



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:25 AM BST

PDB ID : 6VCF
Title : Crystal structure of Nitrosotalea devanaterrea carotenoid cleavage dioxygenase, iron form
Authors : Daruwalla, A.; Shi, W.; Kiser, P.D.
Deposited on : 2019-12-20
Resolution : 2.69 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

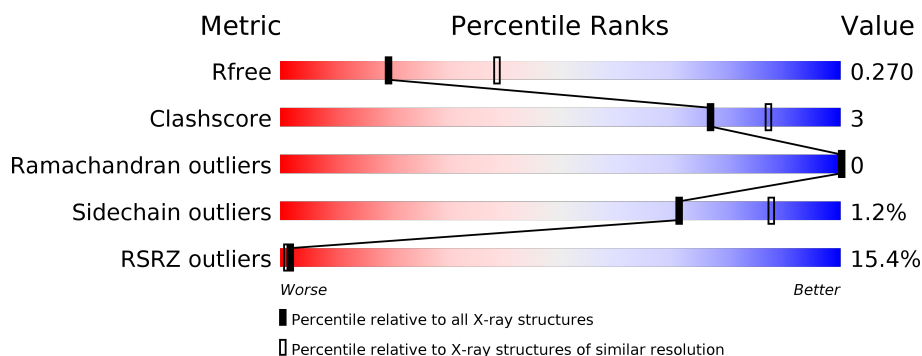
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 on 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	472	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	472	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	C	472	<div> <div>6%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	D	472	<div> <div>7%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	E	472	<div> <div>31%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	F	472	<div> <div>39%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21655 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 carotenoid cleavage dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	1	0
			3636	2343	594	692	7			
1	B	455	Total	C	N	O	S	0	0	0
			3655	2357	599	692	7			
1	C	453	Total	C	N	O	S	0	0	0
			3630	2342	594	687	7			
1	D	452	Total	C	N	O	S	0	0	0
			3617	2332	592	686	7			
1	E	432	Total	C	N	O	S	0	0	0
			3421	2204	556	654	7			
1	F	434	Total	C	N	O	S	0	0	0
			3435	2213	567	648	7			

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

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

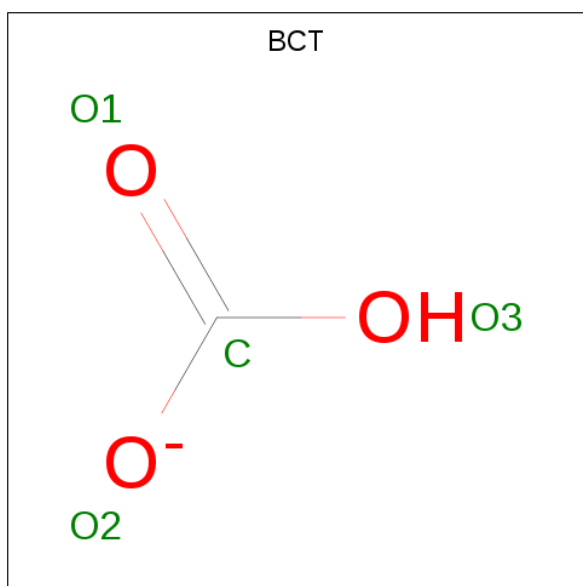
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 1 3	0	0
5	C	1	Total C O 4 1 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	68	Total O 68 68	0	0
6	B	68	Total O 68 68	0	0

