



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:25 PM JST

PDB ID : 7FJL / pdb_00007fjl
Title : Crystal Structure of phthalate dioxygenase from Comamonas testosteroni KF1
Authors : Mahto, J.K.; Kumar, P.
Deposited on : 2021-08-04
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

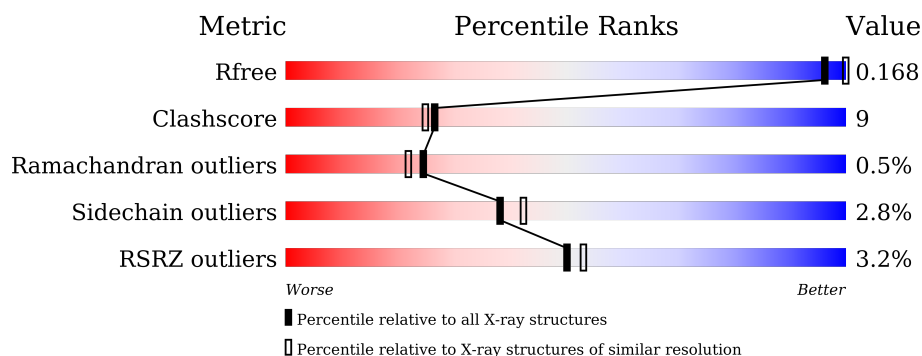
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	3% 73% 18% • 6%
1	B	439	2% 75% 17% • 6%
1	C	439	3% 73% 16% • 7%
1	D	439	2% 77% 15% • 6%
1	E	439	5% 70% 20% •• 7%
1	F	439	2% 74% 17% • 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SRT	B	503	-	X	-	-
5	SRT	C	503	-	X	-	-
5	SRT	D	503	-	X	-	-
5	SRT	E	504	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22171 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.

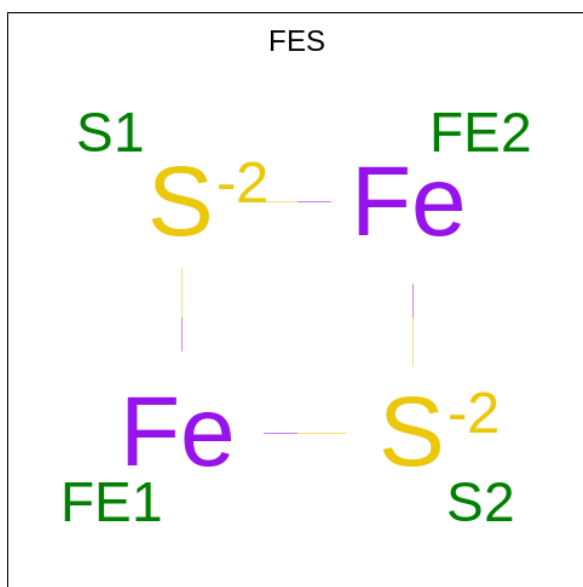
- Molecule 1 is a protein called Rieske (2Fe-2S) domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	1	0
			3249	2043	577	605	24			
1	B	412	Total	C	N	O	S	0	1	0
			3252	2044	578	606	24			
1	C	407	Total	C	N	O	S	0	1	0
			3209	2022	568	595	24			
1	D	412	Total	C	N	O	S	0	1	0
			3249	2043	577	605	24			
1	E	407	Total	C	N	O	S	0	1	0
			3209	2022	568	595	24			
1	F	409	Total	C	N	O	S	0	1	0
			3221	2028	570	599	24			

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

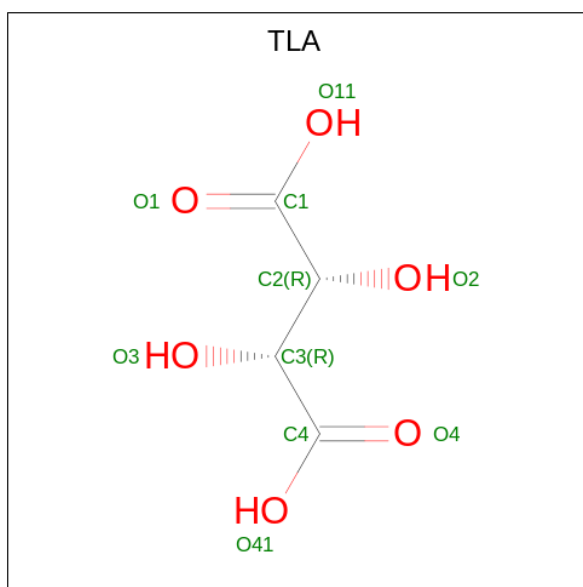
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

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



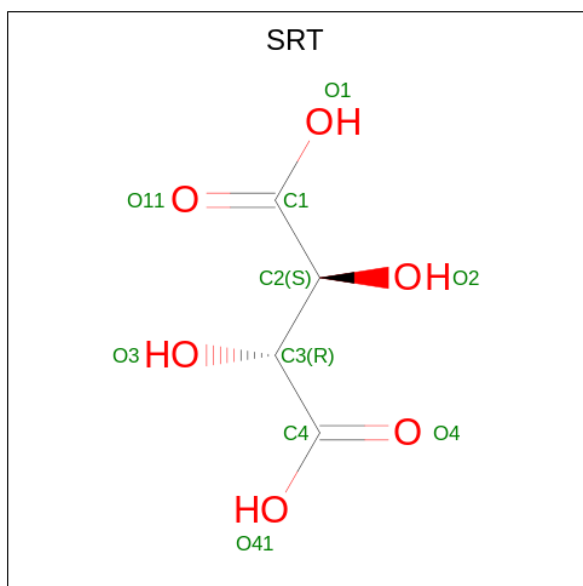
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



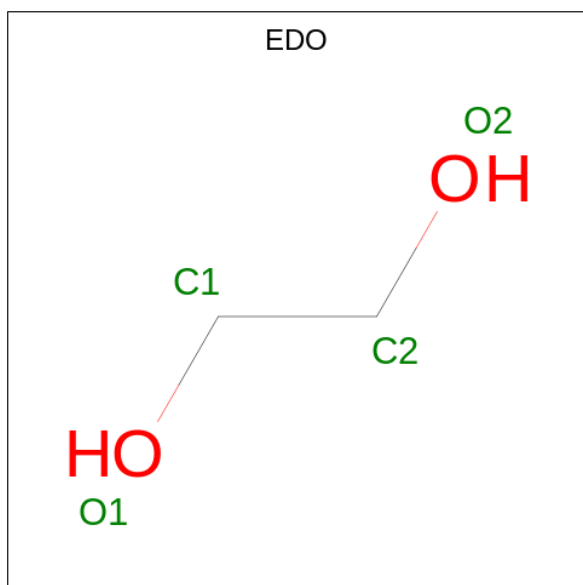
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	4	6		
5	C	1	Total	C	O	0	0
			10	4	6		
5	D	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			10	4	6		
5	F	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0

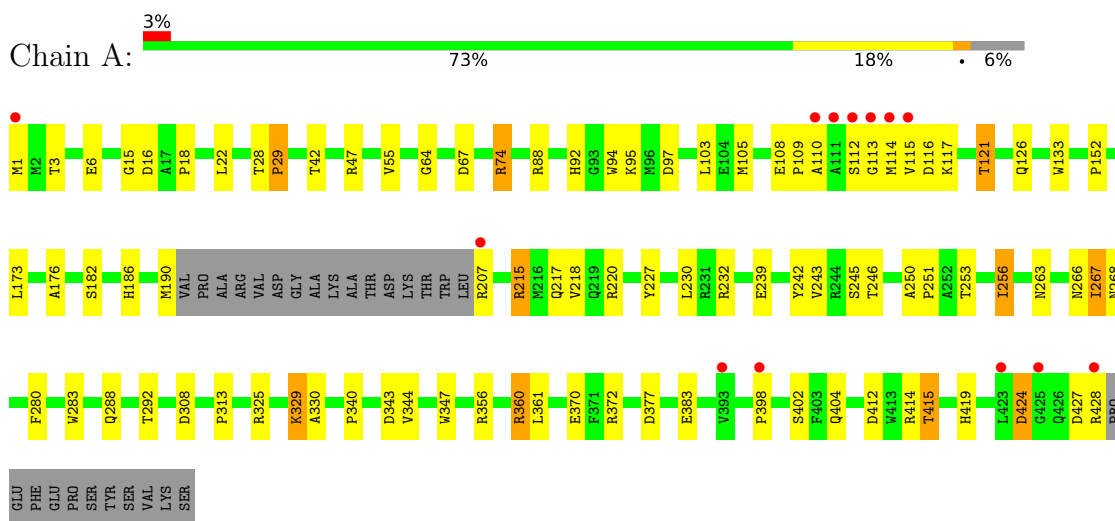
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	488	Total O 488 488	0	0
7	B	438	Total O 438 438	0	0
7	C	429	Total O 429 429	0	0
7	D	447	Total O 447 447	0	0
7	E	416	Total O 416 416	0	0
7	F	410	Total O 410 410	0	0

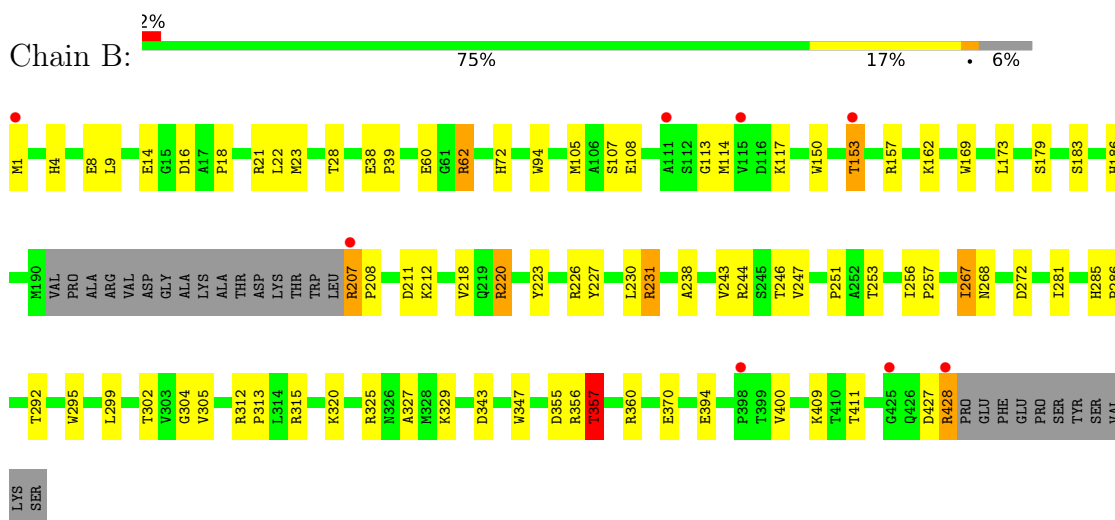
3 Residue-property plots [i](#)

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

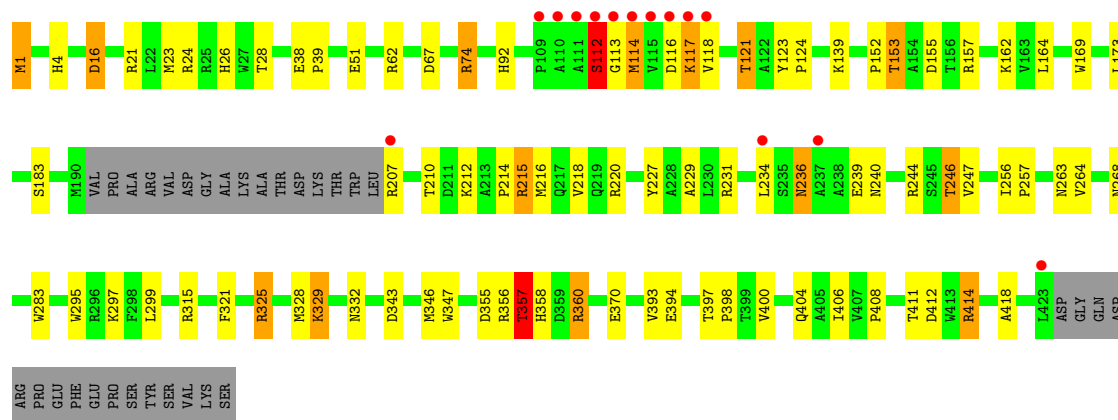


- Molecule 1: Rieske (2Fe-2S) domain protein

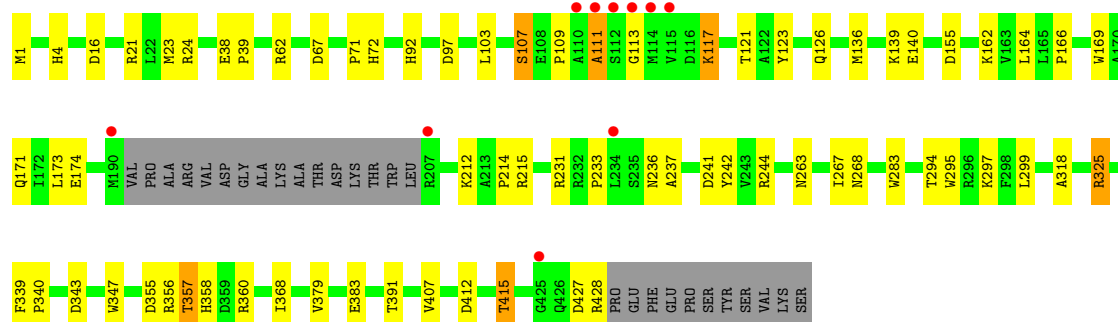
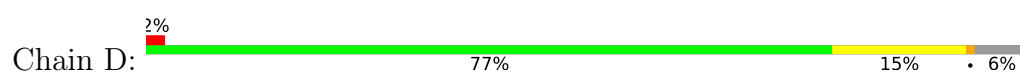


- Molecule 1: Rieske (2Fe-2S) domain protein

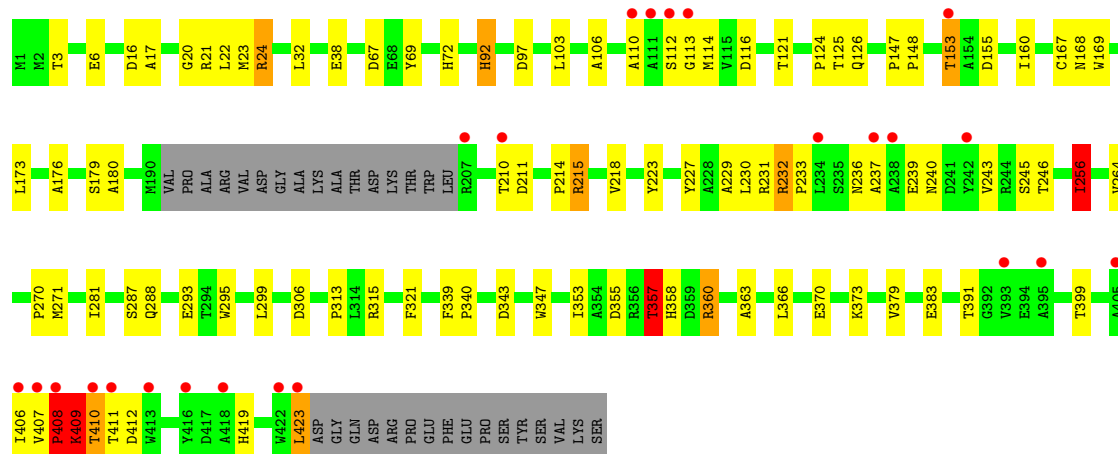




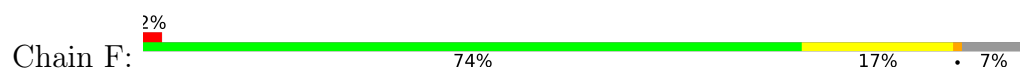
• Molecule 1: Rieske (2Fe-2S) domain protein

