G:299:TRP:CE2	2.45	0.51
5:B:332:HOH:O	2:D:197:SER:HB3	2.08	0.51
2:F:71:LEU:HD21	2:F:111:SER:HA	1.90	0.51
2:H:85:ARG:HG3	2:H:194:VAL:O	2.10	0.51
2:H:170:VAL:HG23	2:H:201:MET:HE3	1.92	0.51
1:E:361:GLN:OE1	2:F:116:ARG:NH1	2.43	0.51
1:A:169:THR:HA	1:A:176:LEU:HD22	1.92	0.51
1:A:124:LYS:O	1:A:128:GLN:HG3	2.10	0.51
1:A:180:GLY:HA2	2:B:100:MET:HG2	1.93	0.51
2:B:56:ILE:HD12	2:D:137:ASN:HA	1.93	0.51
1:E:170:LYS:HD3	1:E:268:VAL:HB	1.93	0.51
2:H:41:LEU:HD21	2:H:142:LEU:HG	1.93	0.51
1:E:255:VAL:HG22	1:E:299:TRP:CE2	2.46	0.51
1:C:40:GLU:CD	1:C:50:ARG:HH22	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:GLU:OE2	1:E:50:ARG:NH2	2.44	0.50
1:E:358:MET:HE3	2:F:113:ARG:HA	1.93	0.50
1:G:161:PHE:HE2	1:G:165:LEU:HD13	1.75	0.50
1:A:97:HIS:HB2	3:A:501:FES:S1	2.52	0.50
2:B:148:HIS:CE1	2:B:179:ARG:HD3	2.47	0.50
1:E:168:TYR:CE1	1:E:284:ILE:HD12	2.47	0.50
2:H:180:ARG:HH11	2:H:183:ASP:HA	1.76	0.49
1:A:373:THR:HG22	5:C:628:HOH:O	2.13	0.49
1:A:206:GLN:HG2	1:C:98:GLY:CA	2.42	0.49
1:C:9:ILE:HD12	1:C:425:LEU:HD13	1.95	0.49
2:B:130:ARG:NH2	2:D:87:THR:OG1	2.45	0.49
1:A:161:PHE:CE2	1:A:289:VAL:HG22	2.48	0.48
1:G:161:PHE:CE2	1:G:165:LEU:HD13	2.47	0.48
1:E:347:LYS:O	1:E:351:MET:HG3	2.13	0.48
1:E:161:PHE:HE2	1:E:165:LEU:HD13	1.78	0.48
1:G:127:GLY:N	5:G:609:HOH:O	2.37	0.48
1:A:134:PRO:HG2	1:A:147:MET:HA	1.95	0.48
1:A:138:SER:OG	1:A:458:THR:CG2	2.61	0.48
2:B:41:LEU:HD21	2:B:142:LEU:HG	1.96	0.48
1:C:79:MET:CE	1:C:95:PRO:HG2	2.44	0.48
2:D:71:LEU:HD21	2:D:111:SER:CB	2.44	0.47
2:D:143:THR:HG22	2:D:150:VAL:HG23	1.96	0.47
2:H:148:HIS:NE2	2:H:179:ARG:HD3	2.28	0.47
1:A:93:ARG:HH12	1:E:206:GLN:HG3	1.80	0.47
2:D:85:ARG:HG3	2:D:194:VAL:O	2.13	0.47
1:E:302:VAL:HG23	1:E:307:ASP:O	2.15	0.47
1:G:414:VAL:HG22	5:G:617:HOH:O	2.15	0.47
2:H:86:VAL:HG23	2:H:88:THR:HG23	1.97	0.47
2:F:125:GLU:OE1	2:F:129:SER:OG	2.33	0.47
2:H:52:HIS:CE1	2:H:138:ILE:HD12	2.49	0.47
1:A:453:ARG:HA	1:A:453:ARG:CZ	2.45	0.46
1:E:106:ARG:HG3	5:E:637:HOH:O	2.12	0.46
2:B:71:LEU:HD21	2:B:111:SER:HA	1.97	0.46
2:B:87:THR:OG1	2:F:130:ARG:NH2	2.49	0.46
1:C:3:ASP:OD1	1:C:6:ARG:NH2	2.49	0.46
1:A:385:ASN:HB2	1:C:444:VAL:O	2.14	0.46
1:C:204:THR:HB	1:C:205:PRO:HD3	1.97	0.46
1:G:106:ARG:HA	1:G:129:THR:HG22	1.97	0.46
1:C:112:PHE:O	1:C:116:ALA:HB3	2.15	0.46
1:C:347:LYS:O	1:C:351:MET:HG3	2.16	0.46
1:E:347:LYS:HB2	2:F:27:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:THR:HG22	2:F:22:SER:H	1.80	0.46
1:A:255:VAL:HG22	1:A:299:TRP:CE2	2.51	0.46
2:D:27:LEU:HB2	2:D:104:ASP:OD1	2.16	0.46
2:F:28:GLY:O	2:F:33:ARG:NH2	2.49	0.46
2:D:180:ARG:NH1	2:D:183:ASP:HA	2.32	0.45
2:D:46:ARG:NH1	2:F:42:ARG:HD3	2.31	0.45
1:G:124:LYS:O	1:G:128:GLN:HG3	2.16	0.45
1:G:51:ARG:HA	1:G:55:ASP:O	2.16	0.45
1:A:53:LEU:HD11	1:A:319:PRO:HG2	1.97	0.45
1:A:161:PHE:CE2	1:A:165:LEU:HD13	2.51	0.45
1:E:402:THR:OG1	1:E:405:GLU:HG3	2.17	0.45
1:A:260:GLU:H	1:A:260:GLU:CD	2.20	0.45
1:G:232:TRP:CE3	1:G:237:GLY:HA3	2.52	0.45
2:D:56:ILE:O	2:D:60:TYR:HD1	1.99	0.45
1:E:161:PHE:CE2	1:E:165:LEU:HD13	2.51	0.45
1:C:335:ARG:CD	5:C:641:HOH:O	2.56	0.45
1:C:84:ALA:HB1	2:D:88:THR:HA	1.99	0.45
1:C:358:MET:HE2	2:D:116:ARG:CD	2.39	0.45
1:E:358:MET:HE1	2:F:116:ARG:HB2	1.98	0.45
1:A:40:GLU:CD	1:A:50:ARG:HH22	2.21	0.45
5:D:321:HOH:O	2:F:197:SER:HB3	2.15	0.44
1:C:224:LYS:HA	1:C:227:ASP:OD2	2.17	0.44
2:F:41:LEU:HD21	2:F:142:LEU:HG	2.00	0.44
1:G:224:LYS:HA	1:G:227:ASP:OD2	2.17	0.44
1:A:206:GLN:HG3	1:C:93:ARG:NH1	2.28	0.44
1:E:358:MET:HE2	2:F:116:ARG:CD	2.35	0.44
1:A:38:GLU:HG2	1:A:67:ILE:CD1	2.47	0.44
1:A:51:ARG:HA	1:A:55:ASP:O	2.17	0.44
1:C:256:GLY:HA3	1:C:310:PRO:HD3	1.99	0.44
2:F:136:THR:HG23	2:F:137:ASN:OD1	2.16	0.44
2:H:155:GLU:OE2	2:H:208:LEU:OXT	2.35	0.44
1:C:298:ASN:O	1:C:310:PRO:HA	2.18	0.44
1:E:53:LEU:HD11	1:E:319:PRO:HG2	2.00	0.44
1:G:347:LYS:HB2	2:H:27:LEU:HD11	2.00	0.44
2:H:143:THR:HG22	2:H:150:VAL:HG23	1.98	0.44
1:C:206:GLN:HG2	1:E:98:GLY:CA	2.47	0.44
1:A:186:VAL:HA	5:A:627:HOH:O	2.17	0.44
2:F:147:ASP:HB3	2:F:180:ARG:HB2	2.00	0.44
1:A:78:GLY:O	1:E:373:THR:HG21	2.18	0.43
1:A:315:ARG:NH1	1:A:360:GLU:OE1	2.51	0.43