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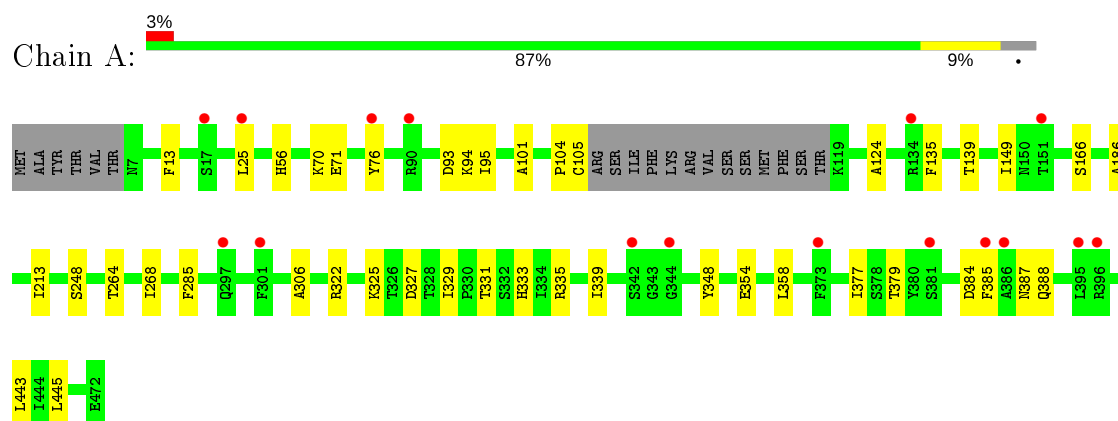
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	42	Total 42	O 42	0	0
6	D	45	Total 45	O 45	0	0
6	E	12	Total 12	O 12	0	0
6	F	9	Total 9	O 9	0	0

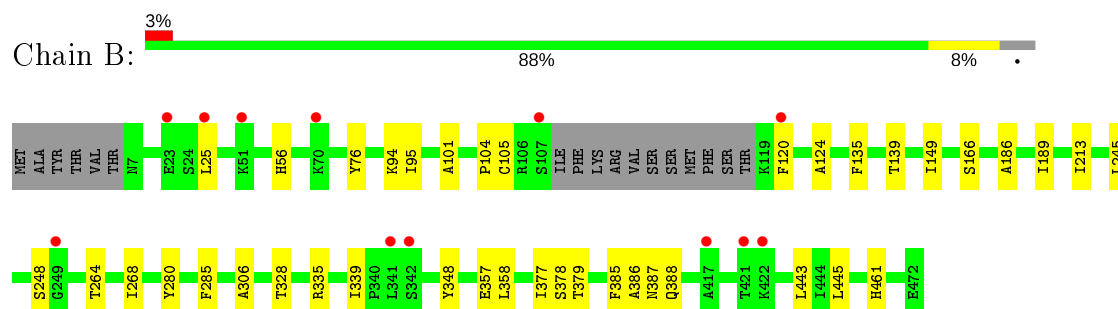
3 Residue-property plots [i](#)

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.

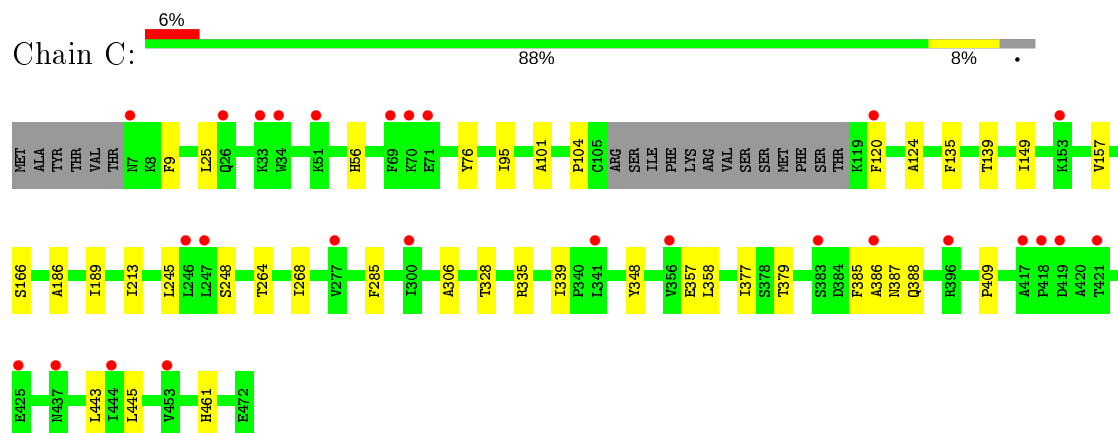
- Molecule 1: carotenoid cleavage dioxygenase