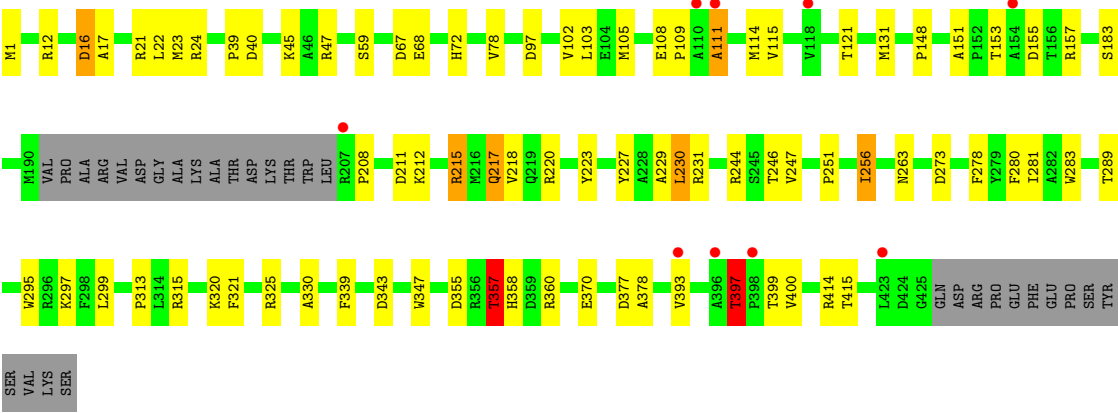


• Molecule 1: Rieske (2Fe-2S) domain protein



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.25Å 121.38Å 161.53Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	158.59 – 2.11 158.59 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.9 (158.59-2.11) 98.9 (158.59-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.220 0.168 , 0.168	Depositor DCC
R_{free} test set	9810 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22171	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, SRT, TLA, EDO, 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	0.82	2/3340 (0.1%)	1.37	16/4547 (0.4%)
1	B	0.80	1/3340 (0.0%)	1.33	19/4547 (0.4%)
1	C	0.80	2/3300 (0.1%)	1.31	13/4494 (0.3%)
1	D	0.81	1/3340 (0.0%)	1.31	17/4547 (0.4%)
1	E	0.78	1/3300 (0.0%)	1.29	21/4494 (0.5%)
1	F	0.76	1/3312 (0.0%)	1.34	18/4510 (0.4%)
All	All	0.80	8/19932 (0.0%)	1.33	104/27139 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	HIS	CE1-NE2	7.93	1.40	1.32
1	C	26	HIS	CE1-NE2	6.74	1.39	1.32
1	D	92	HIS	CE1-NE2	6.66	1.39	1.32
1	E	92	HIS	CE1-NE2	6.33	1.38	1.32
1	B	186	HIS	CE1-NE2	6.04	1.38	1.32
1	F	72	HIS	CE1-NE2	5.97	1.38	1.32
1	C	92	HIS	CE1-NE2	5.77	1.38	1.32
1	A	92	HIS	CE1-NE2	5.50	1.38	1.32

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	CG-CD-NE	-10.62	88.63	112.00
1	F	215	ARG	CB-CA-C	8.82	124.08	109.53
1	A	67	ASP	CA-CB-CG	7.85	120.45	112.60
1	F	24	ARG	CB-CG-CD	-7.55	93.93	111.30
1	C	325	ARG	CB-CG-CD	-7.52	94.01	111.30
1	F	313	PRO	CB-CA-C	-7.43	101.87	111.46
1	E	24	ARG	CB-CG-CD	-7.43	94.22	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	THR	CA-CB-OG1	7.41	120.72	109.60
1	F	397	THR	CB-CA-C	7.40	120.74	109.56
1	F	67	ASP	CA-CB-CG	7.28	119.88	112.60
1	B	220	ARG	CG-CD-NE	7.22	127.88	112.00
1	B	268	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	308	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	292	THR	CA-CB-OG1	-6.96	99.15	109.60
1	F	256	ILE	N-CA-CB	-6.93	101.50	111.21
1	D	24	ARG	CB-CG-CD	-6.90	95.43	111.30
1	D	62	ARG	CG-CD-NE	-6.90	96.83	112.00
1	B	157	ARG	CG-CD-NE	-6.82	97.00	112.00
1	A	256	ILE	N-CA-CB	-6.78	101.71	111.21
1	D	121	THR	CA-CB-OG1	-6.69	99.56	109.60
1	E	313	PRO	CB-CA-C	-6.60	102.43	111.21
1	F	357	THR	CA-CB-OG1	6.53	119.39	109.60
1	B	231	ARG	CD-NE-CZ	6.48	133.48	124.40
1	B	411	THR	CA-CB-OG1	-6.42	99.97	109.60
1	D	391	THR	CA-CB-OG1	-6.16	100.36	109.60
1	E	67	ASP	CA-CB-CG	6.03	118.62	112.60
1	A	28	THR	CA-CB-OG1	-6.02	100.56	109.60
1	E	357	THR	N-CA-CB	-6.00	100.99	110.22
1	D	67	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	62	ARG	CG-CD-NE	-5.92	98.97	112.00
1	C	24	ARG	CG-CD-NE	-5.87	99.08	112.00
1	C	357	THR	OG1-CB-CG2	5.86	121.02	109.30
1	C	74	ARG	CG-CD-NE	5.86	124.89	112.00
1	A	239	GLU	N-CA-CB	-5.82	102.19	110.81
1	C	28	THR	CA-CB-OG1	-5.82	100.87	109.60
1	F	325	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	121	THR	CB-CA-C	-5.77	101.86	110.16
1	A	42	THR	CA-CB-OG1	-5.75	100.97	109.60
1	D	356	ARG	CG-CD-NE	-5.70	99.47	112.00
1	E	167	CYS	CA-C-N	5.63	128.71	120.71
1	E	167	CYS	C-N-CA	5.63	128.71	120.71
1	B	153	THR	CB-CA-C	-5.62	100.84	110.95
1	F	358	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	414	ARG	CG-CD-NE	-5.58	99.71	112.00
1	E	410	THR	CB-CA-C	5.58	119.36	109.65
1	B	231	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	F	339	PHE	CB-CA-C	5.56	122.68	112.05
1	F	16	ASP	CB-CA-C	-5.55	100.01	110.67
1	D	171	GLN	CB-CG-CD	-5.53	103.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	PRO	CB-CA-C	-5.52	104.78	111.46
1	E	110	ALA	CA-C-N	5.51	127.93	120.65
1	E	110	ALA	C-N-CA	5.51	127.93	120.65
1	F	289	THR	CA-CB-OG1	-5.51	101.34	109.60
1	E	306	ASP	CA-CB-CG	-5.49	107.11	112.60
1	E	271	MET	N-CA-C	-5.46	105.36	112.23
1	A	47	ARG	CB-CA-C	5.45	117.97	110.34
1	B	28	THR	CA-CB-OG1	-5.45	101.43	109.60
1	D	166	PRO	CA-C-N	-5.44	113.77	122.53
1	D	166	PRO	C-N-CA	-5.44	113.77	122.53
1	B	292	THR	CA-CB-OG1	-5.42	101.47	109.60
1	B	325	ARG	CB-CG-CD	-5.37	98.95	111.30
1	F	47	ARG	CB-CG-CD	-5.36	98.97	111.30
1	A	360	ARG	CG-CD-NE	-5.33	100.28	112.00
1	B	356	ARG	CG-CD-NE	-5.30	100.35	112.00
1	D	318	ALA	CA-C-N	-5.26	114.39	122.60
1	D	318	ALA	C-N-CA	-5.26	114.39	122.60
1	B	231	ARG	CB-CG-CD	5.25	123.37	111.30
1	C	67	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	157	ARG	CG-CD-NE	-5.25	100.46	112.00
1	E	391	THR	CA-CB-OG1	-5.25	101.73	109.60
1	F	280	PHE	CB-CA-C	5.24	119.18	110.74
1	A	377	ASP	CB-CA-C	-5.23	101.95	110.85
1	E	124	PRO	CB-CA-C	-5.23	104.54	111.23
1	A	280	PHE	CB-CA-C	5.21	118.48	110.14
1	D	294	THR	N-CA-C	-5.21	105.68	111.36
1	E	215	ARG	CB-CA-C	5.19	118.09	109.53
1	C	356	ARG	CG-CD-NE	-5.18	100.61	112.00
1	E	121	THR	CA-CB-OG1	-5.18	101.83	109.60
1	D	166	PRO	N-CA-CB	5.17	106.20	102.79
1	E	408	PRO	CA-C-N	5.17	131.42	121.54
1	E	408	PRO	C-N-CA	5.17	131.42	121.54
1	A	215	ARG	CG-CD-NE	5.17	123.38	112.00
1	D	268	ASN	CA-C-N	-5.16	116.00	123.28
1	D	268	ASN	C-N-CA	-5.16	116.00	123.28
1	A	29	PRO	CB-CA-C	-5.15	105.15	111.64
1	C	268	ASN	CA-CB-CG	-5.13	107.47	112.60
1	F	278	PHE	CA-CB-CG	5.13	118.93	113.80
1	E	69	TYR	CB-CA-C	5.12	118.20	109.80
1	E	256	ILE	CA-CB-CG2	5.12	119.21	110.50
1	D	241	ASP	CA-CB-CG	5.11	117.71	112.60
1	E	270	PRO	CB-CA-C	-5.11	105.28	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ARG	CB-CG-CD	-5.10	99.57	111.30
1	F	357	THR	OG1-CB-CG2	5.09	119.48	109.30
1	F	330	ALA	CA-C-N	-5.08	115.47	122.63
1	F	330	ALA	C-N-CA	-5.08	115.47	122.63
1	B	304	GLY	N-CA-C	-5.07	108.32	114.92
1	E	125	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	327	ALA	N-CA-C	-5.05	105.77	111.28
1	C	246	THR	CA-CB-OG1	-5.05	102.03	109.60
1	C	121	THR	CB-CA-C	-5.04	103.05	110.06
1	A	356	ARG	CG-CD-NE	-5.04	100.92	112.00
1	C	412	ASP	CB-CA-C	5.03	118.53	110.29
1	D	325	ARG	CB-CG-CD	5.02	122.85	111.30
1	B	427	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3249	0	3123	62	0
1	B	3252	0	3122	55	0
1	C	3209	0	3091	78	0
1	D	3249	0	3123	43	0
1	E	3209	0	3091	73	0
1	F	3221	0	3098	52	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	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	4	0	0	0	0
3	F	4	0	0	0	0
4	A	10	0	4	1	0
5	B	10	0	4	1	0
5	C	10	0	4	1	0
5	D	10	0	4	1	0
5	E	10	0	4	0	0
5	F	10	0	4	3	0
6	B	20	0	30	0	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
6	E	20	0	30	1	0
6	F	8	0	12	0	0
7	A	488	0	0	16	0
7	B	438	0	0	10	0
7	C	429	0	0	16	0
7	D	447	0	0	12	0
7	E	416	0	0	10	0
7	F	410	0	0	13	0
All	All	22171	0	18768	357	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 9.