1:C:164:TYR:CG	1:C:231:TYR:CE2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:170:VAL:HG23	2:F:201:MET:HE3	2.00	0.43
2:B:130:ARG:NH1	2:B:160:SER:OG	2.52	0.43
1:G:201:MET:HG2	1:G:225:ARG:NH1	2.32	0.43
2:H:164:VAL:HG23	2:H:165:ASN:ND2	2.33	0.43
1:G:161:PHE:HE2	1:G:165:LEU:CD1	2.32	0.43
1:G:311:PHE:CD1	1:G:311:PHE:C	2.91	0.43
2:H:27:LEU:HB2	2:H:104:ASP:OD1	2.18	0.43
1:A:22:ARG:HG2	1:A:432:LEU:HD22	2.00	0.43
1:A:163:PHE:CZ	1:A:273:GLN:HA	2.54	0.43
1:A:284:ILE:HG13	1:A:297:HIS:HD1	1.83	0.43
1:G:358:MET:HE2	2:H:116:ARG:CD	2.38	0.43
1:A:373:THR:HG21	1:C:78:GLY:O	2.18	0.43
1:A:126:LYS:HD2	5:A:668:HOH:O	2.18	0.43
1:C:179:ARG:NH1	2:D:99:GLY:O	2.49	0.43
1:G:43:GLN:OE1	1:G:43:GLN:CA	2.67	0.43
1:A:308:VAL:O	5:A:601:HOH:O	2.21	0.43
1:E:302:VAL:HG12	1:E:303:GLU:H	1.83	0.43
1:A:256:GLY:HA3	1:A:310:PRO:HD3	2.01	0.43
1:A:362:ASP:CG	2:B:116:ARG:NH2	2.71	0.43
1:E:211:VAL:HG11	1:E:359:PHE:CZ	2.54	0.43
2:H:71:LEU:HD21	2:H:111:SER:CB	2.49	0.43
1:E:51:ARG:HA	1:E:55:ASP:O	2.19	0.43
1:G:358:MET:CE	2:H:116:ARG:CD	2.95	0.43
2:D:130:ARG:HD2	2:F:195:ASP:O	2.19	0.42
1:C:40:GLU:OE2	1:C:50:ARG:NH2	2.47	0.42
2:F:52:HIS:CE1	2:F:138:ILE:HD12	2.55	0.42
1:A:8:MET:C	1:A:9:ILE:HD13	2.39	0.42
1:A:141:GLY:N	1:A:458:THR:HG23	2.32	0.42
1:C:167:TYR:HB2	1:C:284:ILE:HD13	2.00	0.42
1:G:62:ASP:HA	1:G:103:ASN:HD21	1.85	0.42
2:H:161:ARG:HD3	5:H:321:HOH:O	2.19	0.42
1:E:43:GLN:OE1	1:E:43:GLN:CA	2.67	0.42
1:G:339:GLU:O	1:G:343:LYS:HG3	2.19	0.42
1:E:211:VAL:HG11	1:E:359:PHE:CE1	2.54	0.42
2:H:112:ARG:HH11	2:H:112:ARG:HG2	1.84	0.42
1:A:402:THR:OG1	1:A:405:GLU:HG3	2.20	0.42
1:E:290:PHE:HA	1:E:291:PRO:HA	1.78	0.42
1:A:142:MET:SD	1:A:169:THR:HG21	2.60	0.42
1:E:10:PRO:O	1:E:13:ILE:HG23	2.20	0.42
1:E:264:ARG:NH1	5:E:608:HOH:O	2.53	0.42
1:G:22:ARG:HD2	5:G:630:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LEU:O	2:D:177:LEU:HD12	2.19	0.42
1:G:9:ILE:HD12	1:G:425:LEU:HD13	2.01	0.41
1:G:180:GLY:HA3	1:G:181:PRO:HA	1.84	0.41
1:C:315:ARG:HA	1:C:328:LEU:O	2.19	0.41
1:A:98:GLY:HA3	1:E:206:GLN:HG2	2.01	0.41
2:F:19:SER:CB	5:F:336:HOH:O	2.52	0.41
2:B:88:THR:O	2:F:127:PRO:HB3	2.21	0.41
1:E:75:LEU:HD21	1:E:130:LEU:HA	2.02	0.41
2:B:80:TYR:OH	2:B:208:LEU:O	2.28	0.41
1:C:58:ILE:O	1:C:69:ALA:HA	2.20	0.41
1:C:167:TYR:CB	1:C:284:ILE:HD13	2.51	0.41
1:G:73:MET:HG2	1:G:74:CYS:O	2.20	0.41
1:A:11:ALA:HB3	1:A:379:ALA:O	2.21	0.41
1:A:190:TRP:CE2	1:A:191:LYS:HG3	2.56	0.41
1:A:328:LEU:HD12	1:A:328:LEU:N	2.36	0.41
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.92	0.41
1:C:11:ALA:HB3	1:C:379:ALA:O	2.20	0.41
1:C:170:LYS:HD3	1:C:268:VAL:HB	2.03	0.41
2:D:80:TYR:OH	2:D:208:LEU:O	2.30	0.41
2:D:136:THR:HG23	2:D:137:ASN:OD1	2.21	0.41
1:G:264:ARG:NH1	5:G:606:HOH:O	2.47	0.41
1:A:22:ARG:NH1	1:A:22:ARG:CG	2.54	0.41
1:A:40:GLU:OE2	1:A:50:ARG:NH2	2.49	0.41
5:C:666:HOH:O	2:D:164:VAL:HG21	2.21	0.41
1:A:70:MET:HG2	1:A:452:ILE:CD1	2.51	0.40
1:A:224:LYS:CE	5:A:603:HOH:O	2.69	0.40
1:A:362:ASP:CG	2:B:116:ARG:HH22	2.24	0.40
2:B:180:ARG:NH1	2:B:183:ASP:HA	2.36	0.40
2:D:71:LEU:HD21	2:D:111:SER:HA	2.03	0.40
1:G:211:VAL:HG11	1:G:359:PHE:CZ	2.56	0.40
2:H:28:GLY:O	2:H:33:ARG:NH2	2.54	0.40
1:A:230:THR:O	1:A:412:ALA:HA	2.22	0.40
1:G:14:TYR:O	1:G:189:ASN:HB2	2.21	0.40
1:G:97:HIS:HB2	3:G:501:FES:S2	2.62	0.40
2:H:90:LEU:HD23	2:H:90:LEU:HA	1.94	0.40
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.87	0.40
1:C:378:MET:HG2	1:E:147:MET:HE1	2.04	0.40
1:A:73:MET:HG2	1:A:74:CYS:O	2.22	0.40
1:A:161:PHE:HE2	1:A:165:LEU:HD13	1.85	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	445/507 (88%)	433 (97%)	12 (3%)	0	100 100
1	C	432/507 (85%)	409 (95%)	22 (5%)	1 (0%)	44 71
1	E	437/507 (86%)	420 (96%)	17 (4%)	0	100 100
1	G	437/507 (86%)	417 (95%)	18 (4%)	2 (0%)	25 53
2	B	186/208 (89%)	177 (95%)	9 (5%)	0	100 100
2	D	186/208 (89%)	173 (93%)	13 (7%)	0	100 100
2	F	187/208 (90%)	173 (92%)	14 (8%)	0	100 100
2	H	186/208 (89%)	173 (93%)	13 (7%)	0	100 100
All	All	2496/2860 (87%)	2375 (95%)	118 (5%)	3 (0%)	48 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	303	GLU
1	C	15	ASN
1	G	53	LEU