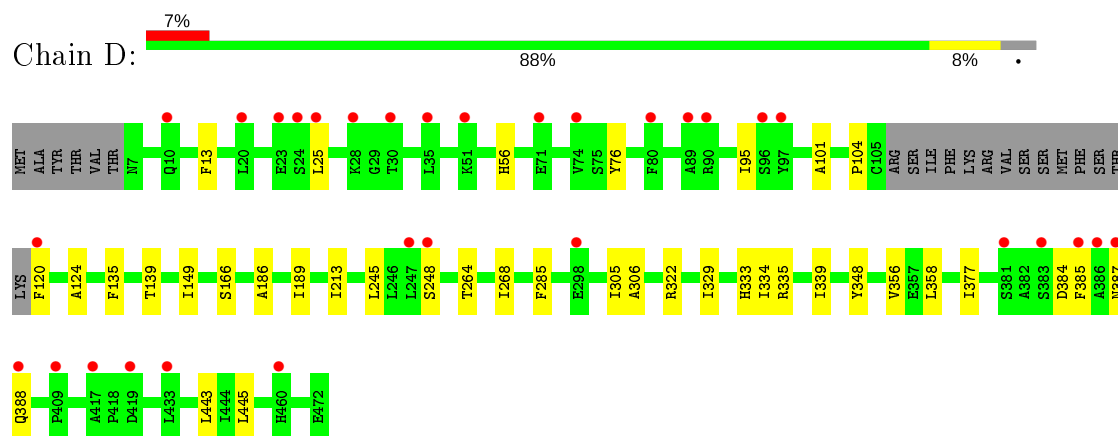
- Molecule 1: carotenoid cleavage dioxygenase



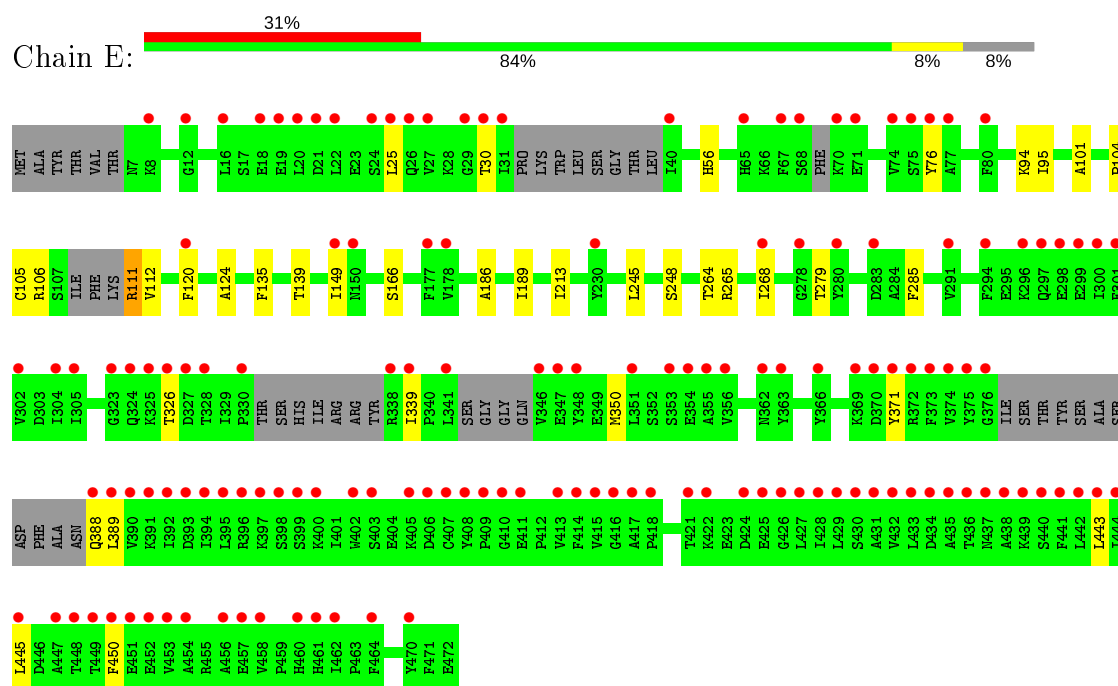
- Molecule 1: carotenoid cleavage dioxygenase