All (357) 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:E:360:ARG:HB2	1:E:360:ARG:NH1	1.35	1.36
1:E:360:ARG:HH11	1:E:360:ARG:CB	1.66	1.09
1:C:360:ARG:HG3	1:C:360:ARG:HH11	1.17	1.01
1:E:360:ARG:NH1	1:E:360:ARG:CB	2.27	0.95
1:E:355:ASP:OD1	1:E:357:THR:HB	1.68	0.94
1:F:153:THR:HG23	1:F:155:ASP:OD2	1.68	0.93
1:D:355:ASP:OD1	1:D:357:THR:HB	1.69	0.93
1:C:218:VAL:HG11	1:C:370:GLU:HG2	1.50	0.93
1:E:218:VAL:HG11	1:E:370:GLU:HG2	1.48	0.93
1:C:216:MET:HE1	1:C:229:ALA:CB	1.98	0.91
1:E:360:ARG:HB2	1:E:360:ARG:HH11	0.78	0.91
1:C:394:GLU:OE2	1:C:394:GLU:HA	1.71	0.89
1:B:329:LYS:HE3	7:B:978:HOH:O	1.74	0.88
1:E:153:THR:HG23	1:E:155:ASP:OD1	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASP:O	1:B:231:ARG:HD3	1.74	0.87
1:A:16:ASP:HB2	7:A:888:HOH:O	1.74	0.86
1:F:297:LYS:HE2	7:F:965:HOH:O	1.74	0.86
1:C:355:ASP:OD1	1:C:357:THR:HB	1.79	0.82
1:F:217:GLN:HE21	1:F:414:ARG:HH21	1.27	0.82
1:B:207:ARG:HB2	1:B:208:PRO:HD2	1.61	0.82
1:A:288:GLN:HE22	1:A:424:ASP:H	1.28	0.82
1:E:408:PRO:O	1:E:410:THR:N	2.12	0.81
1:C:360:ARG:HH11	1:C:360:ARG:CG	1.93	0.81
1:B:218:VAL:HG11	1:B:370:GLU:HG2	1.63	0.80
1:E:176:ALA:HB1	1:E:256:ILE:HD11	1.61	0.80
1:C:212:LYS:O	1:D:107:SER:HB3	1.83	0.79
1:C:216:MET:HE2	1:C:229:ALA:HA	1.63	0.78
1:C:216:MET:HE1	1:C:229:ALA:HB2	1.64	0.78
1:E:239:GLU:O	1:E:409:LYS:HB2	1.84	0.76
1:A:16:ASP:HA	7:A:738:HOH:O	1.85	0.76
1:C:112:SER:HB3	7:C:617:HOH:O	1.85	0.75
1:D:140:GLU:OE1	1:D:140:GLU:N	2.15	0.74
1:C:360:ARG:CG	1:C:360:ARG:NH1	2.49	0.74
1:F:153:THR:CG2	1:F:155:ASP:OD2	2.35	0.73
1:E:419:HIS:HB3	7:E:999:HOH:O	1.87	0.73
1:C:360:ARG:HG3	1:C:360:ARG:NH1	1.94	0.73
1:A:15:GLY:HA3	7:A:726:HOH:O	1.88	0.73
1:B:117:LYS:HD2	7:B:884:HOH:O	1.88	0.73
1:B:231:ARG:HD2	7:B:739:HOH:O	1.89	0.73
1:A:220:ARG:HD3	1:A:370:GLU:OE2	1.87	0.73
1:F:218:VAL:HG21	1:F:370:GLU:HG3	1.73	0.71
1:F:355:ASP:OD1	1:F:357:THR:HB	1.90	0.71
1:C:220:ARG:NH1	1:C:370:GLU:OE2	2.22	0.70
1:B:16:ASP:O	1:B:21:ARG:NH1	2.25	0.70
1:C:23:MET:HE1	1:C:169:TRP:CE2	2.27	0.70
1:E:3:THR:OG1	1:E:6:GLU:HG3	1.91	0.70
1:A:419:HIS:HB3	1:A:428:ARG:NH1	2.05	0.70
1:C:207:ARG:HD3	7:C:818:HOH:O	1.91	0.70
1:C:329:LYS:NZ	7:C:601:HOH:O	2.21	0.70
1:C:216:MET:CE	1:C:229:ALA:HA	2.21	0.70
7:B:760:HOH:O	1:F:297:LYS:HE3	1.92	0.69
1:F:217:GLN:HE21	1:F:414:ARG:NH2	1.90	0.69
1:C:1:MET:N	7:C:603:HOH:O	2.23	0.69
1:C:162:LYS:HE2	1:C:164:LEU:HD21	1.74	0.69
1:B:428:ARG:HB3	7:B:741:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:GLU:HG3	7:C:687:HOH:O	1.92	0.68
1:A:230:LEU:CD2	1:A:243:VAL:HG22	2.24	0.67
1:D:155:ASP:OD2	1:D:428:ARG:NH2	2.27	0.67
1:A:288:GLN:NE2	1:A:424:ASP:H	1.92	0.66
1:C:397:THR:HB	1:C:398:PRO:CD	2.25	0.66
1:F:148:PRO:HG2	1:F:151:ALA:HB3	1.77	0.66
1:D:297:LYS:HG3	7:D:973:HOH:O	1.94	0.66
1:A:74:ARG:HG3	1:A:74:ARG:HH11	1.59	0.66
1:E:126:GLN:HG3	7:E:702:HOH:O	1.94	0.66
1:C:112:SER:CB	7:C:617:HOH:O	2.43	0.66
1:E:179:SER:OG	1:E:231:ARG:NH2	2.27	0.66
1:F:360:ARG:NH2	7:F:602:HOH:O	2.28	0.66
1:C:121:THR:HG21	7:C:934:HOH:O	1.97	0.65
1:E:240:ASN:HD22	1:E:406:ILE:HG21	1.62	0.65
1:E:360:ARG:HD2	7:E:973:HOH:O	1.96	0.65
1:E:153:THR:CG2	1:E:155:ASP:OD1	2.44	0.65
1:F:377:ASP:HB2	7:F:788:HOH:O	1.96	0.65
1:C:62:ARG:HD2	7:C:825:HOH:O	1.96	0.64
1:C:210:THR:HG23	1:C:234:LEU:HD21	1.79	0.63
1:F:131:MET:HE1	1:F:281:ILE:HD11	1.80	0.63
1:A:207:ARG:HD3	1:A:242:TYR:HE2	1.63	0.63
1:F:217:GLN:NE2	1:F:414:ARG:NH2	2.46	0.63
1:E:211:ASP:O	1:E:231:ARG:HD3	1.99	0.63
1:E:358:HIS:HD2	7:E:968:HOH:O	1.82	0.62
1:B:22:LEU:C	1:B:22:LEU:HD23	2.25	0.62
1:F:16:ASP:O	1:F:21:ARG:HD3	1.98	0.62
1:A:176:ALA:HB1	1:A:256:ILE:HD11	1.81	0.62
1:B:179:SER:OG	1:B:231:ARG:NH2	2.25	0.61
1:C:297:LYS:HE2	7:E:650:HOH:O	2.00	0.61
1:F:397:THR:HG23	1:F:399:THR:H	1.65	0.61
1:B:295:TRP:CE2	1:B:299:LEU:HD11	2.36	0.61
1:F:211:ASP:HB3	1:F:231:ARG:HB3	1.82	0.61
1:E:240:ASN:ND2	1:E:406:ILE:HG21	2.16	0.61
1:E:360:ARG:NH2	7:E:604:HOH:O	2.34	0.60
1:E:22:LEU:HD23	1:E:22:LEU:C	2.26	0.60
1:A:1:MET:N	7:A:604:HOH:O	2.30	0.60
1:A:288:GLN:HE22	1:A:424:ASP:N	1.96	0.59
1:A:419:HIS:HB3	1:A:428:ARG:HH11	1.65	0.59
1:F:229:ALA:C	1:F:230:LEU:HD23	2.27	0.59
1:C:394:GLU:OE2	1:C:394:GLU:CA	2.43	0.59
1:B:38:GLU:HB3	1:B:39:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:LYS:HE2	7:F:644:HOH:O	2.02	0.59
1:B:207:ARG:HB2	1:B:208:PRO:CD	2.32	0.58
1:E:240:ASN:ND2	1:E:406:ILE:CG2	2.66	0.58
1:E:240:ASN:HB3	1:E:406:ILE:HG23	1.85	0.58
1:A:218:VAL:HG11	1:A:370:GLU:HG2	1.85	0.58
1:C:315:ARG:HB3	1:C:321:PHE:HA	1.86	0.57
1:A:109:PRO:O	1:A:112:SER:N	2.32	0.57
1:C:216:MET:HE1	1:C:229:ALA:HB1	1.86	0.57
1:D:427:ASP:O	1:D:428:ARG:C	2.48	0.57
1:A:330:ALA:HB1	1:C:329:LYS:HD2	1.87	0.57
1:E:339:PHE:CG	1:E:340:PRO:HD3	2.40	0.56
1:F:1:MET:N	7:F:605:HOH:O	2.38	0.56
7:A:1040:HOH:O	1:B:329:LYS:HE2	2.04	0.56
1:F:102:VAL:HG11	1:F:105:MET:HE3	1.87	0.56
1:A:182:SER:OG	4:A:503:TLA:H3	2.06	0.56
1:F:1:MET:HE1	7:F:839:HOH:O	2.05	0.56
1:D:415:THR:HG21	7:D:853:HOH:O	2.04	0.56
1:A:126:GLN:NE2	7:A:607:HOH:O	2.38	0.55
1:E:358:HIS:HE1	7:E:922:HOH:O	1.89	0.55
1:B:108:GLU:OE2	1:E:363:ALA:N	2.35	0.55
1:C:117:LYS:CD	7:C:696:HOH:O	2.55	0.54
1:A:74:ARG:HH11	1:A:74:ARG:CG	2.20	0.54
1:C:227:TYR:CE1	1:C:246:THR:HB	2.42	0.54
1:C:152:PRO:HB2	1:C:153:THR:HG23	1.89	0.54
1:B:183:SER:HB3	1:B:212:LYS:HG2	1.90	0.53
1:E:408:PRO:C	1:E:410:THR:H	2.13	0.53
1:C:23:MET:CE	1:C:169:TRP:CZ2	2.91	0.53
1:D:297:LYS:HE3	7:D:973:HOH:O	2.06	0.53
1:F:16:ASP:O	1:F:17:ALA:C	2.52	0.53
1:E:173:LEU:HD13	1:E:173:LEU:C	2.33	0.53
1:E:218:VAL:HG11	1:E:370:GLU:CG	2.31	0.53
1:C:216:MET:CE	1:C:229:ALA:CB	2.81	0.53
1:C:117:LYS:HD2	7:C:696:HOH:O	2.08	0.53
1:A:428:ARG:H	1:A:428:ARG:HD3	1.74	0.52
1:C:139:LYS:HD2	1:C:139:LYS:O	2.09	0.52
1:C:173:LEU:HD13	1:C:173:LEU:C	2.34	0.52
1:F:256:ILE:HG23	5:F:504:SRT:O3	2.08	0.52
1:F:397:THR:CG2	1:F:399:THR:H	2.23	0.52
1:A:173:LEU:HD13	1:A:173:LEU:C	2.34	0.52
1:E:23:MET:HE1	1:E:169:TRP:CE2	2.45	0.52
1:E:379:VAL:O	1:E:383:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:HD21	1:A:268:ASN:HD21	1.58	0.51
1:D:379:VAL:O	1:D:383:GLU:HG3	2.10	0.51
1:F:227:TYR:CE2	1:F:246:THR:HB	2.44	0.51
1:A:113:GLY:O	1:A:117:LYS:HE3	2.10	0.51
1:B:244:ARG:HH11	5:B:503:SRT:H2	1.76	0.51
1:C:397:THR:CB	1:C:398:PRO:CD	2.88	0.51
1:C:214:PRO:HB3	1:C:231:ARG:HG3	1.93	0.51
1:E:295:TRP:CE2	1:E:299:LEU:HD11	2.46	0.51
1:D:295:TRP:CE2	1:D:299:LEU:HD11	2.46	0.51
1:C:263:ASN:HB2	1:C:283:TRP:CE2	2.46	0.50
1:B:320:LYS:HE2	7:B:983:HOH:O	2.10	0.50
1:D:23:MET:HE1	1:D:169:TRP:CE2	2.47	0.50
1:A:112:SER:C	1:A:114:MET:H	2.19	0.50
1:E:218:VAL:HG23	1:E:366:LEU:HD23	1.93	0.50
1:F:212:LYS:HE3	7:F:716:HOH:O	2.11	0.50
1:B:4[B]:HIS:CE1	7:B:861:HOH:O	2.64	0.50
1:C:247:VAL:HG11	1:C:400:VAL:CG1	2.41	0.50
1:D:236:ASN:ND2	7:D:611:HOH:O	2.45	0.50
1:D:244:ARG:HH11	5:D:503:SRT:H2	1.75	0.50
1:E:232:ARG:NH1	1:E:409:LYS:HZ1	2.09	0.50
1:B:173:LEU:C	1:B:173:LEU:HD13	2.36	0.50
1:E:223:TYR:CD1	1:E:223:TYR:C	2.89	0.50
1:B:4[A]:HIS:CD2	7:B:901:HOH:O	2.65	0.50
1:C:220:ARG:HD3	1:C:370:GLU:OE2	2.12	0.50
1:E:406:ILE:HD12	1:E:406:ILE:N	2.26	0.49
1:B:38:GLU:HB3	1:B:39:PRO:CD	2.42	0.49
1:D:38:GLU:HB3	1:D:39:PRO:HD2	1.95	0.49
1:D:357:THR:HG22	1:D:358:HIS:CE1	2.48	0.49
1:F:297:LYS:CE	7:F:965:HOH:O	2.44	0.49
1:B:23:MET:HE1	1:B:169:TRP:CE2	2.48	0.49
1:F:97:ASP:HB3	1:F:103:LEU:HD21	1.95	0.49
1:B:9:LEU:CD1	1:B:18:PRO:HG2	2.43	0.48
1:E:211:ASP:HB3	1:E:231:ARG:HG2	1.94	0.48
1:F:223:TYR:CD1	1:F:223:TYR:C	2.91	0.48
1:C:328:MET:HA	1:C:332:ASN:O	2.13	0.48
1:A:109:PRO:HG2	1:A:112:SER:HB2	1.95	0.48
1:A:217:GLN:OE1	1:A:414:ARG:NH2	2.47	0.48
1:A:343:ASP:HB3	1:A:347:TRP:CZ2	2.48	0.48
1:D:212:LYS:HE2	7:D:972:HOH:O	2.13	0.48
1:F:183:SER:HB3	1:F:212:LYS:HG2	1.96	0.48
1:B:14:GLU:OE1	1:B:272:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:THR:HG22	1:D:358:HIS:ND1	2.29	0.48
1:B:94:TRP:CZ2	1:B:105:MET:HE3	2.49	0.48
1:C:343:ASP:HB3	1:C:347:TRP:CZ2	2.49	0.48
1:E:20:GLY:O	1:E:24:ARG:HG3	2.14	0.47
1:A:230:LEU:HD23	1:A:243:VAL:HG22	1.94	0.47
1:C:215:ARG:NH2	7:C:623:HOH:O	2.47	0.47
1:E:232:ARG:HG3	1:E:237:ALA:HB1	1.97	0.47
1:C:117:LYS:O	1:C:117:LYS:HG2	2.14	0.47
1:E:97:ASP:HB3	1:E:103:LEU:HD11	1.96	0.47
1:B:4[B]:HIS:HE1	7:B:861:HOH:O	1.97	0.47
1:F:115:VAL:HG21	7:F:844:HOH:O	2.15	0.47
1:A:22:LEU:C	1:A:22:LEU:HD23	2.40	0.47
1:C:244:ARG:HH11	5:C:503:SRT:H2	1.80	0.47
1:C:408:PRO:HG2	1:C:411:THR:OG1	2.14	0.47
1:E:227:TYR:CE2	1:E:246:THR:HB	2.50	0.47
1:C:23:MET:CE	1:C:169:TRP:CE2	2.96	0.47
1:C:240:ASN:OD1	1:C:408:PRO:HA	2.14	0.47
1:E:112:SER:O	1:E:114:MET:N	2.48	0.47
1:B:60:GLU:HG2	1:B:62:ARG:HH21	1.80	0.47
1:B:107:SER:HB2	1:E:180:ALA:HB1	1.97	0.47
1:F:230:LEU:HD23	1:F:230:LEU:N	2.30	0.47
1:C:51:GLU:OE2	1:C:123:TYR:OH	2.24	0.46
1:C:216:MET:CE	1:C:229:ALA:CA	2.93	0.46
1:D:267:ILE:HD12	7:D:716:HOH:O	2.14	0.46
1:A:230:LEU:HD22	1:A:243:VAL:HG22	1.98	0.46
1:E:236:ASN:OD1	1:E:239:GLU:CB	2.64	0.46
1:A:227:TYR:CE2	1:A:246:THR:HB	2.51	0.46
1:B:238:ALA:O	1:B:409:LYS:HE3	2.15	0.46
1:D:113:GLY:O	1:D:117:LYS:HE3	2.15	0.46
1:D:297:LYS:NZ	7:D:616:HOH:O	2.48	0.46
1:E:218:VAL:HG23	1:E:366:LEU:CD2	2.45	0.46
1:A:97:ASP:HB3	1:A:103:LEU:HD11	1.97	0.46
1:A:109:PRO:O	1:A:110:ALA:C	2.59	0.46
1:D:325:ARG:HD3	7:D:644:HOH:O	2.15	0.46
1:E:287:SER:HA	6:E:501:EDO:H21	1.98	0.46
1:F:68:GLU:HG3	1:F:78:VAL:HG23	1.97	0.46
1:E:16:ASP:O	1:E:21:ARG:HD3	2.16	0.46
1:B:227:TYR:CE2	1:B:246:THR:HB	2.51	0.46
1:C:38:GLU:HB3	1:C:39:PRO:HD2	1.97	0.46
1:A:115:VAL:HG22	7:A:866:HOH:O	2.14	0.46
1:B:23:MET:HG2	1:B:251:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:HB3	1:B:347:TRP:CZ2	2.51	0.45
1:D:415:THR:CG2	7:D:1027:HOH:O	2.65	0.45
1:E:407:VAL:O	1:E:409:LYS:N	2.49	0.45
1:F:23:MET:HG2	1:F:251:PRO:CG	2.47	0.45
1:E:215:ARG:HD3	7:E:936:HOH:O	2.15	0.45
1:E:288:GLN:OE1	1:E:423:LEU:HA	2.17	0.45
1:F:109:PRO:HB2	1:F:111:ALA:HB3	1.98	0.45
1:A:245:SER:O	1:A:402:SER:HB2	2.17	0.45
1:A:360:ARG:HG3	7:A:645:HOH:O	2.16	0.45
1:B:113:GLY:O	1:B:117:LYS:HG3	2.17	0.45
1:A:152:PRO:HB3	1:A:398:PRO:HB3	1.97	0.45
1:D:173:LEU:C	1:D:173:LEU:HD13	2.41	0.45
1:A:340:PRO:O	1:A:344:VAL:HG23	2.16	0.45
1:C:346:MET:HA	1:C:346:MET:HE2	1.99	0.45
1:C:357:THR:HG22	1:C:358:HIS:CD2	2.51	0.45
1:D:162:LYS:HE3	1:D:164:LEU:HD21	1.99	0.45
1:E:411:THR:HG22	1:E:412:ASP:O	2.16	0.45
1:A:3:THR:OG1	1:A:6:GLU:HG3	2.16	0.45
1:A:29:PRO:HD3	1:A:133:TRP:CZ3	2.51	0.45
1:D:117:LYS:HD3	7:D:1043:HOH:O	2.17	0.45
1:D:174:GLU:HG2	1:D:368:ILE:HG23	1.98	0.45
1:B:256:ILE:HG23	1:B:257:PRO:HD2	1.98	0.44
1:B:162:LYS:NZ	7:B:624:HOH:O	2.51	0.44
1:B:1:MET:HE1	1:B:357:THR:O	2.17	0.44
1:E:214:PRO:HB2	1:E:229:ALA:HB1	2.00	0.44
1:F:12:ARG:HD3	1:F:273:ASP:OD2	2.17	0.44
1:A:207:ARG:HD3	1:A:242:TYR:CE2	2.48	0.44
1:C:183:SER:HB3	1:C:212:LYS:HG2	2.00	0.44
1:C:397:THR:HB	1:C:398:PRO:HD3	1.96	0.44
1:D:263:ASN:HB2	1:D:283:TRP:CE2	2.52	0.44
1:E:236:ASN:OD1	1:E:239:GLU:HB3	2.17	0.44
1:E:373:LYS:HD2	7:E:739:HOH:O	2.17	0.44
1:F:315:ARG:HB3	1:F:321:PHE:HA	1.99	0.44
1:A:263:ASN:HB2	1:A:283:TRP:CE2	2.52	0.44
1:A:329:LYS:NZ	7:A:626:HOH:O	2.49	0.44
1:C:236:ASN:OD1	1:C:236:ASN:N	2.50	0.44
1:C:297:LYS:HD3	1:E:293:GLU:HG3	2.00	0.44
1:D:139:LYS:O	1:D:139:LYS:HG3	2.17	0.44
1:F:263:ASN:HB2	1:F:283:TRP:CE2	2.53	0.44
1:A:105:MET:SD	1:A:114:MET:HE3	2.57	0.43
1:B:105:MET:HE2	1:B:108:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ASP:O	1:E:17:ALA:C	2.61	0.43
1:E:32:LEU:HD21	1:E:160:ILE:HG21	2.00	0.43
1:F:157:ARG:O	1:F:283:TRP:HA	2.17	0.43
1:C:216:MET:HE2	1:C:216:MET:HA	1.99	0.43
1:C:404:GLN:O	7:C:602:HOH:O	2.21	0.43
1:B:223:TYR:CD1	1:B:223:TYR:C	2.96	0.43
1:D:412:ASP:O	1:D:415:THR:HB	2.18	0.43
1:B:105:MET:HE2	1:B:108:GLU:HB2	2.01	0.43
1:C:360:ARG:HB2	1:D:71:PRO:O	2.18	0.43
1:D:16:ASP:O	1:D:21:ARG:NH1	2.51	0.43
1:D:109:PRO:HB2	1:D:111:ALA:HB3	1.99	0.43
1:A:215:ARG:NH1	7:A:631:HOH:O	2.52	0.43
1:D:343:ASP:HB3	1:D:347:TRP:CZ2	2.54	0.43
1:F:22:LEU:C	1:F:22:LEU:HD23	2.44	0.43
1:E:232:ARG:NH1	1:E:409:LYS:NZ	2.66	0.43
1:D:126:GLN:NE2	7:D:623:HOH:O	2.52	0.43
1:E:406:ILE:N	1:E:406:ILE:CD1	2.82	0.43
1:A:55:VAL:HA	1:A:64:GLY:O	2.19	0.43
1:A:88:ARG:HA	1:A:95:LYS:HA	2.00	0.43
1:C:418:ALA:HA	7:C:830:HOH:O	2.18	0.43
1:B:105:MET:HE1	1:B:114:MET:SD	2.58	0.42
1:A:190:MET:O	7:A:601:HOH:O	2.22	0.42
1:A:250:ALA:HB1	1:A:251:PRO:HA	2.00	0.42
1:B:4[B]:HIS:O	1:B:8:GLU:HG2	2.18	0.42
1:D:4[A]:HIS:NE2	1:D:357:THR:HG21	2.34	0.42
1:E:38:GLU:HG3	7:E:696:HOH:O	2.19	0.42
1:A:94:TRP:CZ3	1:A:105:MET:HE2	2.55	0.42
1:A:253:THR:OG1	1:A:267:ILE:HD12	2.19	0.42
1:B:253:THR:OG1	1:B:267:ILE:HD12	2.19	0.42
1:F:256:ILE:CG2	5:F:504:SRT:O3	2.66	0.42
1:F:320:LYS:CE	7:F:644:HOH:O	2.66	0.42
1:F:343:ASP:HB3	1:F:347:TRP:CZ2	2.54	0.42
1:A:412:ASP:O	1:A:415:THR:HG22	2.19	0.42
1:F:244:ARG:HH11	5:F:504:SRT:H2	1.84	0.42
1:E:92:HIS:O	1:E:106:ALA:HB3	2.18	0.42
1:E:168:ASN:HB2	1:E:353:ILE:HG12	2.01	0.42
1:C:23:MET:HE1	1:C:169:TRP:CD2	2.55	0.42
1:F:21:ARG:HD2	7:F:800:HOH:O	2.19	0.42
1:C:16:ASP:O	1:C:21:ARG:NH1	2.53	0.42
1:D:1:MET:N	7:D:625:HOH:O	2.52	0.42
1:E:147:PRO:HA	1:E:148:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:404:GLN:HA	2.20	0.42
1:B:230:LEU:HD22	1:B:243:VAL:HG22	2.01	0.42
1:B:355:ASP:OD1	1:B:357:THR:HB	2.19	0.42
1:C:256:ILE:HB	1:C:257:PRO:CD	2.50	0.42
1:F:115:VAL:HG23	7:F:826:HOH:O	2.18	0.42
1:A:18:PRO:HB3	1:A:383:GLU:HG3	2.02	0.42
1:B:105:MET:HE2	1:B:108:GLU:CB	2.50	0.42
1:C:113:GLY:O	1:C:117:LYS:HD3	2.20	0.42
1:C:153:THR:OG1	1:C:155:ASP:OD1	2.38	0.42
1:A:232:ARG:HA	7:A:798:HOH:O	2.20	0.41
1:C:397:THR:HB	1:C:398:PRO:HD2	1.99	0.41
1:F:23:MET:HG2	1:F:251:PRO:HG2	2.00	0.41
1:F:39:PRO:O	1:F:40:ASP:HB2	2.20	0.41
1:B:223:TYR:HB3	1:B:394:GLU:O	2.20	0.41
1:C:114:MET:O	1:C:118:VAL:HG23	2.19	0.41
1:D:97:ASP:HB3	1:D:103:LEU:HD11	2.02	0.41
1:A:109:PRO:HG3	7:A:1081:HOH:O	2.19	0.41
1:C:256:ILE:HD11	1:C:264:VAL:HG11	2.02	0.41
1:E:22:LEU:HD12	1:E:379:VAL:HA	2.02	0.41
1:E:343:ASP:HB3	1:E:347:TRP:CZ2	2.56	0.41
1:E:360:ARG:HB2	1:E:360:ARG:CZ	2.31	0.41
1:B:226:ARG:HG2	1:B:247:VAL:HG22	2.01	0.41
7:C:649:HOH:O	1:F:360:ARG:HG3	2.19	0.41
1:D:123:TYR:CD1	1:D:136:MET:HA	2.55	0.41
1:B:247:VAL:HG11	1:B:400:VAL:CG1	2.51	0.41
1:D:140:GLU:H	1:D:140:GLU:CD	2.20	0.41
7:A:627:HOH:O	1:B:360:ARG:HG3	2.21	0.41
1:C:62:ARG:HG2	7:C:791:HOH:O	2.19	0.41
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.79	0.41
1:E:233:PRO:HD2	1:E:237:ALA:HA	2.01	0.41
1:B:105:MET:CE	1:B:108:GLU:HG2	2.51	0.41
1:E:264:VAL:HA	1:E:281:ILE:O	2.20	0.41
1:B:285:HIS:HA	1:B:286:PRO:HD3	1.95	0.41
1:C:295:TRP:CE2	1:C:299:LEU:HD11	2.56	0.41
1:D:214:PRO:HB3	1:D:231:ARG:HG3	2.03	0.41
1:D:233:PRO:HD2	1:D:237:ALA:HA	2.03	0.41
1:E:230:LEU:HD22	1:E:243:VAL:HG22	2.02	0.41
1:E:315:ARG:HB3	1:E:321:PHE:HA	2.03	0.41
1:A:121:THR:HA	7:A:1033:HOH:O	2.20	0.41
1:A:325:ARG:HA	1:A:325:ARG:HD3	1.85	0.41
1:A:207:ARG:N	7:A:637:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4[A]:HIS:CE1	7:C:816:HOH:O	2.74	0.40
1:C:124:PRO:HG3	1:C:139:LYS:HE3	2.03	0.40
1:D:242:TYR:CE2	1:D:244:ARG:HD2	2.56	0.40
1:E:227:TYR:O	1:E:245:SER:HA	2.21	0.40
1:F:378:ALA:HA	7:F:958:HOH:O	2.20	0.40
1:A:108:GLU:HG2	1:A:114:MET:HE2	2.02	0.40
1:B:150:TRP:CZ3	1:B:281:ILE:HD13	2.56	0.40
1:F:295:TRP:CE2	1:F:299:LEU:HD11	2.56	0.40
1:A:361:LEU:HD11	1:A:372:ARG:NH1	2.37	0.40
1:B:302:THR:HB	1:B:305:VAL:HB	2.03	0.40
1:C:74:ARG:HH11	1:C:74:ARG:HD2	1.73	0.40
1:E:211:ASP:HB3	1:E:231:ARG:CG	2.52	0.40
1:B:312:ARG:HA	1:B:313:PRO:HD3	1.94	0.40
1:D:339:PHE:CG	1:D:340:PRO:HD3	2.57	0.40
1:F:247:VAL:HG11	1:F:400:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	409/439 (93%)	385 (94%)	22 (5%)	2 (0%)	24	22
1	B	409/439 (93%)	390 (95%)	18 (4%)	1 (0%)	43	44
1	C	404/439 (92%)	381 (94%)	22 (5%)	1 (0%)	43	44
1	D	409/439 (93%)	391 (96%)	16 (4%)	2 (0%)	24	22
1	E	404/439 (92%)	382 (95%)	18 (4%)	4 (1%)	12	8
1	F	406/439 (92%)	390 (96%)	14 (3%)	2 (0%)	24	22
All	All	2441/2634 (93%)	2319 (95%)	110 (4%)	12 (0%)	24	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	112	SER
1	D	111	ALA
1	E	408	PRO
1	E	409	LYS
1	A	424	ASP
1	E	113	GLY
1	F	111	ALA
1	B	72	HIS
1	D	72	HIS
1	A	427	ASP
1	E	72	HIS
1	F	208	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/363 (94%)	336 (98%)	5 (2%)	57	65
1	B	341/363 (94%)	335 (98%)	6 (2%)	51	59
1	C	337/363 (93%)	321 (95%)	16 (5%)	23	23
1	D	341/363 (94%)	334 (98%)	7 (2%)	47	54
1	E	337/363 (93%)	327 (97%)	10 (3%)	36	40
1	F	338/363 (93%)	325 (96%)	13 (4%)	29	30
All	All	2035/2178 (93%)	1978 (97%)	57 (3%)	38	42