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	381/426 (89%)	357 (94%)	24 (6%)	15 39
1	C	369/426 (87%)	341 (92%)	28 (8%)	11 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	371/426 (87%)	342 (92%)	29 (8%)	10 28
1	G	373/426 (88%)	346 (93%)	27 (7%)	12 32
2	B	167/183 (91%)	160 (96%)	7 (4%)	25 56
2	D	167/183 (91%)	159 (95%)	8 (5%)	21 51
2	F	169/183 (92%)	161 (95%)	8 (5%)	22 52
2	H	167/183 (91%)	159 (95%)	8 (5%)	21 51
All	All	2164/2436 (89%)	2025 (94%)	139 (6%)	14 38

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	81	VAL
1	A	96	TYR
1	A	106	ARG
1	A	131	LEU
1	A	135	ASN
1	A	170	LYS
1	A	174	SER
1	A	178	VAL
1	A	209	THR
1	A	211	VAL
1	A	225	ARG
1	A	226	LYS
1	A	230	THR
1	A	239	THR
1	A	249	ASP
1	A	298	ASN
1	A	304	ASP
1	A	315	ARG
1	A	318	GLN
1	A	373	THR
1	A	380	ARG
1	A	382	LEU
1	A	453	ARG
2	B	37	THR
2	B	52	HIS
2	B	136	THR
2	B	139	ARG
2	B	140	THR

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Mol	Chain	Res	Type
2	B	164	VAL
2	B	180	ARG
1	C	22	ARG
1	C	53	LEU
1	C	60	SER
1	C	81	VAL
1	C	96	TYR
1	C	106	ARG
1	C	135	ASN
1	C	170	LYS
1	C	176	LEU
1	C	178	VAL
1	C	205	PRO
1	C	209	THR
1	C	211	VAL
1	C	218	ARG
1	C	225	ARG
1	C	226	LYS
1	C	230	THR
1	C	239	THR
1	C	249	ASP
1	C	255	VAL
1	C	298	ASN
1	C	315	ARG
1	C	360	GLU
1	C	373	THR
1	C	380	ARG
1	C	382	LEU
1	C	432	LEU
1	C	444	VAL
2	D	37	THR
2	D	52	HIS
2	D	136	THR
2	D	139	ARG
2	D	140	THR
2	D	164	VAL
2	D	180	ARG
2	D	201	MET
1	E	17	LYS
1	E	22	ARG
1	E	53	LEU
1	E	68	ARG

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Mol	Chain	Res	Type
1	E	81	VAL
1	E	96	TYR
1	E	106	ARG
1	E	135	ASN
1	E	170	LYS
1	E	176	LEU
1	E	178	VAL
1	E	209	THR
1	E	211	VAL
1	E	218	ARG
1	E	225	ARG
1	E	226	LYS
1	E	230	THR
1	E	239	THR
1	E	253	GLN
1	E	255	VAL
1	E	298	ASN
1	E	304	ASP
1	E	315	ARG
1	E	318	GLN
1	E	360	GLU
1	E	373	THR
1	E	380	ARG
1	E	382	LEU
1	E	444	VAL
2	F	37	THR
2	F	81	LEU
2	F	136	THR
2	F	139	ARG
2	F	140	THR
2	F	164	VAL
2	F	180	ARG
2	F	201	MET
1	G	22	ARG
1	G	73	MET
1	G	81	VAL
1	G	96	TYR
1	G	102	ARG
1	G	106	ARG
1	G	135	ASN
1	G	170	LYS
1	G	176	LEU

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Mol	Chain	Res	Type
1	G	209	THR
1	G	218	ARG
1	G	224	LYS
1	G	225	ARG
1	G	226	LYS
1	G	230	THR
1	G	239	THR
1	G	249	ASP
1	G	255	VAL
1	G	298	ASN
1	G	304	ASP
1	G	315	ARG
1	G	318	GLN
1	G	360	GLU
1	G	371	THR
1	G	380	ARG
1	G	382	LEU
1	G	444	VAL
2	H	37	THR
2	H	52	HIS
2	H	87	THR
2	H	130	ARG
2	H	131	LEU
2	H	136	THR
2	H	164	VAL
2	H	180	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	253	GLN
1	A	366	ASN
2	B	65	GLN
1	C	366	ASN
2	D	65	GLN
1	E	103	ASN
1	E	366	ASN
2	H	121	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	G	501	1	0,4,4	-	-	-		
3	FES	E	501	1	0,4,4	-	-	-		
3	FES	C	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	G	501	1	-	-	0/1/1/1
3	FES	E	501	1	-	-	0/1/1/1
3	FES	C	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.

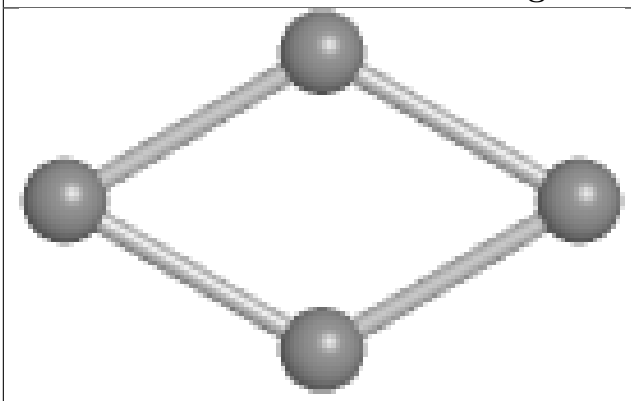
There are no ring outliers.

3 monomers are involved in 3 short contacts:

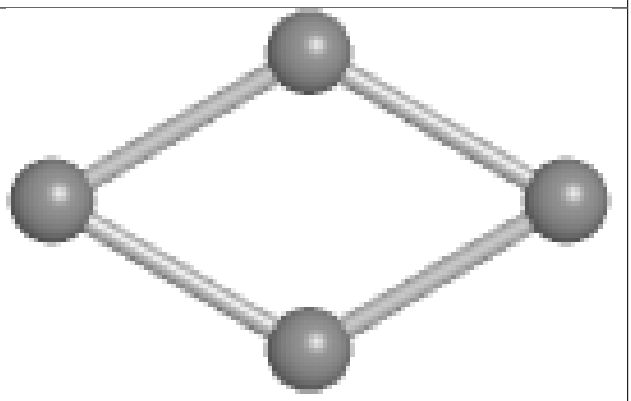
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	FES	1	0
3	G	501	FES	1	0
3	E	501	FES	1	0

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 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.