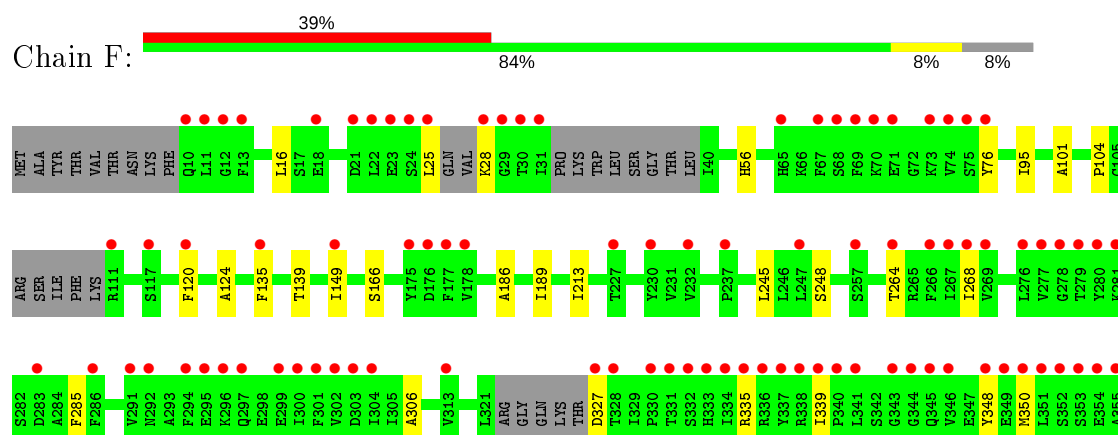
• Molecule 1: carotenoid cleavage dioxygenase

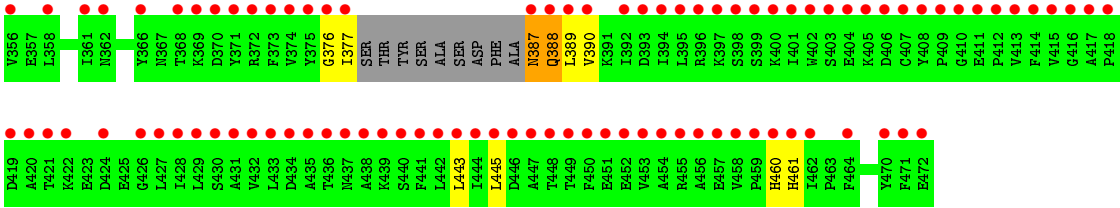


• Molecule 1: carotenoid cleavage dioxygenase



• Molecule 1: carotenoid cleavage dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	107.27Å 107.27Å 491.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 2.69 49.15 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.15-2.69) 99.8 (49.15-2.69)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.252 , 0.271 0.252 , 0.270	Depositor DCC
R_{free} test set	4373 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21655	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: BCT, NA, FE2, CL

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	0.64	0/3729	0.72	0/5061
1	B	0.63	0/3748	0.71	0/5080
1	C	0.64	0/3723	0.71	0/5050
1	D	0.64	0/3710	0.71	0/5034
1	E	0.65	0/3502	0.71	0/4747
1	F	0.65	0/3518	0.71	0/4771
All	All	0.64	0/21930	0.71	0/29743