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	116	ASP
1	A	267	ILE
1	A	329	LYS
1	A	415	THR
1	B	153	THR
1	B	207	ARG

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Mol	Chain	Res	Type
1	B	220	ARG
1	B	267	ILE
1	B	357	THR
1	B	428	ARG
1	C	1	MET
1	C	16	ASP
1	C	112	SER
1	C	114	MET
1	C	116	ASP
1	C	117	LYS
1	C	153	THR
1	C	215	ARG
1	C	236	ASN
1	C	239	GLU
1	C	329	LYS
1	C	357	THR
1	C	360	ARG
1	C	393	VAL
1	C	406	ILE
1	C	414	ARG
1	D	107	SER
1	D	117	LYS
1	D	215	ARG
1	D	357	THR
1	D	360	ARG
1	D	407	VAL
1	D	415	THR
1	E	116	ASP
1	E	153	THR
1	E	210	THR
1	E	232	ARG
1	E	256	ILE
1	E	357	THR
1	E	360	ARG
1	E	399	THR
1	E	409	LYS
1	E	423	LEU
1	F	45	LYS
1	F	59	SER
1	F	108	GLU
1	F	114	MET
1	F	121	THR

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Mol	Chain	Res	Type
1	F	215	ARG
1	F	217	GLN
1	F	220	ARG
1	F	230	LEU
1	F	357	THR
1	F	393	VAL
1	F	397	THR
1	F	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	288	GLN
1	A	419	HIS
1	B	266	ASN
1	B	268	ASN
1	B	419	HIS
1	C	126	GLN
1	C	266	ASN
1	C	268	ASN
1	C	358	HIS
1	D	309	GLN
1	E	240	ASN
1	E	301	GLN
1	E	384	GLN
1	F	217	GLN
1	F	266	ASN
1	F	268	ASN
1	F	288	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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	$\# Z > 2$
6	EDO	D	504	-	3,3,3	0.44	0	2,2,2	0.45	0
3	FES	D	502	1	0,4,4	-	-	-		
3	FES	C	502	1	0,4,4	-	-	-		
6	EDO	D	505	-	3,3,3	0.40	0	2,2,2	0.15	0
6	EDO	B	508	-	3,3,3	0.36	0	2,2,2	0.59	0
6	EDO	B	507	-	3,3,3	0.28	0	2,2,2	0.23	0
3	FES	F	503	1	0,4,4	-	-	-		
5	SRT	F	504	-	9,9,9	1.37	1 (11%)	12,12,12	1.40	1 (8%)
5	SRT	C	503	-	9,9,9	0.75	0	12,12,12	1.68	3 (25%)
6	EDO	E	505	-	3,3,3	0.31	0	2,2,2	0.57	0
5	SRT	E	504	-	9,9,9	1.10	1 (11%)	12,12,12	2.08	7 (58%)
6	EDO	C	505	-	3,3,3	0.73	0	2,2,2	0.80	0
6	EDO	E	507	-	3,3,3	0.34	0	2,2,2	0.52	0
6	EDO	F	501	-	3,3,3	0.20	0	2,2,2	0.33	0
6	EDO	F	505	-	3,3,3	0.48	0	2,2,2	0.49	0
4	TLA	A	503	-	9,9,9	0.80	0	12,12,12	1.05	0
5	SRT	D	503	-	9,9,9	1.15	0	12,12,12	2.06	6 (50%)
6	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.59	0
3	FES	B	502	1	0,4,4	-	-	-		
6	EDO	E	506	-	3,3,3	0.31	0	2,2,2	0.63	0
3	FES	E	503	1	0,4,4	-	-	-		
3	FES	A	502	1	0,4,4	-	-	-		
6	EDO	B	505	-	3,3,3	0.36	0	2,2,2	0.73	0
6	EDO	B	506	-	3,3,3	0.64	0	2,2,2	0.60	0
6	EDO	E	508	-	3,3,3	0.11	0	2,2,2	0.15	0
6	EDO	E	501	-	3,3,3	0.36	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SRT	B	503	-	9,9,9	1.25	1 (11%)	12,12,12	2.37	6 (50%)
6	EDO	C	504	-	3,3,3	0.48	0	2,2,2	0.83	0

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
6	EDO	D	504	-	-	1/1/1/1	-
3	FES	D	502	1	-	-	0/1/1/1
3	FES	C	502	1	-	-	0/1/1/1
6	EDO	D	505	-	-	0/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	B	507	-	-	0/1/1/1	-
3	FES	F	503	1	-	-	0/1/1/1
5	SRT	F	504	-	-	9/12/12/12	-
5	SRT	C	503	-	-	12/12/12/12	-
6	EDO	E	505	-	-	1/1/1/1	-
5	SRT	E	504	-	-	11/12/12/12	-
6	EDO	C	505	-	-	1/1/1/1	-
6	EDO	E	507	-	-	0/1/1/1	-
6	EDO	F	501	-	-	1/1/1/1	-
6	EDO	F	505	-	-	0/1/1/1	-
5	SRT	D	503	-	-	12/12/12/12	-
4	TLA	A	503	-	-	0/12/12/12	-
6	EDO	B	504	-	-	1/1/1/1	-
3	FES	B	502	1	-	-	0/1/1/1
6	EDO	E	506	-	-	0/1/1/1	-
3	FES	E	503	1	-	-	0/1/1/1
3	FES	A	502	1	-	-	0/1/1/1
6	EDO	B	505	-	-	1/1/1/1	-
6	EDO	B	506	-	-	1/1/1/1	-
6	EDO	E	508	-	-	1/1/1/1	-
6	EDO	E	501	-	-	1/1/1/1	-
5	SRT	B	503	-	-	9/12/12/12	-
6	EDO	C	504	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	SRT	C3-C4	2.31	1.55	1.52
5	F	504	SRT	C2-C1	2.17	1.55	1.52
5	E	504	SRT	C3-C4	2.12	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	SRT	O2-C2-C3	3.81	117.79	110.23
5	B	503	SRT	O3-C3-C2	-3.56	103.16	110.23
5	B	503	SRT	O2-C2-C1	3.48	117.95	110.66
5	B	503	SRT	C2-C3-C4	3.44	117.55	109.87
5	D	503	SRT	O2-C2-C3	3.22	116.63	110.23
5	E	504	SRT	O3-C3-C2	-3.21	103.85	110.23
5	D	503	SRT	O2-C2-C1	2.99	116.92	110.66
5	D	503	SRT	C2-C3-C4	2.97	116.51	109.87
5	B	503	SRT	C3-C2-C1	2.75	116.02	109.87
5	C	503	SRT	O11-C1-C2	-2.61	114.78	121.63
5	F	504	SRT	C3-C2-C1	2.58	115.62	109.87
5	E	504	SRT	C2-C3-C4	2.57	115.61	109.87
5	E	504	SRT	O41-C4-C3	2.54	120.14	113.27
5	E	504	SRT	O1-C1-C2	2.51	120.05	113.27
5	E	504	SRT	O11-C1-C2	-2.49	115.09	121.63
5	C	503	SRT	O2-C2-C3	2.43	115.06	110.23
5	D	503	SRT	O4-C4-C3	-2.42	115.26	121.63
5	D	503	SRT	O3-C3-C2	-2.40	105.47	110.23
5	E	504	SRT	C3-C2-C1	2.21	114.80	109.87
5	E	504	SRT	O4-C4-C3	-2.09	116.14	121.63
5	B	503	SRT	O41-C4-C3	2.04	118.78	113.27
5	D	503	SRT	O41-C4-C3	2.04	118.77	113.27
5	C	503	SRT	O3-C3-C2	-2.00	106.26	110.23