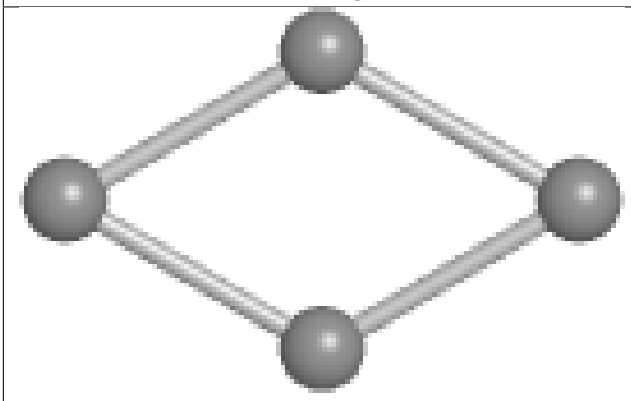
Ligand FES A 501



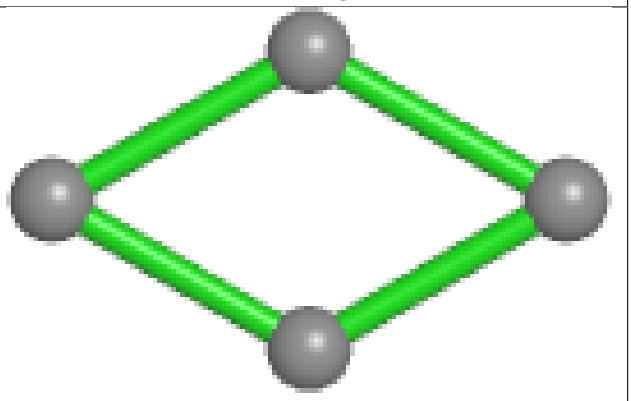
Bond lengths



Bond angles

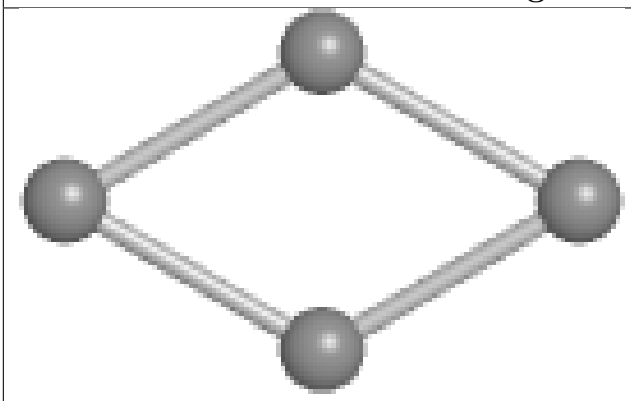


Torsions

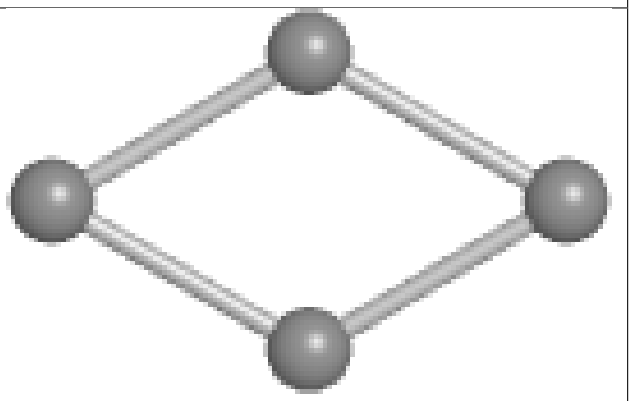


Rings

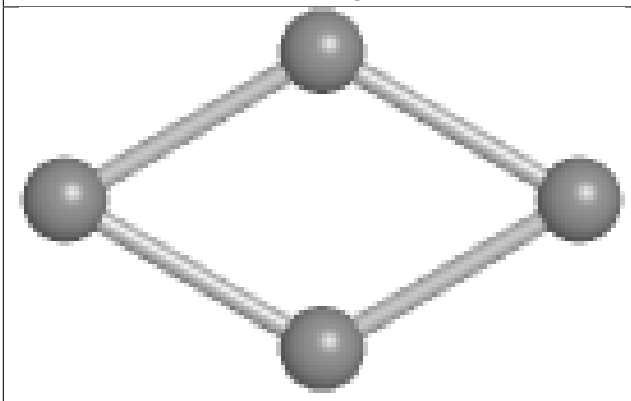
Ligand FES G 501



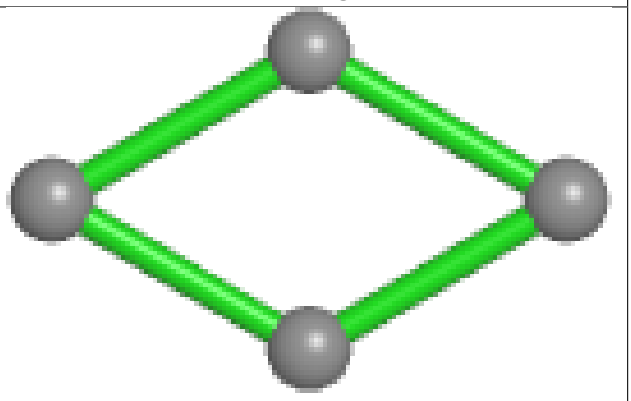
Bond lengths



Bond angles

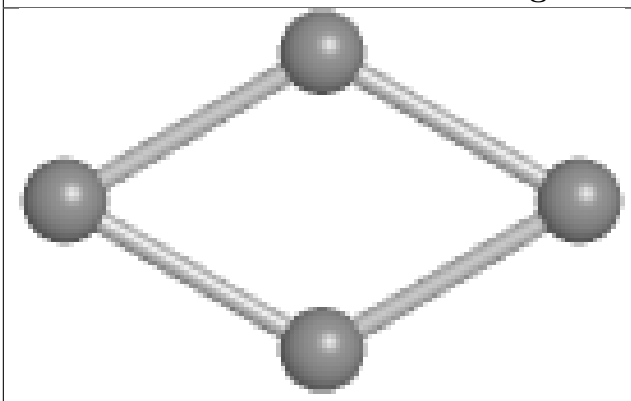


Torsions

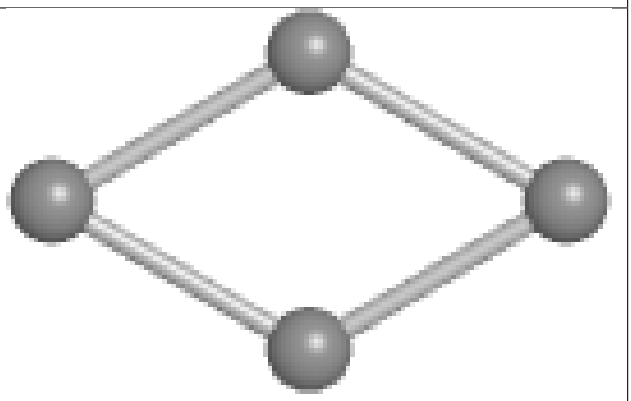


Rings

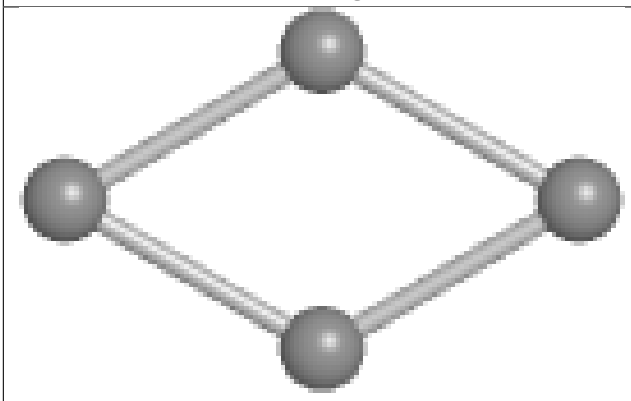
Ligand FES E 501



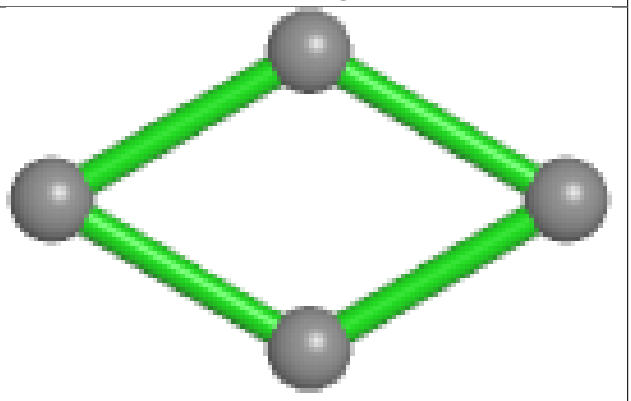
Bond lengths



Bond angles

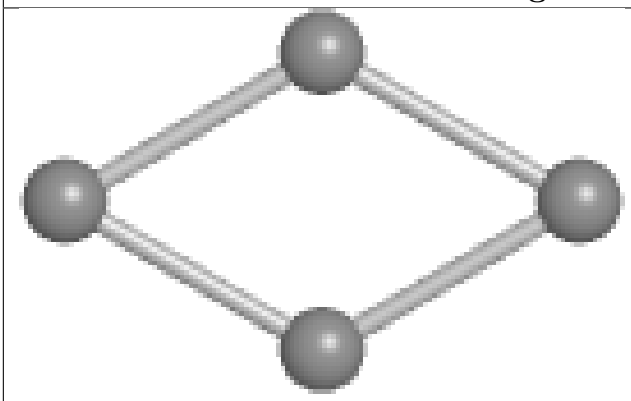


Torsions

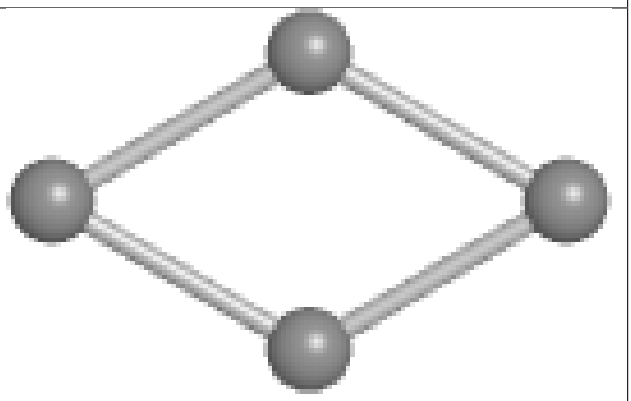


Rings

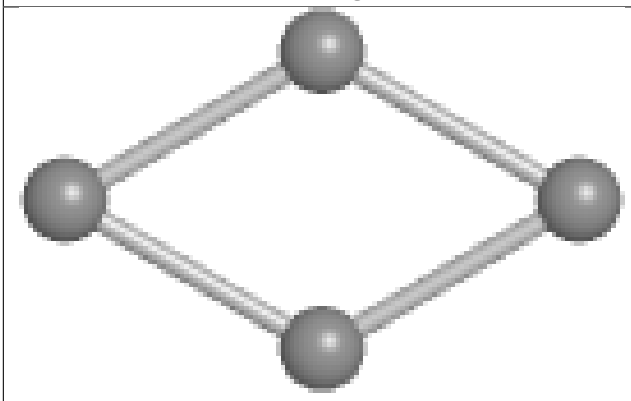
Ligand FES C 501



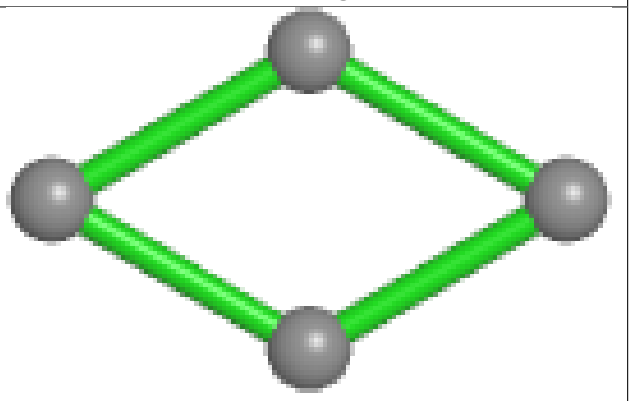
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	449/507 (88%)	-0.05	4 (0%)	81	77	7, 16, 36, 54	2 (0%)
1	C	438/507 (86%)	-0.04	4 (0%)	81	77	6, 18, 38, 59	0
1	E	441/507 (86%)	0.09	7 (1%)	70	65	8, 19, 42, 63	0
1	G	443/507 (87%)	-0.02	6 (1%)	73	68	4, 13, 34, 72	0
2	B	188/208 (90%)	0.09	3 (1%)	70	65	9, 22, 40, 60	0
2	D	188/208 (90%)	0.07	1 (0%)	87	85	12, 25, 41, 61	0
2	F	191/208 (91%)	0.24	5 (2%)	57	52	12, 25, 45, 63	0