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3636	0	3505	26	0
1	B	3655	0	3558	20	0
1	C	3630	0	3518	21	0
1	D	3617	0	3495	22	0
1	E	3421	0	3263	23	0
1	F	3435	0	3281	22	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
6	A	68	0	0	0	0
6	B	68	0	0	0	0
6	C	42	0	0	0	0
6	D	45	0	0	0	0
6	E	12	0	0	0	0
6	F	9	0	0	0	0
All	All	21655	0	20620	127	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 3.

All (127) 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:354[B]:GLU:N	1:A:354[B]:GLU:OE1	2.12	0.82
1:F:376:GLY:O	1:F:377:ILE:HG22	1.80	0.80
1:D:334:ILE:HG13	1:D:356:VAL:HG21	1.73	0.70
1:E:389:LEU:HG	1:E:450:PHE:CZ	2.27	0.69
1:D:306:ALA:HB3	1:D:335:ARG:HD3	1.76	0.67
1:A:306:ALA:HB3	1:A:335:ARG:HD3	1.76	0.67
1:C:306:ALA:HB3	1:C:335:ARG:HD3	1.76	0.67
1:B:306:ALA:HB3	1:B:335:ARG:HD3	1.75	0.66
1:F:306:ALA:HB3	1:F:335:ARG:HD3	1.76	0.66
1:D:13:PHE:O	1:D:322:ARG:NH1	2.29	0.66
1:A:13:PHE:O	1:A:322:ARG:NH1	2.29	0.65
1:F:377:ILE:HG22	1:F:390:VAL:HG12	1.79	0.63
1:E:389:LEU:HG	1:E:450:PHE:HZ	1.64	0.61
1:F:387:ASN:HD22	1:F:387:ASN:N	1.99	0.60
1:E:166:SER:HB2	1:E:186:ALA:HB1	1.84	0.60
1:F:166:SER:HB2	1:F:186:ALA:HB1	1.84	0.59
1:D:166:SER:HB2	1:D:186:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD12	1:A:377:ILE:HD12	1.85	0.59
1:A:166:SER:HB2	1:A:186:ALA:HB1	1.85	0.58
1:C:166:SER:HB2	1:C:186:ALA:HB1	1.84	0.58
1:A:384:ASP:HB3	1:A:387:ASN:HB3	1.84	0.58
1:B:166:SER:HB2	1:B:186:ALA:HB1	1.84	0.58
1:C:379:THR:HA	1:C:387:ASN:OD1	2.03	0.58
1:B:379:THR:HA	1:B:387:ASN:OD1	2.03	0.57
1:F:377:ILE:HG23	1:F:388:GLN:O	2.05	0.57
1:D:358:LEU:HD12	1:D:377:ILE:HD12	1.86	0.57
1:D:384:ASP:HB3	1:D:387:ASN:HB3	1.86	0.56
1:A:333:HIS:NE2	1:C:328:THR:HG21	2.22	0.54
1:B:213:ILE:N	1:B:213:ILE:HD12	2.25	0.52
1:B:95:ILE:O	1:B:104:PRO:HB3	2.09	0.52
1:E:105:CYS:SG	1:E:106:ARG:N	2.82	0.52
1:C:213:ILE:HD12	1:C:213:ILE:N	2.25	0.52
1:D:305:ILE:HD12	1:D:356:VAL:HG23	1.91	0.52
1:E:213:ILE:HD12	1:E:213:ILE:N	2.25	0.51
1:E:265:ARG:HG3	1:E:279:THR:HG23	1.92	0.51
1:A:213:ILE:HD12	1:A:213:ILE:N	2.25	0.51
1:F:213:ILE:HD12	1:F:213:ILE:N	2.25	0.51
1:D:213:ILE:N	1:D:213:ILE:HD12	2.25	0.51
1:A:95:ILE:O	1:A:104:PRO:HB3	2.10	0.51
1:B:94:LYS:NZ	1:B:105:CYS:SG	2.81	0.51
1:E:56:HIS:HB2	1:E:101:ALA:HB3	1.92	0.51