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	SRT	O2-C2-C3-O3
5	C	503	SRT	O11-C1-C2-O2
5	C	503	SRT	C1-C2-C3-O3
5	C	503	SRT	C1-C2-C3-C4
5	C	503	SRT	O2-C2-C3-O3
5	D	503	SRT	O2-C2-C3-O3
5	E	504	SRT	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	E	504	SRT	O11-C1-C2-O2
5	E	504	SRT	C1-C2-C3-O3
5	E	504	SRT	O2-C2-C3-O3
5	F	504	SRT	C1-C2-C3-O3
5	F	504	SRT	C1-C2-C3-C4
5	F	504	SRT	O2-C2-C3-O3
5	B	503	SRT	C1-C2-C3-O3
5	C	503	SRT	O2-C2-C3-C4
5	D	503	SRT	C1-C2-C3-O3
5	E	504	SRT	O2-C2-C3-C4
5	F	504	SRT	O2-C2-C3-C4
5	B	503	SRT	C1-C2-C3-C4
5	E	504	SRT	C1-C2-C3-C4
5	B	503	SRT	O2-C2-C3-C4
5	D	503	SRT	O2-C2-C3-C4
5	C	503	SRT	O1-C1-C2-O2
5	B	503	SRT	O1-C1-C2-C3
5	B	503	SRT	O11-C1-C2-C3
5	C	503	SRT	O1-C1-C2-C3
5	D	503	SRT	O1-C1-C2-C3
5	D	503	SRT	O11-C1-C2-C3
5	E	504	SRT	O1-C1-C2-C3
5	F	504	SRT	O1-C1-C2-C3
5	F	504	SRT	O11-C1-C2-C3
5	B	503	SRT	O11-C1-C2-O2
5	D	503	SRT	O1-C1-C2-O2
5	C	503	SRT	O11-C1-C2-C3
5	B	503	SRT	O1-C1-C2-O2
5	D	503	SRT	O11-C1-C2-O2
5	F	504	SRT	O1-C1-C2-O2
5	F	504	SRT	O11-C1-C2-O2
5	D	503	SRT	C1-C2-C3-C4
5	D	503	SRT	O3-C3-C4-O41
5	E	504	SRT	O11-C1-C2-C3
6	B	505	EDO	O1-C1-C2-O2
5	C	503	SRT	O3-C3-C4-O41
5	C	503	SRT	C2-C3-C4-O41
5	C	503	SRT	C2-C3-C4-O4
5	B	503	SRT	C2-C3-C4-O4
6	E	508	EDO	O1-C1-C2-O2
5	C	503	SRT	O3-C3-C4-O4
5	E	504	SRT	C2-C3-C4-O41

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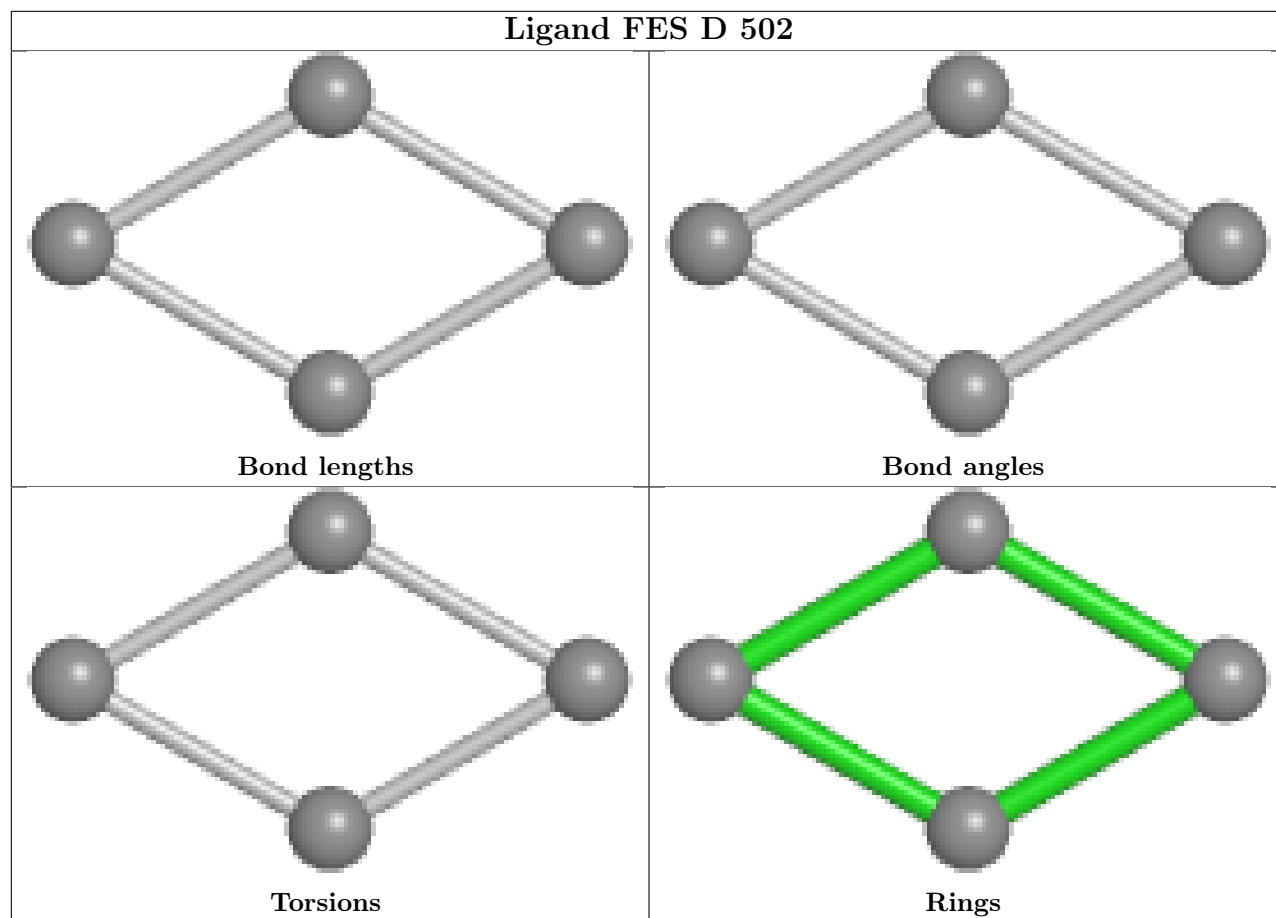
Mol	Chain	Res	Type	Atoms
5	D	503	SRT	C2-C3-C4-O4
6	B	506	EDO	O1-C1-C2-O2
6	C	505	EDO	O1-C1-C2-O2
6	E	501	EDO	O1-C1-C2-O2
6	B	504	EDO	O1-C1-C2-O2
6	D	504	EDO	O1-C1-C2-O2
6	E	505	EDO	O1-C1-C2-O2
5	F	504	SRT	C2-C3-C4-O4
5	E	504	SRT	C2-C3-C4-O4
6	F	501	EDO	O1-C1-C2-O2
5	D	503	SRT	C2-C3-C4-O41
5	D	503	SRT	O3-C3-C4-O4
5	E	504	SRT	O3-C3-C4-O41

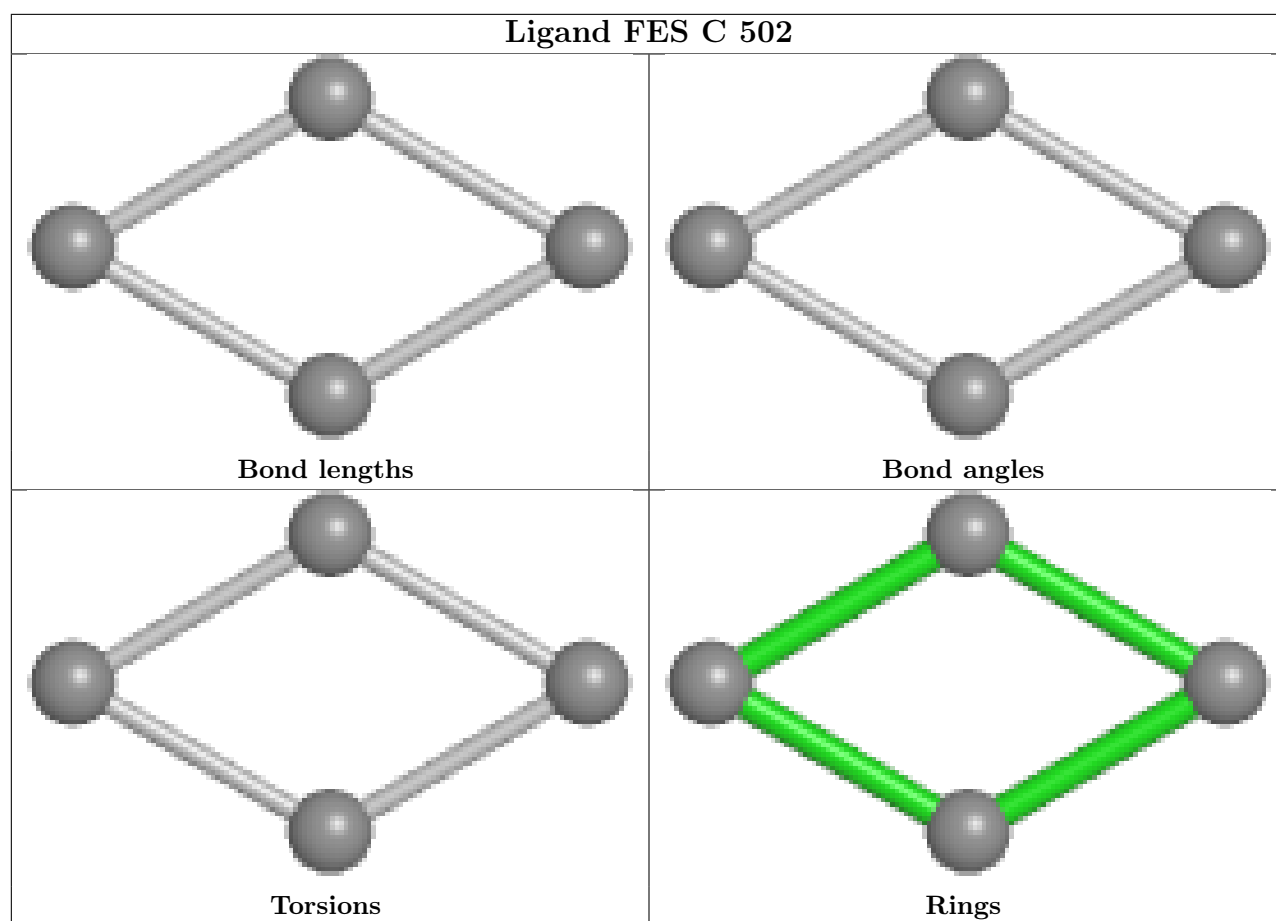
There are no ring outliers.

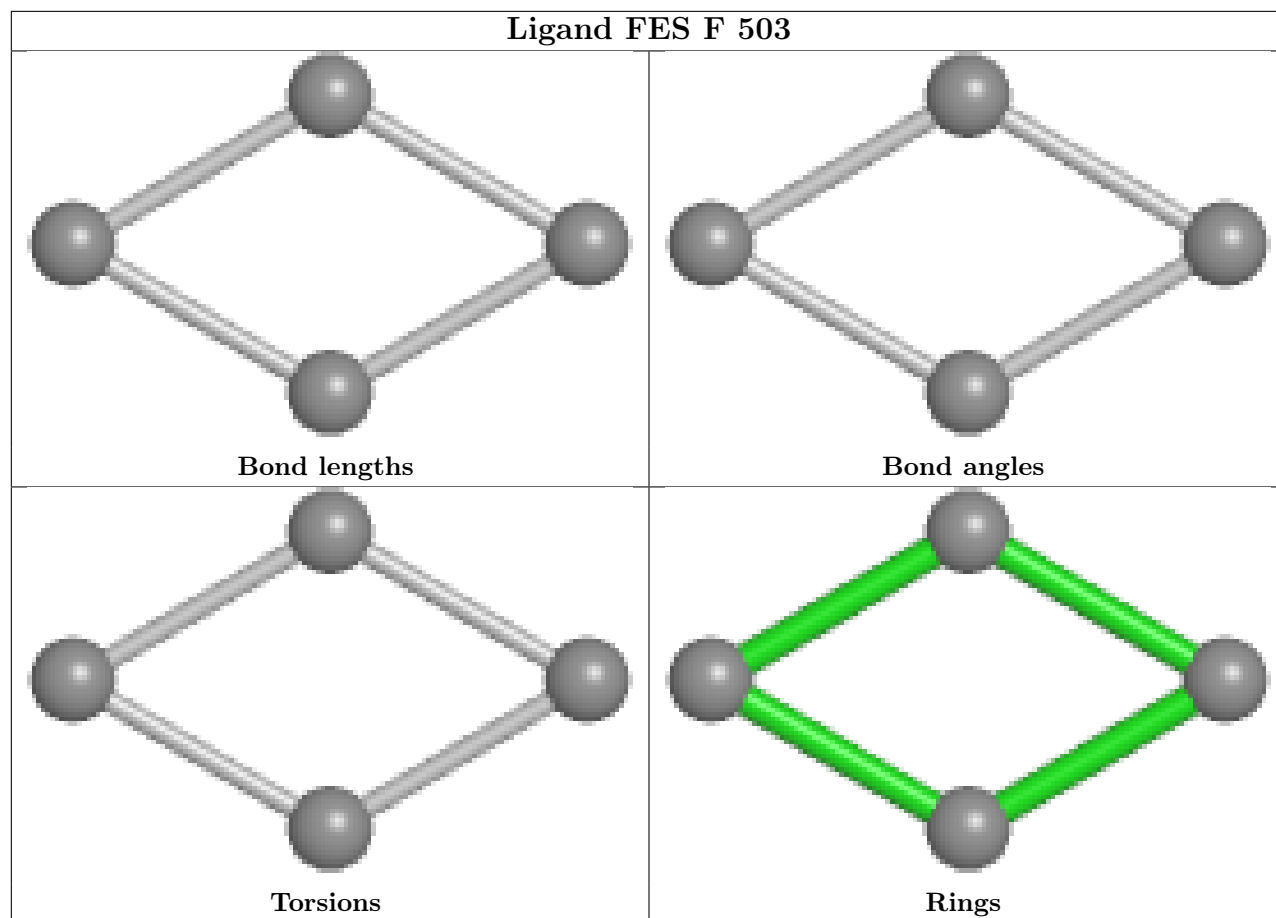
6 monomers are involved in 8 short contacts:

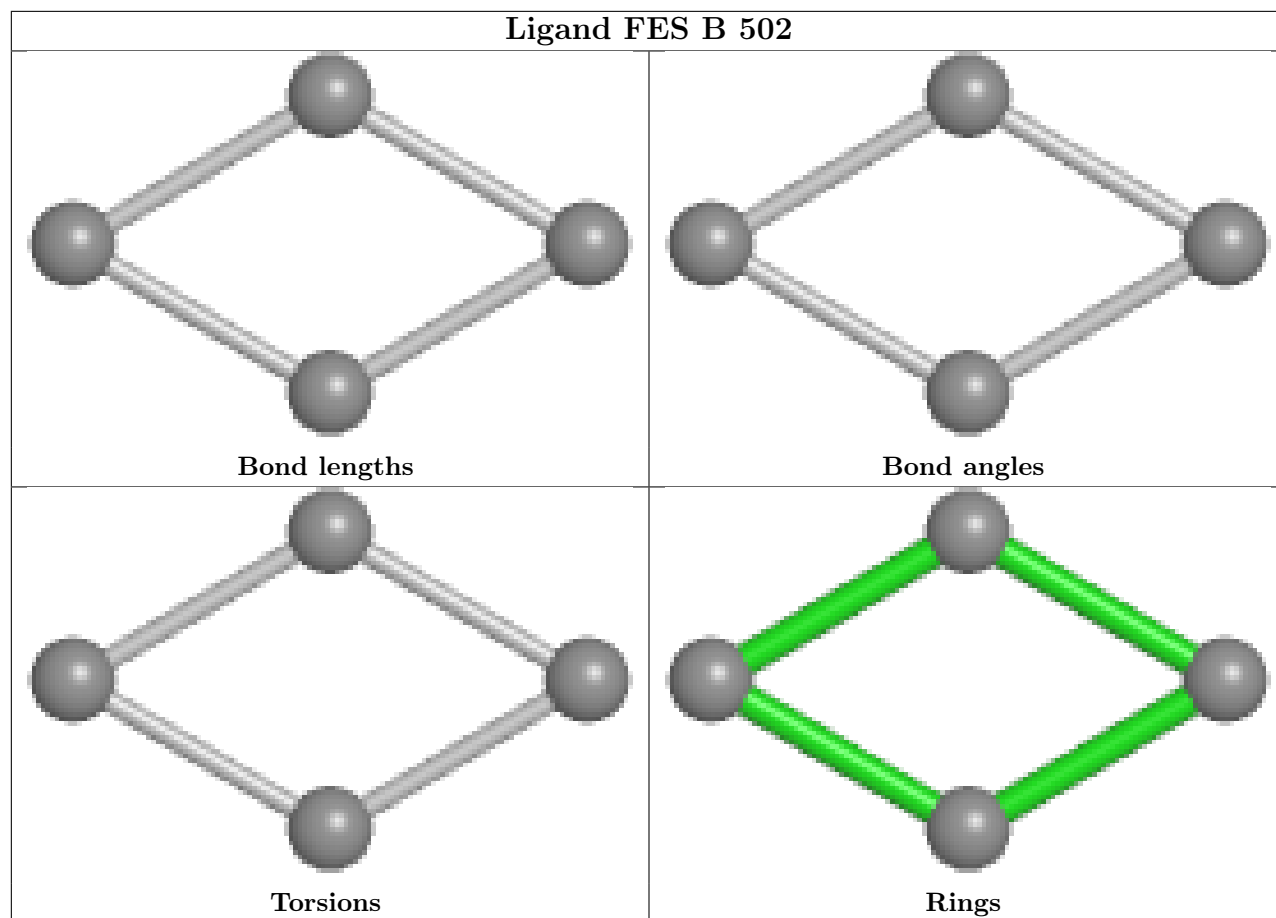
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	504	SRT	3	0
5	C	503	SRT	1	0
4	A	503	TLA	1	0
5	D	503	SRT	1	0
6	E	501	EDO	1	0
5	B	503	SRT	1	0