2	H	188/208 (90%)	0.20	3 (1%)	70	65	9, 22, 40, 68	0
All	All	2526/2860 (88%)	0.04	33 (1%)	74	70	4, 19, 40, 72	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	454	PRO	5.0
1	G	455	LEU	3.8
2	H	30	HIS	3.3
1	E	304	ASP	3.3
2	F	30	HIS	3.3
1	G	93	ARG	3.2
2	F	20	THR	3.2
2	F	17	GLU	3.1
1	G	224	LYS	2.8
1	E	2	GLU	2.8
1	G	206	GLN	2.7
1	E	1	MET	2.7
2	F	18	GLY	2.6
1	C	392	GLU	2.6
2	H	87	THR	2.5
2	B	30	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	THR	2.5
1	C	2	GLU	2.4
1	A	77	ARG	2.3
2	B	21	TYR	2.2
2	F	99	GLY	2.2
1	G	77	ARG	2.2
1	A	304	ASP	2.2
1	C	1	MET	2.1
1	E	224	LYS	2.1
2	B	91	ASN	2.1
1	E	438	GLU	2.1
1	A	1	MET	2.1
1	E	396	ARG	2.1
1	C	126	LYS	2.0
2	H	146	GLU	2.0
2	D	91	ASN	2.0
1	E	437	LEU	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
3	FES	E	501	4/4	0.98	0.04	16,18,19,19	0
3	FES	C	501	4/4	0.99	0.03	13,13,13,14	0
3	FES	A	501	4/4	0.99	0.04	17,18,18,18	0
4	FE2	C	502	1/1	0.99	0.02	4,4,4,4	0
4	FE2	E	502	1/1	0.99	0.03	6,6,6,6	0
3	FES	G	501	4/4	1.00	0.02	9,9,9,9	0

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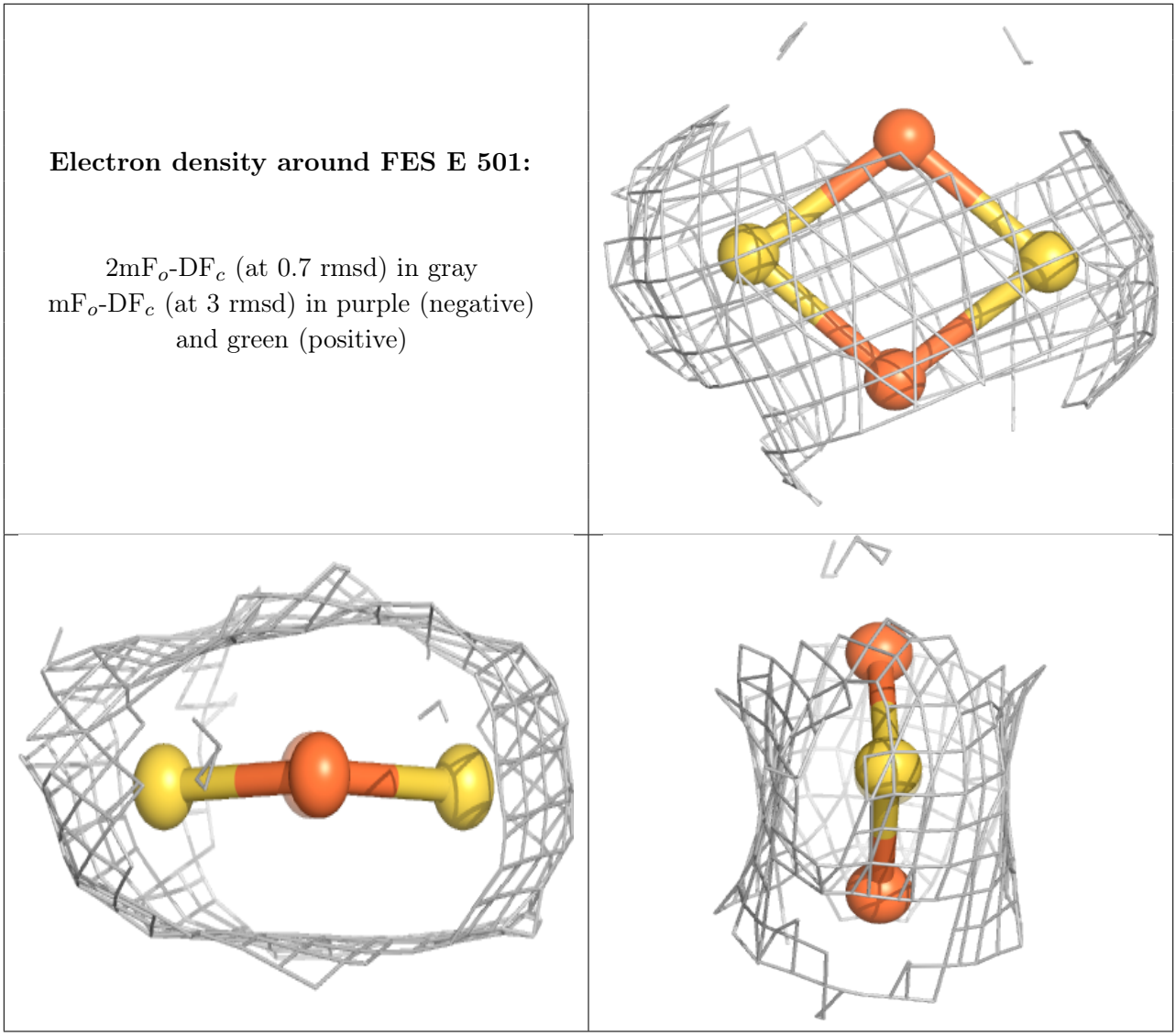
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FE2	A	502	1/1	1.00	0.02	2,2,2,2	0
4	FE2	G	502	1/1	1.00	0.01	3,3,3,3	0

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.