1:A:56:HIS:HB2	1:A:101:ALA:HB3	1.93	0.51
1:C:9:PHE:CZ	1:C:385:PHE:HB2	2.46	0.51
1:F:16:LEU:HD21	1:F:460:HIS:CE1	2.47	0.50
1:D:56:HIS:HB2	1:D:101:ALA:HB3	1.94	0.50
1:C:95:ILE:O	1:C:104:PRO:HB3	2.12	0.50
1:E:95:ILE:O	1:E:104:PRO:HB3	2.11	0.49
1:D:95:ILE:O	1:D:104:PRO:HB3	2.12	0.49
1:B:56:HIS:HB2	1:B:101:ALA:HB3	1.93	0.49
1:C:56:HIS:HB2	1:C:101:ALA:HB3	1.94	0.49
1:F:56:HIS:HB2	1:F:101:ALA:HB3	1.94	0.49
1:B:358:LEU:HD12	1:B:377:ILE:HD13	1.95	0.49
1:C:166:SER:CB	1:C:186:ALA:HB1	2.43	0.49
1:D:329:ILE:HG21	1:D:385:PHE:CZ	2.48	0.49
1:C:358:LEU:HD12	1:C:377:ILE:HD13	1.94	0.48
1:F:95:ILE:O	1:F:104:PRO:HB3	2.13	0.48
1:A:94:LYS:NZ	1:A:105:CYS:SG	2.83	0.48
1:D:166:SER:CB	1:D:186:ALA:HB1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:LYS:NZ	1:E:105:CYS:SG	2.82	0.47
1:E:166:SER:CB	1:E:186:ALA:HB1	2.44	0.47
1:B:166:SER:CB	1:B:186:ALA:HB1	2.44	0.47
1:F:166:SER:CB	1:F:186:ALA:HB1	2.44	0.47
1:F:377:ILE:HG23	1:F:389:LEU:HA	1.97	0.47
1:E:350:MET:SD	1:F:327:ASP:HB3	2.55	0.47
1:F:268:ILE:HD11	1:F:339:ILE:HG21	1.98	0.46
1:A:166:SER:CB	1:A:186:ALA:HB1	2.44	0.46
1:E:326:THR:CG2	1:F:350:MET:HB2	2.45	0.46
1:B:328:THR:HG21	1:D:333:HIS:CE1	2.51	0.46
1:B:335:ARG:HG2	1:B:348:TYR:CE2	2.51	0.45
1:B:124:ALA:HA	1:B:139:THR:HB	1.98	0.45
1:D:124:ALA:HA	1:D:139:THR:HB	1.99	0.45
1:E:265:ARG:HD2	1:E:279:THR:HG21	1.99	0.45
1:A:124:ALA:HA	1:A:139:THR:HB	1.99	0.45
1:C:189:ILE:HG21	1:C:245:LEU:HD23	1.99	0.45
1:C:335:ARG:HG2	1:C:348:TYR:CE2	2.51	0.45
1:E:268:ILE:HD11	1:E:339:ILE:HG21	1.98	0.45
1:B:378:SER:O	1:B:386:ALA:HA	2.17	0.45
1:C:268:ILE:HD11	1:C:339:ILE:HG21	1.98	0.45
1:A:268:ILE:HD11	1:A:339:ILE:HG21	1.99	0.45
1:B:268:ILE:HD11	1:B:339:ILE:HG21	1.99	0.45
1:A:329:ILE:HG21	1:A:385:PHE:CZ	2.52	0.45
1:B:25:LEU:HD11	1:B:76:TYR:HB2	1.99	0.44
1:C:124:ALA:HA	1:C:139:THR:HB	1.99	0.44
1:F:124:ALA:HA	1:F:139:THR:HB	1.99	0.44
1:A:335:ARG:HG2	1:A:348:TYR:CE2	2.52	0.44
1:A:358:LEU:HD12	1:A:377:ILE:CD1	2.47	0.44
1:A:93:ASP:CG	1:E:30:THR:HB	2.38	0.44
1:D:268:ILE:HD11	1:D:339:ILE:HG21	1.98	0.44
1:D:358:LEU:HD12	1:D:377:ILE:CD1	2.47	0.44
1:E:111:ARG:NH2	1:E:112:VAL:O	2.51	0.44
1:F:335:ARG:HG2	1:F:348:TYR:CE2	2.52	0.44
1:D:264:THR:HG21	1:D:285:PHE:CE1	2.53	0.44
1:D:335:ARG:HG2	1:D:348:TYR:CE2	2.52	0.44