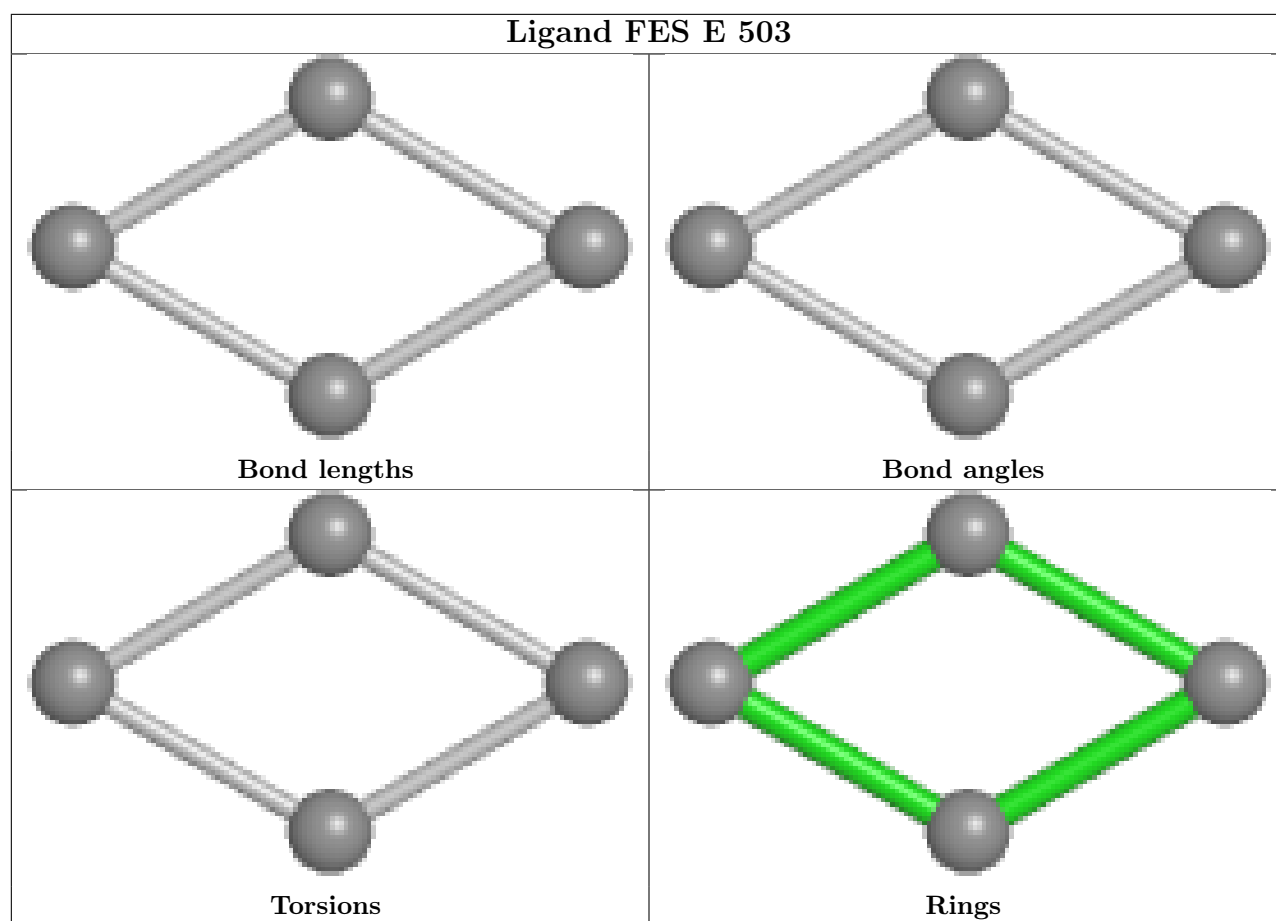
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

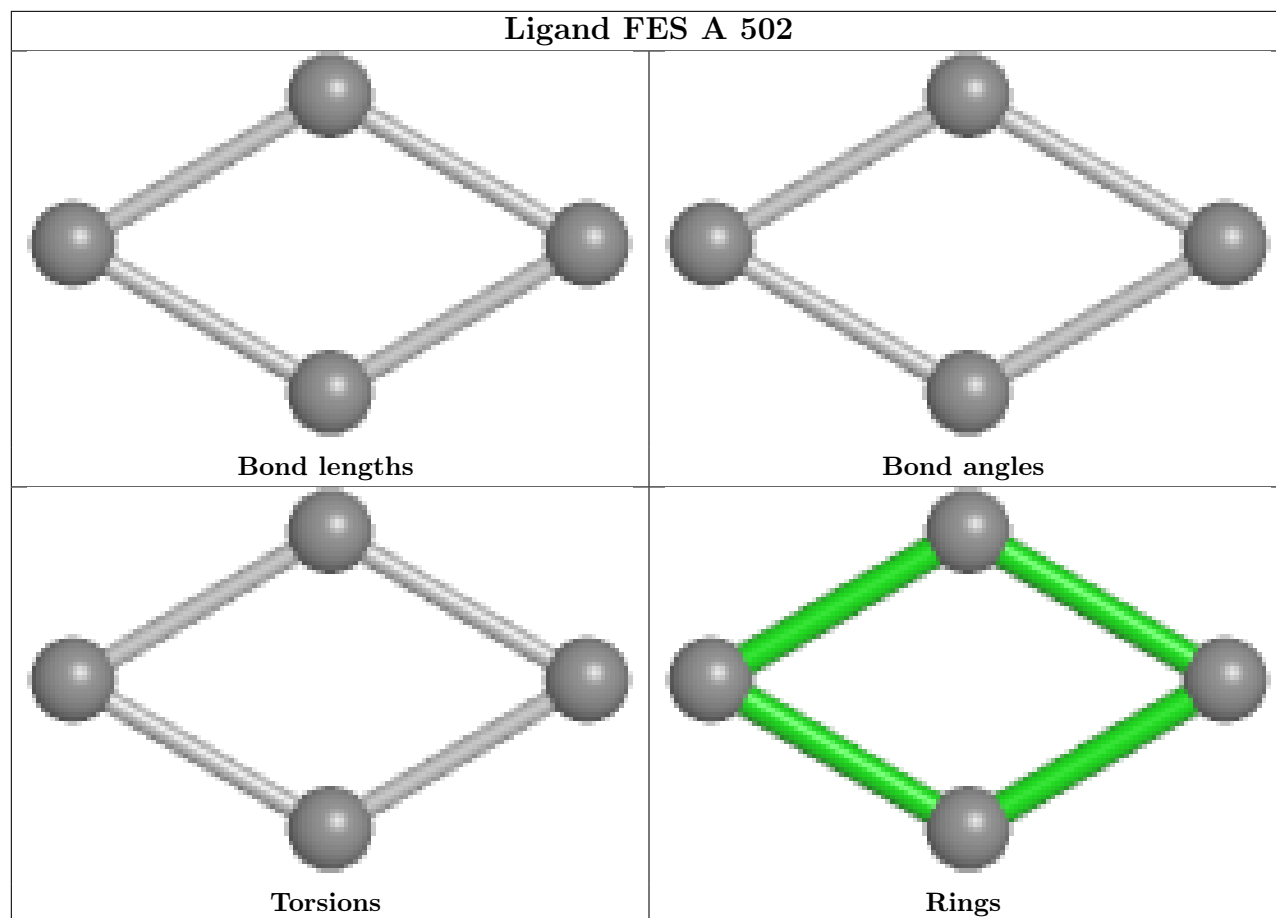












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	412/439 (93%)	-0.35	13 (3%) 50 53	18, 29, 59, 124	1 (0%)
1	B	412/439 (93%)	-0.26	8 (1%) 66 69	18, 31, 64, 96	1 (0%)
1	C	407/439 (92%)	-0.19	14 (3%) 48 51	19, 32, 74, 156	1 (0%)
1	D	412/439 (93%)	-0.34	10 (2%) 59 62	19, 29, 60, 121	1 (0%)
1	E	407/439 (92%)	-0.11	24 (5%) 28 30	21, 32, 77, 110	1 (0%)
1	F	409/439 (93%)	-0.14	9 (2%) 62 65	20, 33, 71, 105	1 (0%)
All	All	2459/2634 (93%)	-0.23	78 (3%) 50 53	18, 31, 71, 156	6 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	VAL	7.8
1	C	113	GLY	5.1
1	C	114	MET	4.8
1	C	111	ALA	4.5
1	F	111	ALA	3.9
1	D	115	VAL	3.8
1	D	110	ALA	3.8
1	D	111	ALA	3.7
1	C	110	ALA	3.7
1	A	112	SER	3.5
1	E	423	LEU	3.4
1	C	116	ASP	3.3
1	C	109	PRO	3.2
1	B	207	ARG	3.1
1	C	207	ARG	3.1
1	C	423	LEU	3.1
1	C	112	SER	3.1
1	E	237	ALA	3.1
1	E	207	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	111	ALA	3.0
1	E	238	ALA	3.0
1	E	153	THR	3.0
1	A	110	ALA	2.9
1	A	111	ALA	2.9
1	E	112	SER	2.9
1	E	395	ALA	2.9
1	B	398	PRO	2.9
1	D	113	GLY	2.9
1	A	115	VAL	2.8
1	C	118	VAL	2.8
1	F	393	VAL	2.8
1	C	234	LEU	2.8
1	E	407	VAL	2.7
1	D	207	ARG	2.7
1	E	411	THR	2.7
1	B	115	VAL	2.7
1	A	425	GLY	2.6
1	E	405	ALA	2.6
1	E	416	TYR	2.6
1	E	410	THR	2.5
1	E	406	ILE	2.5
1	F	110	ALA	2.5
1	C	237	ALA	2.5
1	E	234	LEU	2.5
1	A	207	ARG	2.5
1	E	422	TRP	2.5
1	F	154	ALA	2.4
1	D	112	SER	2.4
1	C	117	LYS	2.4
1	F	207	ARG	2.4
1	B	153	THR	2.4
1	B	428	ARG	2.4
1	E	113	GLY	2.3
1	F	396	ALA	2.3
1	D	425	GLY	2.3
1	E	413	TRP	2.3
1	E	408	PRO	2.2
1	A	428	ARG	2.2
1	B	425	GLY	2.2
1	A	1	MET	2.2
1	A	398	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.2
1	D	190	MET	2.2
1	F	423	LEU	2.2
1	B	111	ALA	2.1
1	E	242	TYR	2.1
1	A	393	VAL	2.1
1	E	393	VAL	2.1
1	F	118	VAL	2.1
1	E	418	ALA	2.1
1	A	114	MET	2.0
1	D	114	MET	2.0
1	A	423	LEU	2.0
1	D	234	LEU	2.0
1	E	110	ALA	2.0
1	E	210	THR	2.0
1	F	398	PRO	2.0
1	A	113	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	E	507	4/4	0.77	0.21	60,61,61,62	0
6	EDO	F	501	4/4	0.83	0.16	63,63,63,64	0
6	EDO	E	501	4/4	0.85	0.19	58,64,68,68	0
6	EDO	E	508	4/4	0.87	0.14	65,68,68,70	0
6	EDO	C	505	4/4	0.88	0.16	43,43,43,48	0
6	EDO	B	507	4/4	0.89	0.14	53,55,56,57	0

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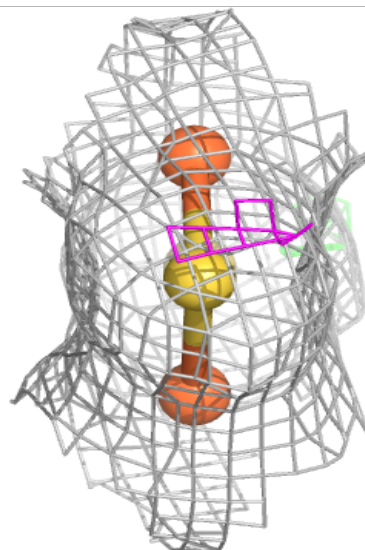
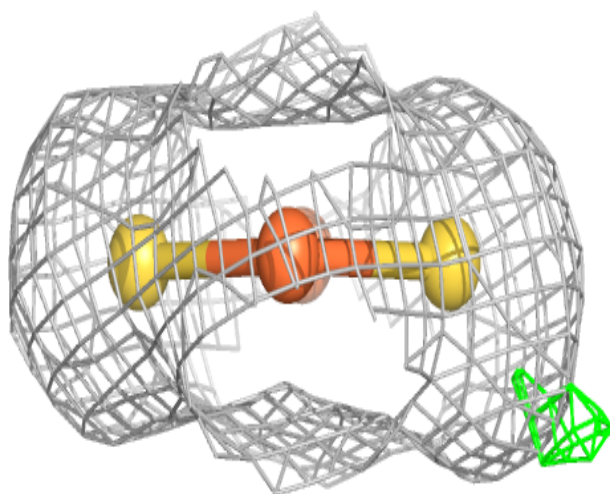
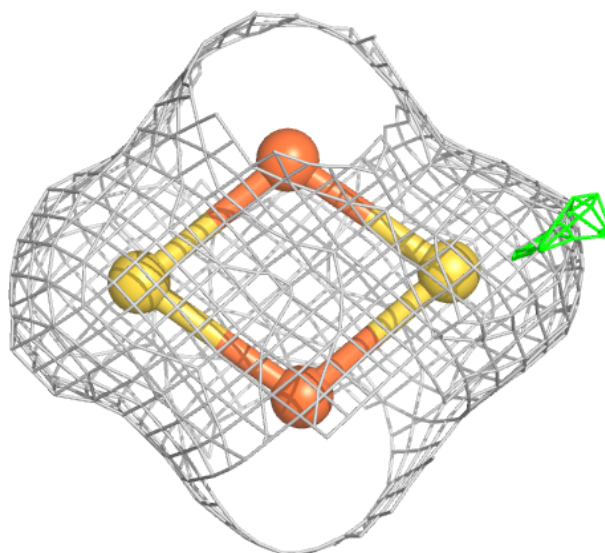
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SRT	D	503	10/10	0.90	0.10	38,47,51,52	0
6	EDO	B	505	4/4	0.90	0.13	50,50,51,52	0
5	SRT	E	504	10/10	0.91	0.09	49,53,55,55	0
5	SRT	C	503	10/10	0.92	0.10	44,49,58,63	0
6	EDO	F	505	4/4	0.92	0.10	33,35,39,40	0
5	SRT	B	503	10/10	0.93	0.09	34,46,52,55	0
5	SRT	F	504	10/10	0.93	0.08	52,56,57,59	0
6	EDO	B	506	4/4	0.94	0.08	32,33,35,39	0
6	EDO	B	508	4/4	0.94	0.12	42,42,47,53	0
4	TLA	A	503	10/10	0.95	0.07	35,39,46,51	0
6	EDO	B	504	4/4	0.95	0.08	32,34,39,40	0
6	EDO	C	504	4/4	0.96	0.07	29,34,36,42	0
6	EDO	E	506	4/4	0.96	0.07	43,44,44,46	0
6	EDO	E	505	4/4	0.97	0.07	25,31,33,39	0
6	EDO	D	505	4/4	0.97	0.08	28,33,41,42	0
6	EDO	D	504	4/4	0.97	0.07	36,37,38,44	0
3	FES	A	502	4/4	0.99	0.02	24,24,24,27	0
3	FES	D	502	4/4	0.99	0.02	25,27,27,29	0
2	FE2	E	502	1/1	1.00	0.01	27,27,27,27	0
2	FE2	F	502	1/1	1.00	0.01	26,26,26,26	0
2	FE2	A	501	1/1	1.00	0.01	21,21,21,21	0
3	FES	B	502	4/4	1.00	0.03	26,27,30,30	0
3	FES	C	502	4/4	1.00	0.02	27,27,28,31	0
2	FE2	B	501	1/1	1.00	0.01	24,24,24,24	0
3	FES	E	503	4/4	1.00	0.02	23,24,25,27	0
3	FES	F	503	4/4	1.00	0.02	26,26,27,29	0
2	FE2	C	501	1/1	1.00	0.01	26,26,26,26	0
2	FE2	D	501	1/1	1.00	0.01	26,26,26,26	0