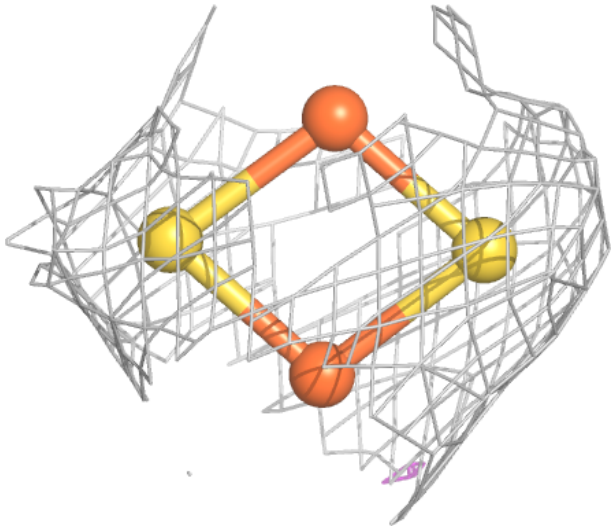
Electron density around FES E 501:

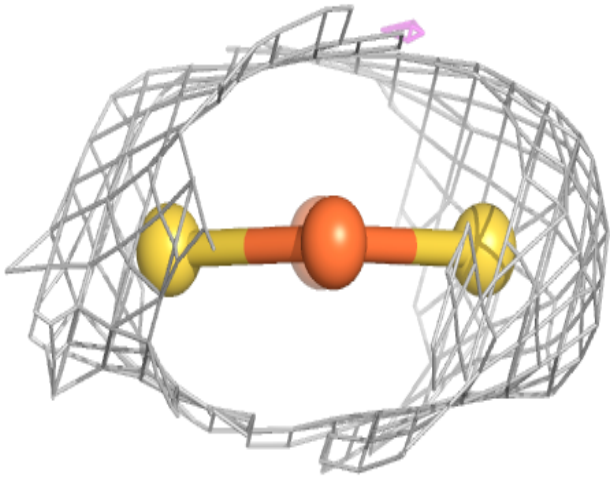
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

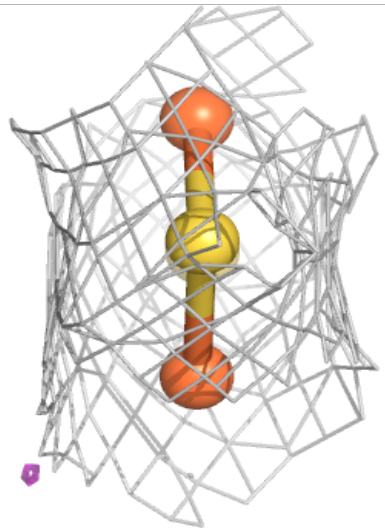


Electron density around FES C 501:

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

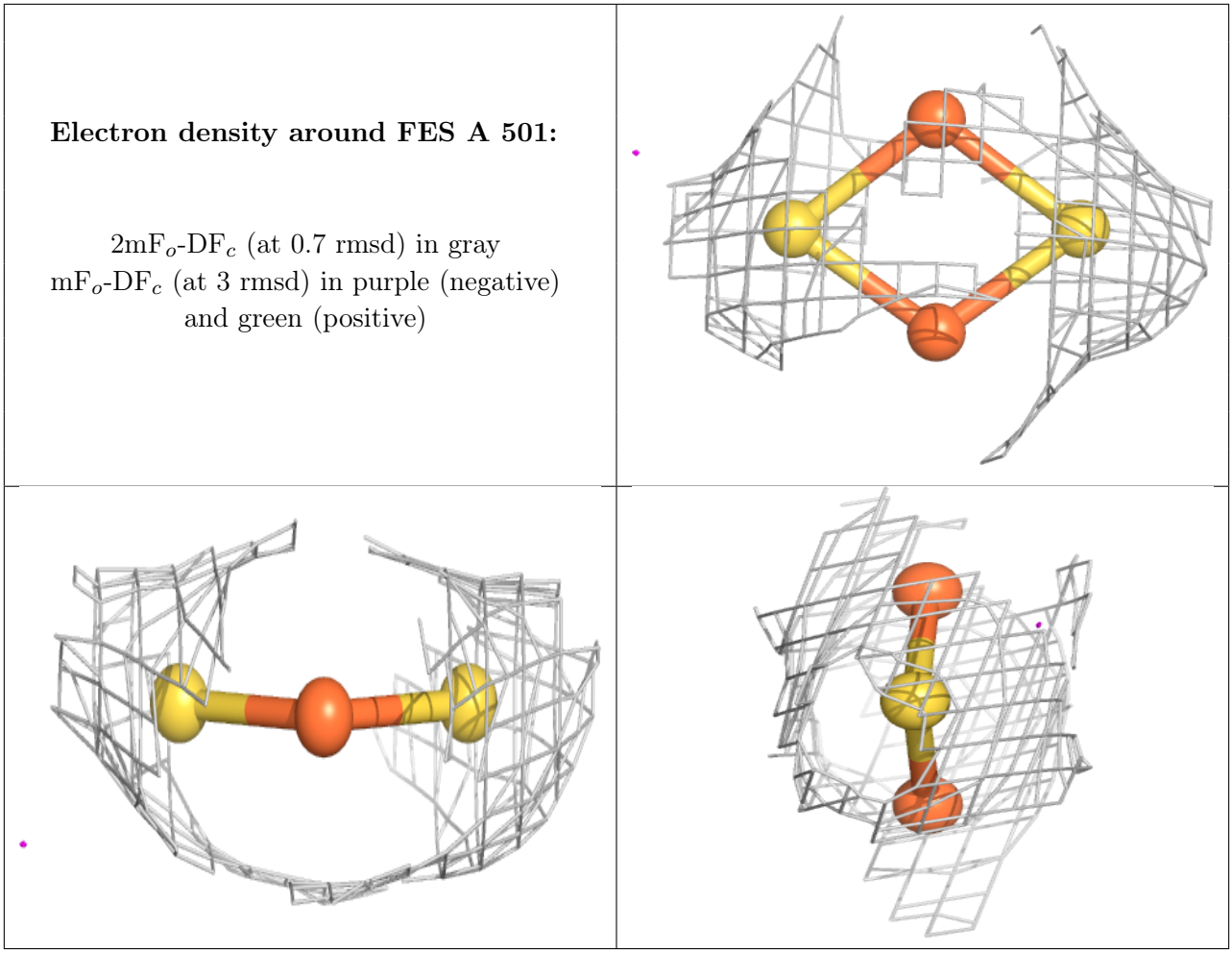






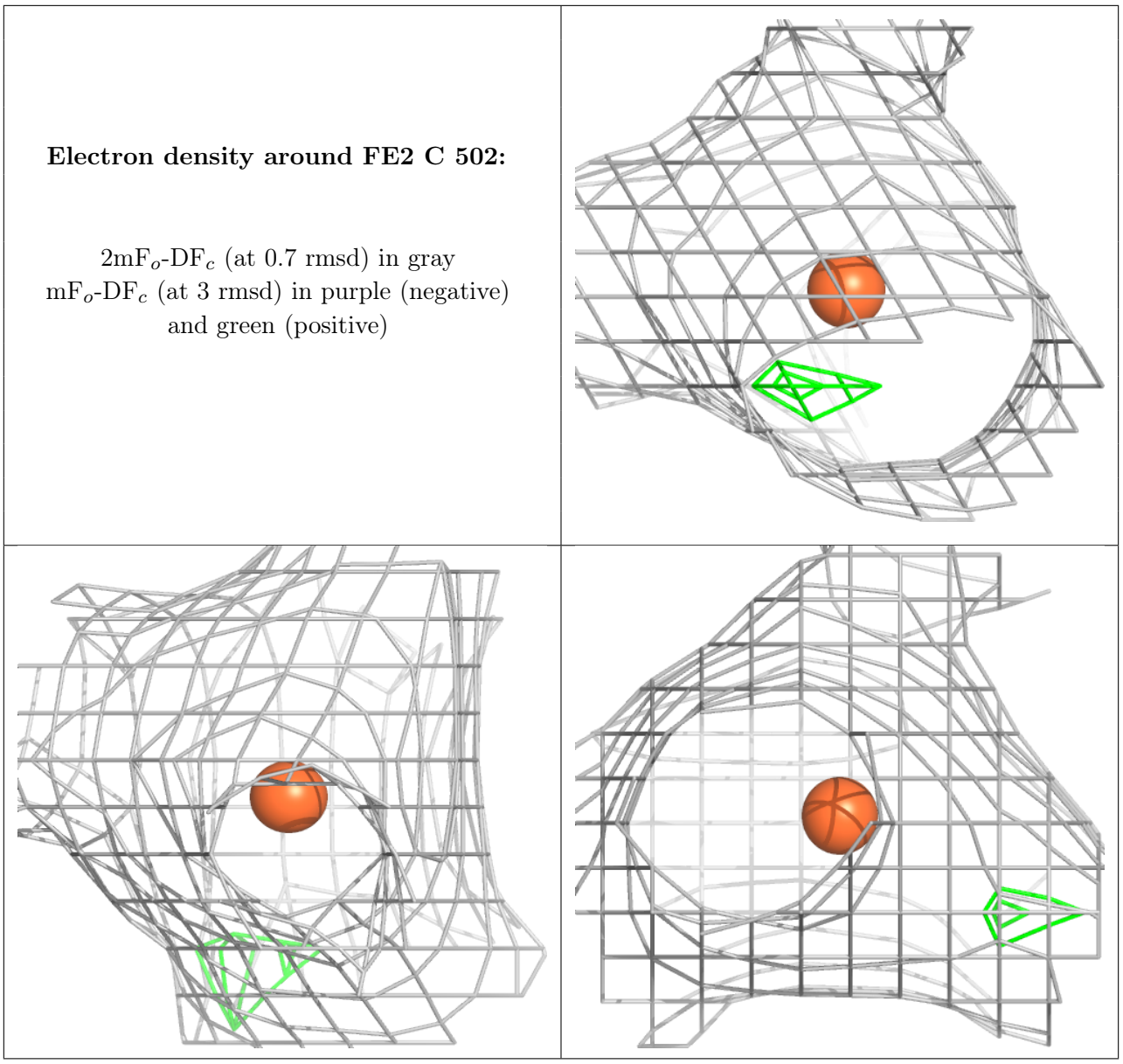
Electron density around FES A 501:

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



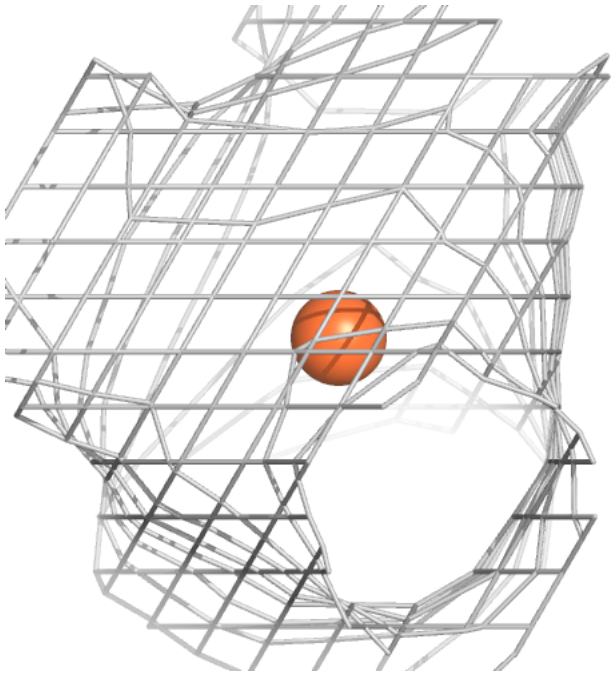
Electron density around FE2 C 502:

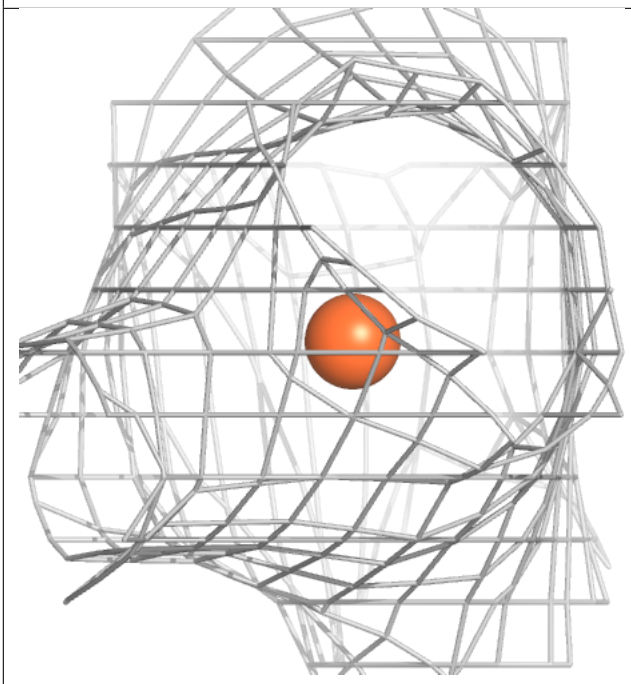
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

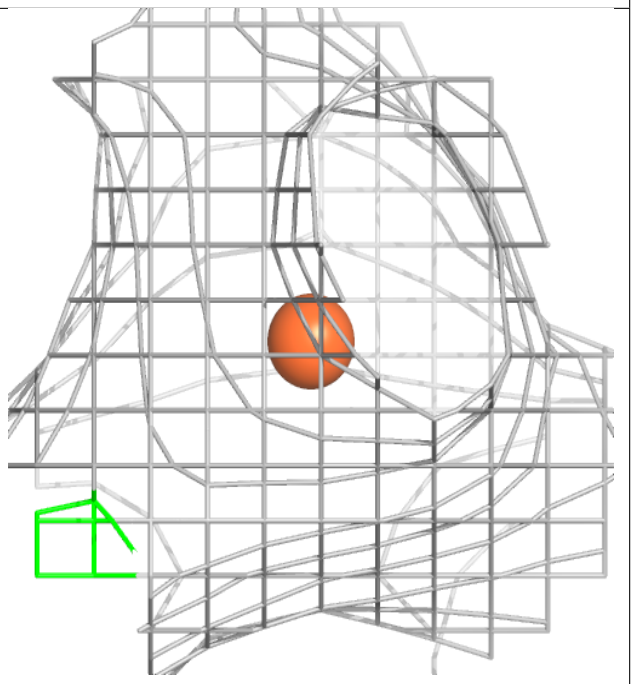


Electron density around FE2 E 502:

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

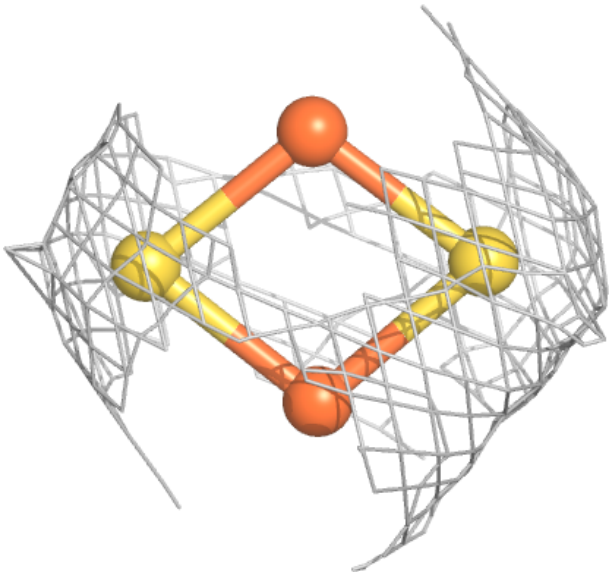


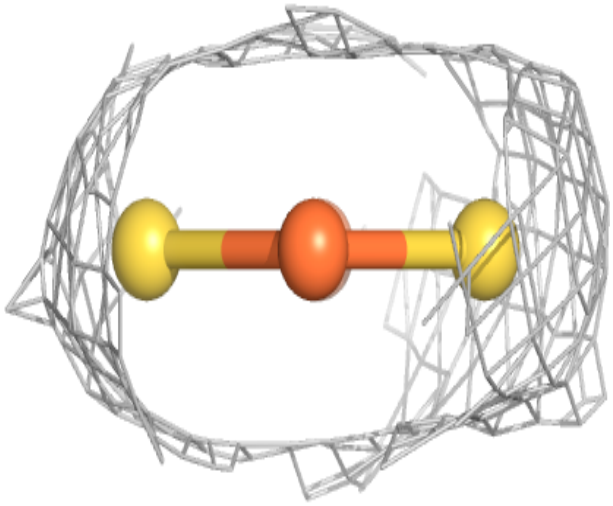


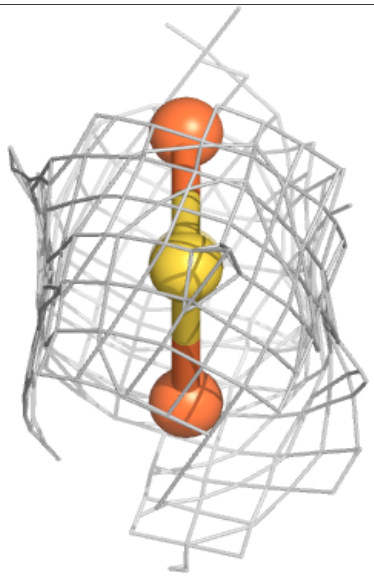


Electron density around FES G 501:

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

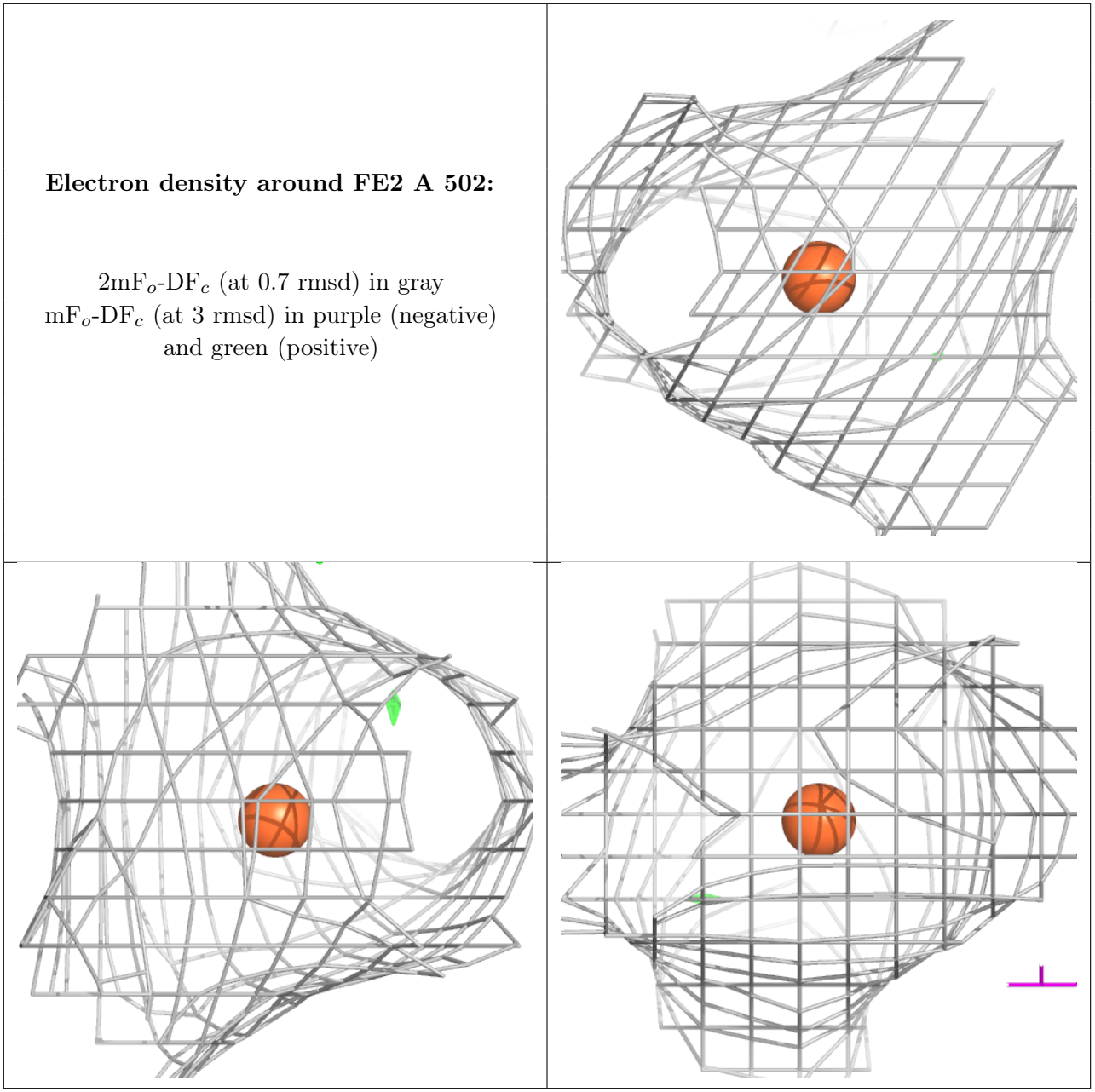






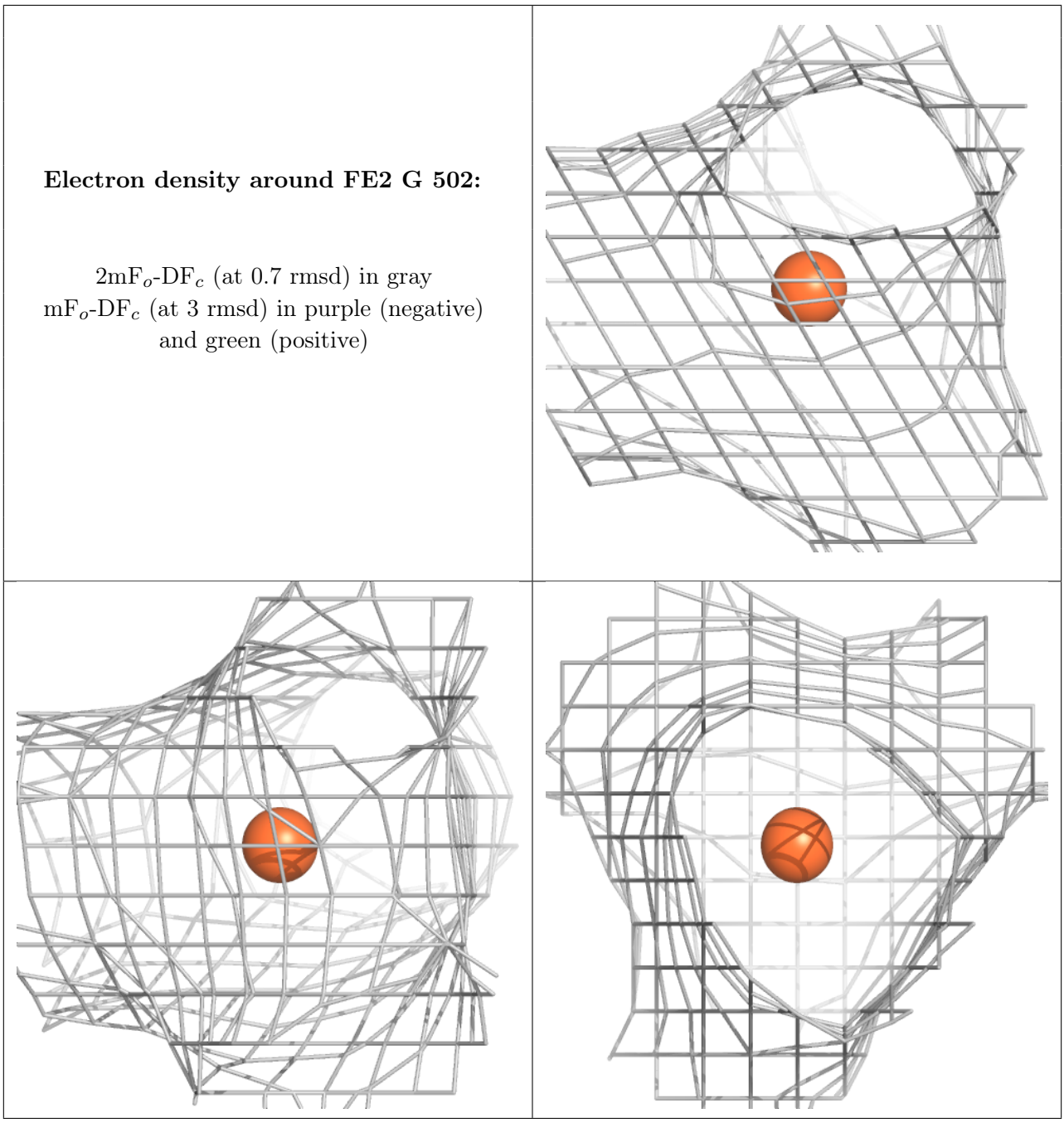
Electron density around FE2 A 502:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.