1:F:264:THR:HG21	1:F:285:PHE:CE1	2.53	0.44
1:C:25:LEU:HD11	1:C:76:TYR:HB2	2.00	0.43
1:E:124:ALA:HA	1:E:139:THR:HB	1.99	0.43
1:E:25:LEU:HD11	1:E:76:TYR:HB2	1.99	0.43
1:B:264:THR:HG21	1:B:285:PHE:CE1	2.53	0.43
1:E:264:THR:HG21	1:E:285:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:THR:HG21	1:C:285:PHE:CE1	2.54	0.43
1:F:25:LEU:HD11	1:F:76:TYR:HB2	2.00	0.43
1:B:189:ILE:HG21	1:B:245:LEU:HD23	2.00	0.43
1:A:25:LEU:HD11	1:A:76:TYR:HB2	2.01	0.42
1:E:443:LEU:HD21	1:E:445:LEU:HD21	2.01	0.42
1:D:25:LEU:HD11	1:D:76:TYR:HB2	2.00	0.42
1:D:443:LEU:HD21	1:D:445:LEU:HD21	2.01	0.42
1:F:443:LEU:HD21	1:F:445:LEU:HD21	2.01	0.42
1:A:264:THR:HG21	1:A:285:PHE:CE1	2.54	0.42
1:A:443:LEU:HD21	1:A:445:LEU:HD21	2.01	0.42
1:D:189:ILE:HG21	1:D:245:LEU:HD23	2.00	0.42
1:A:135:PHE:CE1	1:A:149:ILE:HD12	2.55	0.42
1:B:443:LEU:HD21	1:B:445:LEU:HD21	2.02	0.42
1:E:265:ARG:CG	1:E:279:THR:HG23	2.50	0.42
1:B:135:PHE:CE1	1:B:149:ILE:HD12	2.56	0.41
1:A:327:ASP:OD2	1:C:335:ARG:HD2	2.21	0.41
1:F:135:PHE:CE1	1:F:149:ILE:HD12	2.56	0.41
1:A:70:LYS:C	1:A:71:GLU:HG2	2.41	0.41
1:C:135:PHE:CE1	1:C:149:ILE:HD12	2.56	0.41
1:C:443:LEU:HD21	1:C:445:LEU:HD21	2.02	0.41
1:D:135:PHE:CE1	1:D:149:ILE:HD12	2.56	0.41
1:E:189:ILE:HG21	1:E:245:LEU:HD23	2.03	0.41
1:A:331:THR:HG22	1:A:379:THR:O	2.21	0.41
1:B:268:ILE:HD12	1:B:280:TYR:CE2	2.56	0.41
1:F:189:ILE:HG21	1:F:245:LEU:HD23	2.03	0.41
1:A:325:LYS:HD2	1:C:348:TYR:CZ	2.56	0.40
1:C:386:ALA:O	1:C:409:PRO:HD2	2.22	0.40
1:E:135:PHE:CE1	1:E:149:ILE:HD12	2.56	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	450/472 (95%)	423 (94%)	27 (6%)	0	100	100
1	B	451/472 (96%)	425 (94%)	26 (6%)	0	100	100
1	C	449/472 (95%)	421 (94%)	28 (6%)	0	100	100
1	D	448/472 (95%)	419 (94%)	29 (6%)	0	100	100
1	E	418/472 (89%)	390 (93%)	28 (7%)	0	100	100
1	F	422/472 (89%)	397 (94%)	25 (6%)	0	100	100
All	All	2638/2832 (93%)	2475 (94%)	163 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	392/417 (94%)	390 (100%)	2 (0%)	88	95
1	B	397/417 (95%)	391 (98%)	6 (2%)	65	84
1	C	392/417 (94%)	386 (98%)	6 (2%)	65	84
1	D	390/417 (94%)	387 (99%)	3 (1%)	81	92
1	E	365/417 (88%)	360 (99%)	5 (1%)	67	85
1	F	363/417 (87%)	357 (98%)	6 (2%)	60	82
All	All	2299/2502 (92%)	2271 (99%)	28 (1%)	71	87