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

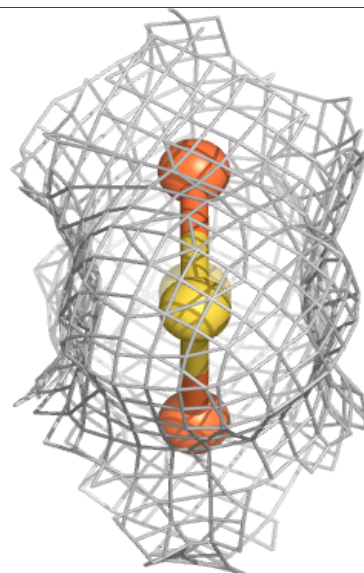
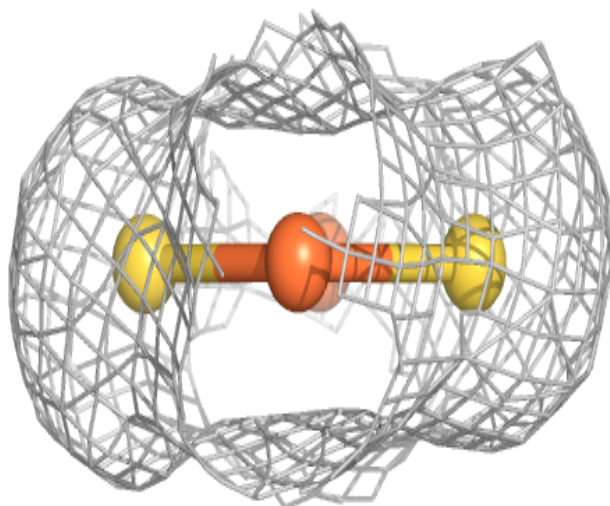
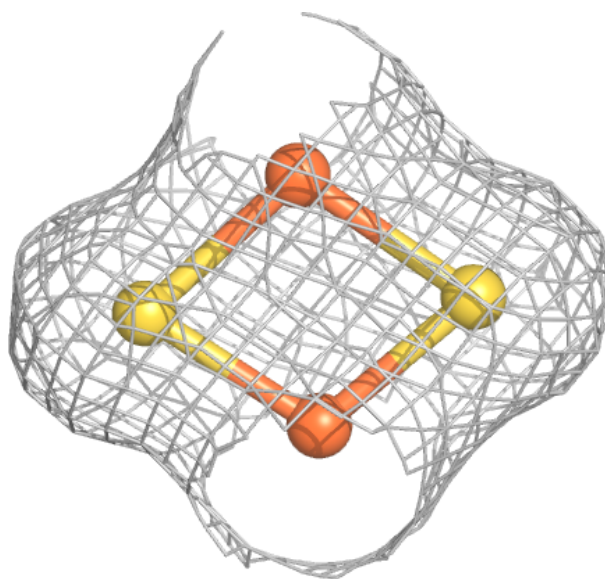
Electron density around FES A 502:

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



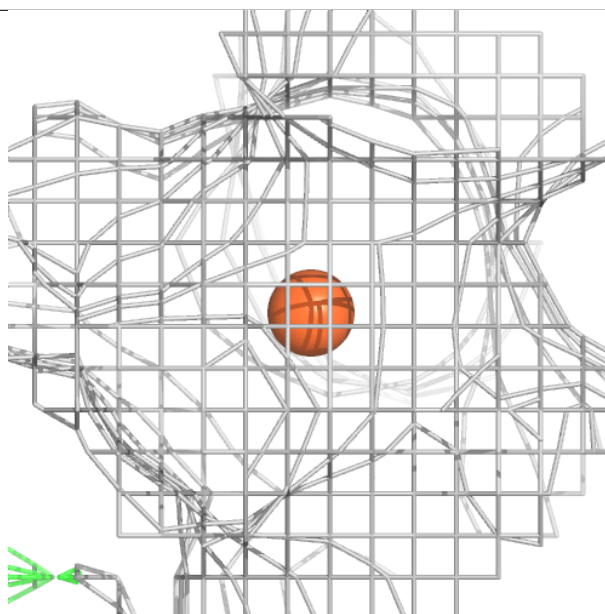
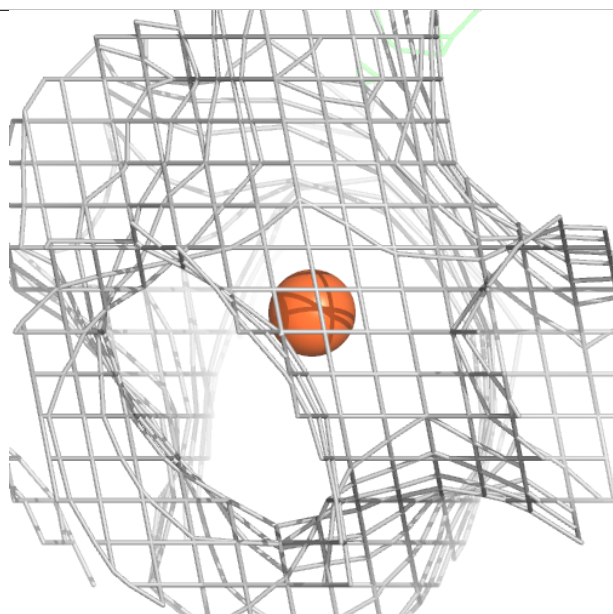
Electron density around FES D 502:

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



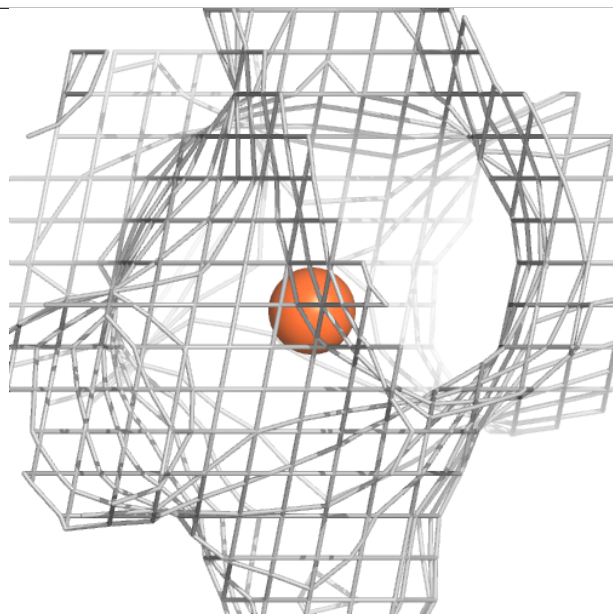
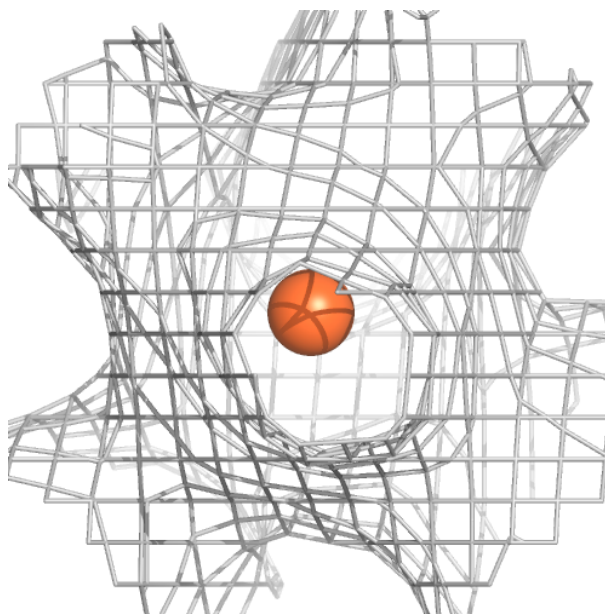
Electron density around FE2 E 502:

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



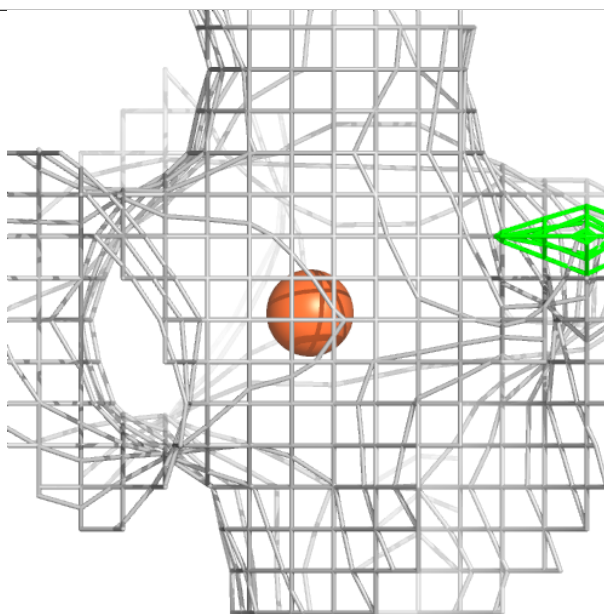
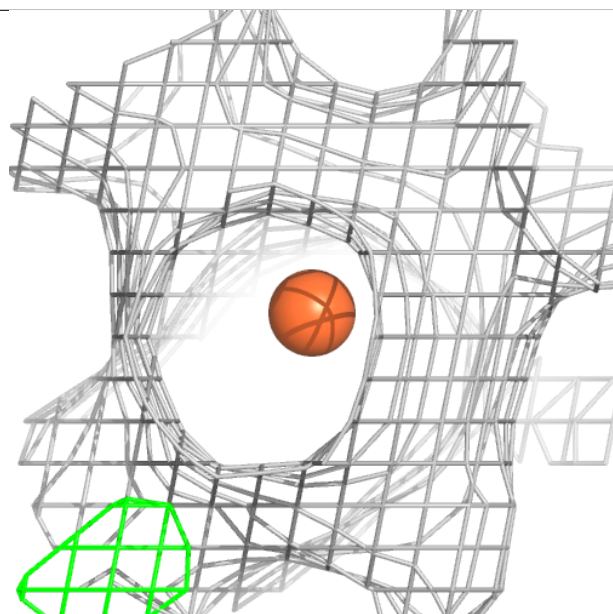
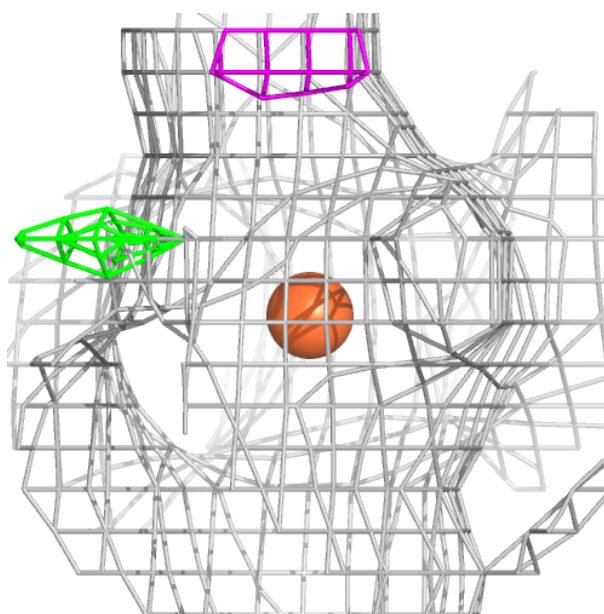
Electron density around FE2 F 502:

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



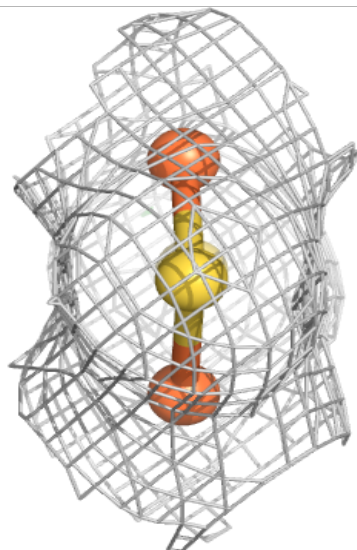
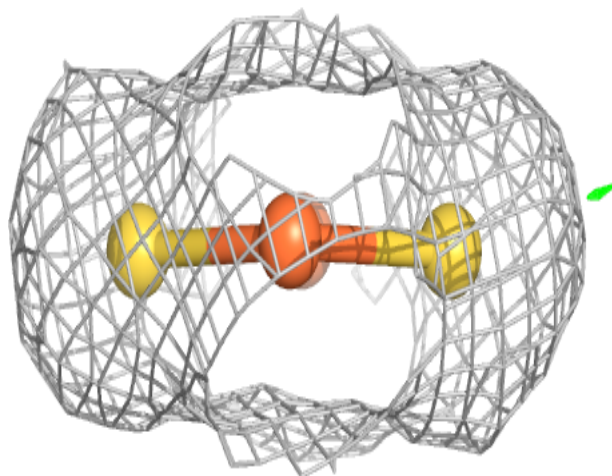
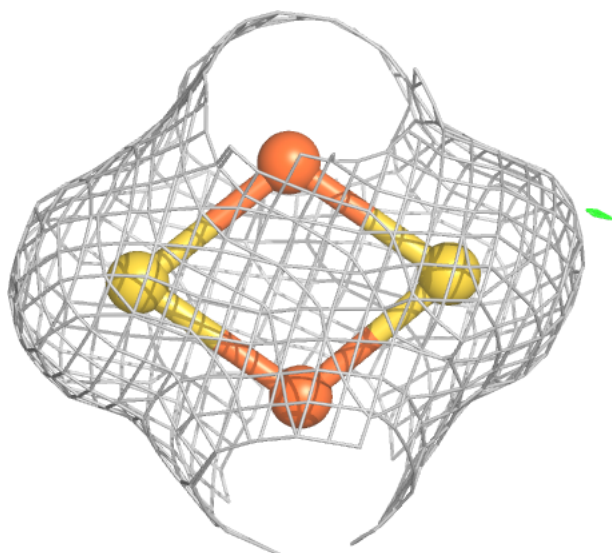
Electron density around FE2 A 501:

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



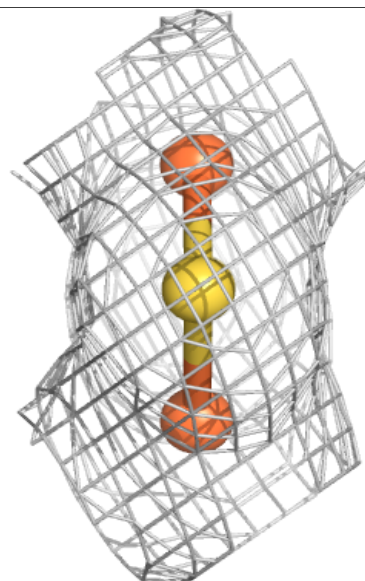
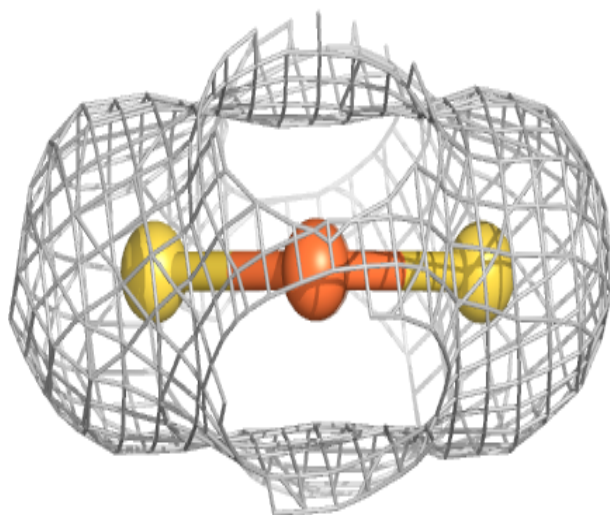
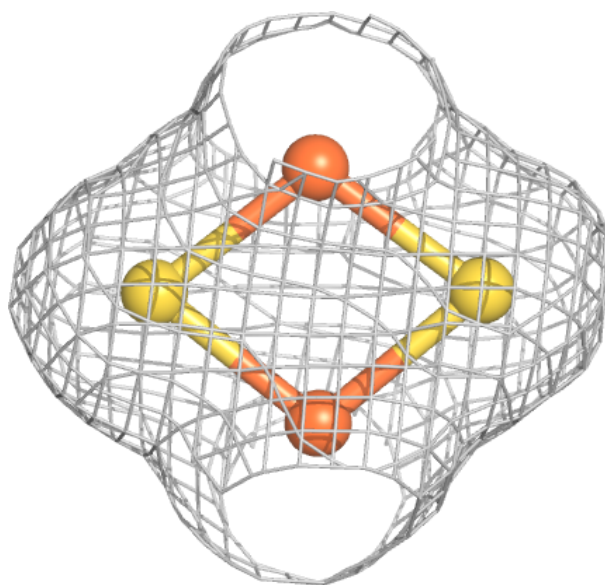
Electron density around FES B 502:

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



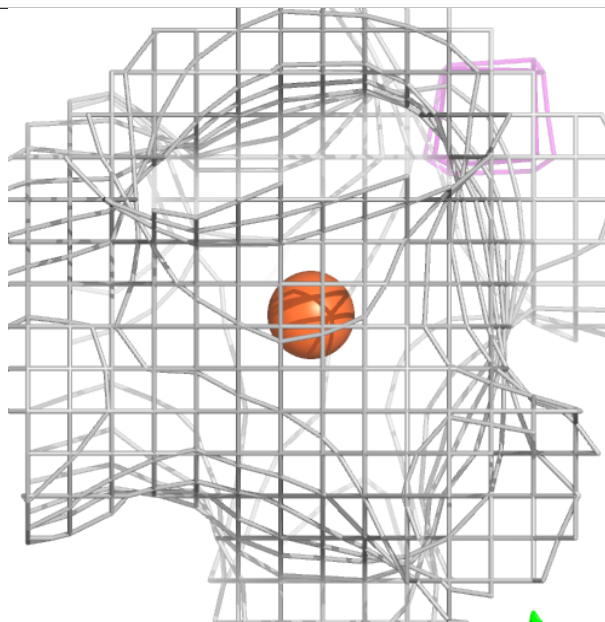
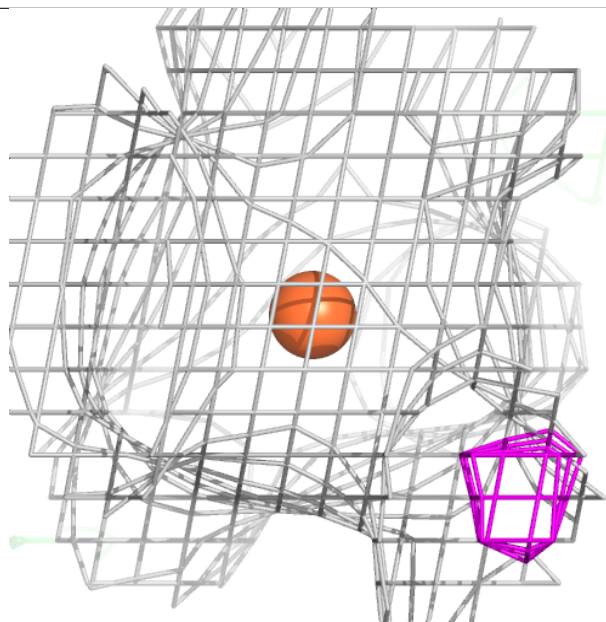
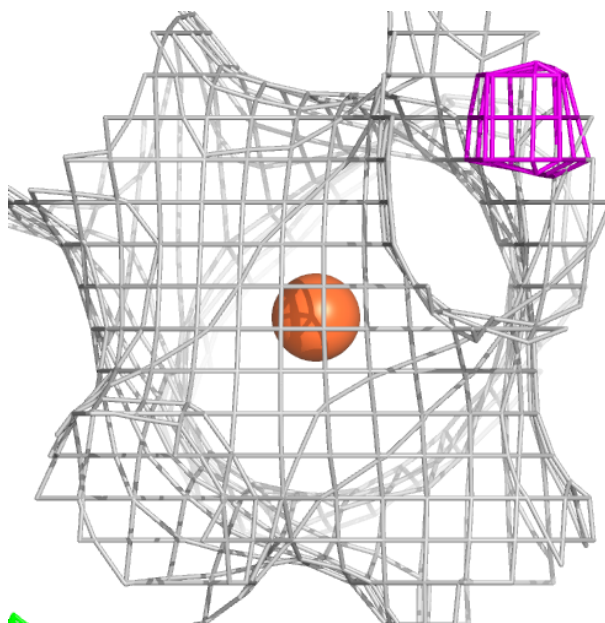
Electron density around FES C 502:

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



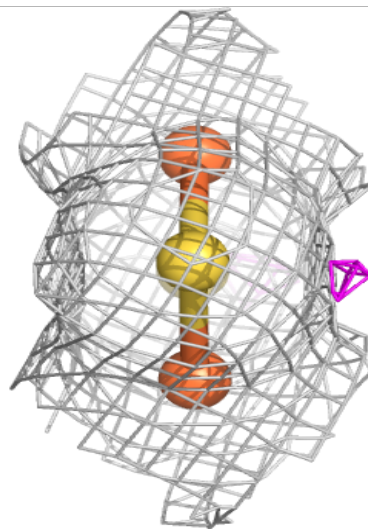
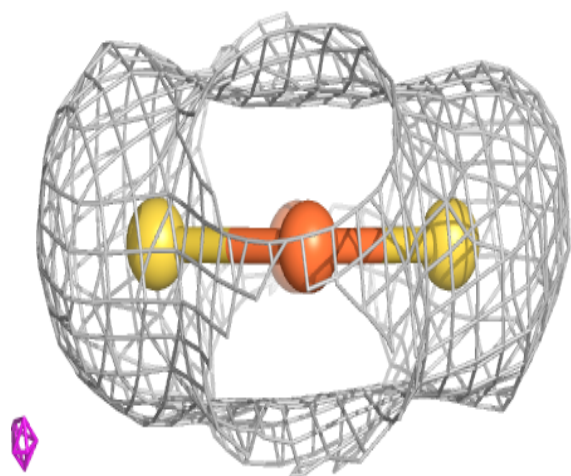
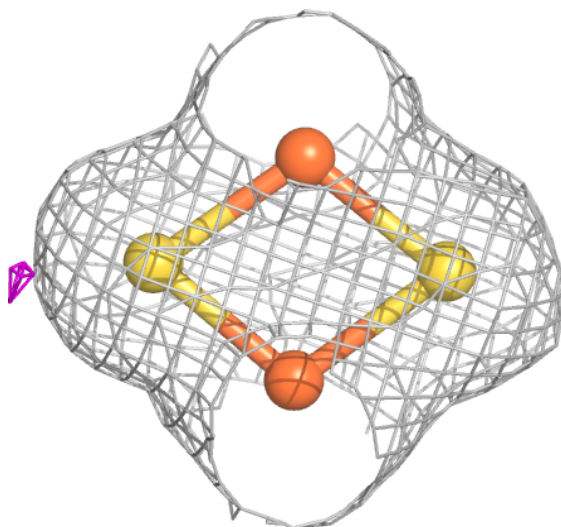
Electron density around FE2 B 501:

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



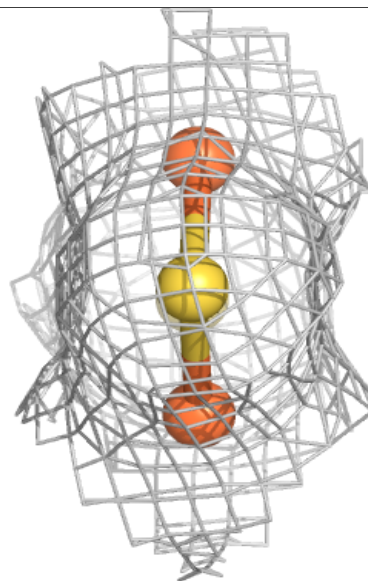
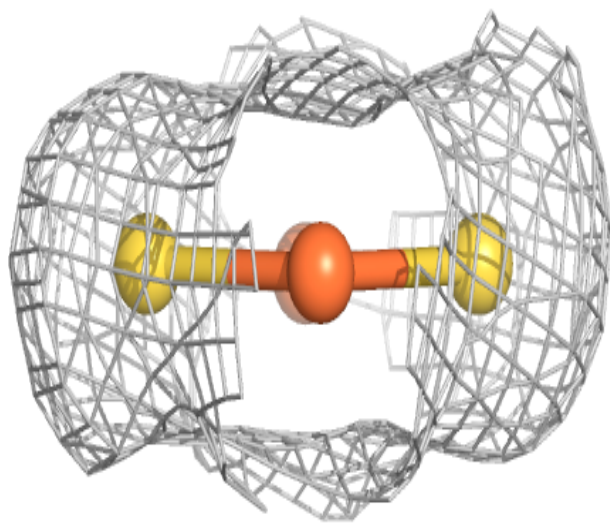
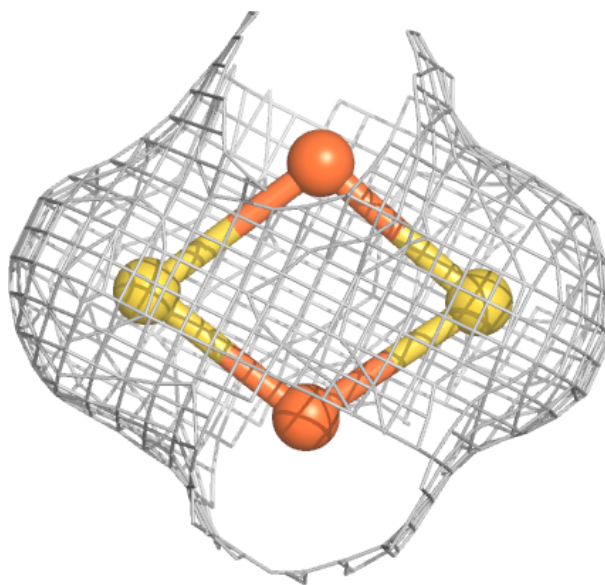
Electron density around FES E 503:

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



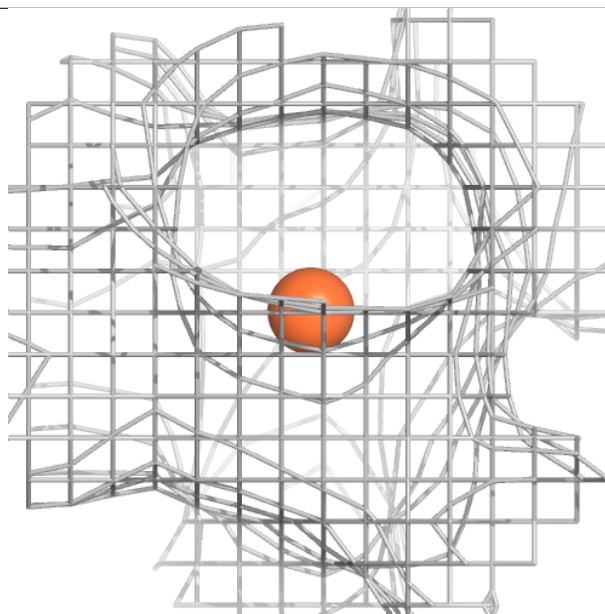
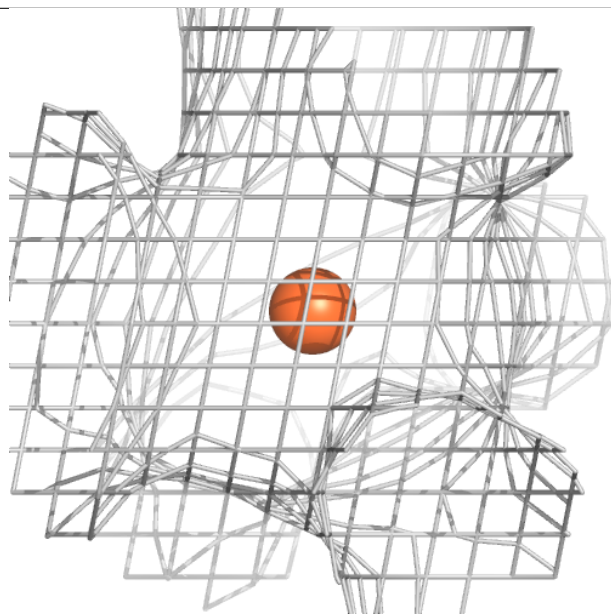
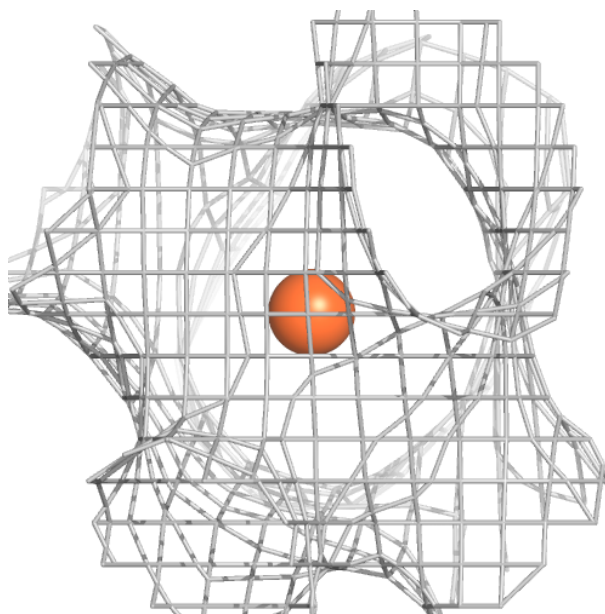
Electron density around FES F 503:

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



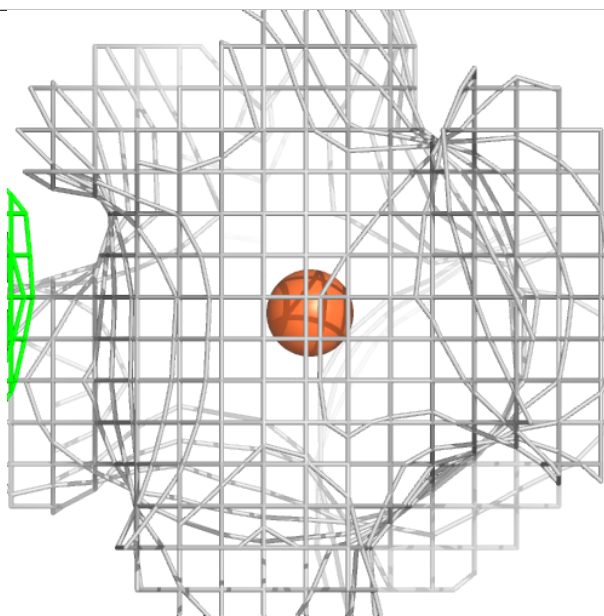
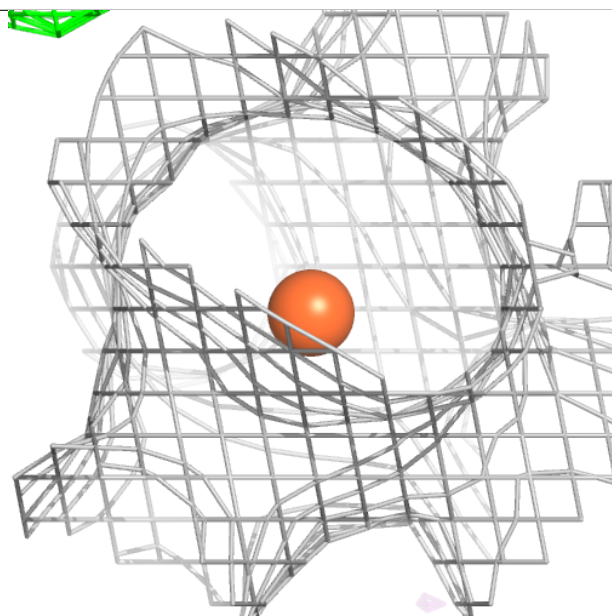
Electron density around FE2 C 501:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.