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	A	388	GLN
1	B	120	PHE
1	B	248	SER
1	B	357	GLU
1	B	385	PHE
1	B	388	GLN

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Mol	Chain	Res	Type
1	B	461	HIS
1	C	120	PHE
1	C	157	VAL
1	C	248	SER
1	C	357	GLU
1	C	388	GLN
1	C	461	HIS
1	D	120	PHE
1	D	248	SER
1	D	388	GLN
1	E	111	ARG
1	E	120	PHE
1	E	248	SER
1	E	371	TYR
1	E	388	GLN
1	F	28	LYS
1	F	120	PHE
1	F	248	SER
1	F	387	ASN
1	F	388	GLN
1	F	461	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z > 2$
5	BCT	C	502	2	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	B	502	2	0,3,3	0.00	-	0,3,3	0.00	-

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.

No monomer is involved in short contacts.

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	453/472 (95%)	0.29	16 (3%) 44 43	44, 74, 105, 127	0
1	B	455/472 (96%)	0.26	12 (2%) 56 55	38, 70, 107, 126	0
1	C	453/472 (95%)	0.40	27 (5%) 21 20	47, 79, 115, 138	0
1	D	452/472 (95%)	0.50	31 (6%) 16 14	47, 87, 133, 168	0
1	E	432/472 (91%)	1.70	144 (33%) 0 0	49, 101, 203, 246	0
1	F	434/472 (91%)	2.23	183 (42%) 0 0	61, 114, 215, 244	0
All	All	2679/2832 (94%)	0.88	413 (15%) 2 1	38, 84, 175, 246	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31	ILE	14.2
1	F	374	VAL	14.2
1	F	394	ILE	12.4
1	E	31	ILE	12.3
1	E	25	LEU	11.0
1	E	20	LEU	10.5
1	F	376	GLY	10.0
1	E	407	CYS	9.7
1	F	443	LEU	9.7
1	F	375	TYR	9.4
1	F	373	PHE	9.2
1	F	409	PRO	9.2
1	E	376	GLY	8.8
1	F	414	PHE	8.8
1	E	457	GLU	8.7
1	F	74	VAL	8.4
1	E	427	LEU	8.2
1	F	389	LEU	8.1
1	F	454	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
1	F	392	ILE	7.9
1	E	396	ARG	7.7
1	F	351	LEU	7.6
1	E	395	LEU	7.5
1	F	458	VAL	7.4
1	F	67	PHE	7.3
1	F	387	ASN	7.3
1	E	375	TYR	7.3
1	E	76	TYR	7.3
1	F	22	LEU	7.2
1	F	445	LEU	7.2
1	E	422	LYS	7.1
1	F	294	PHE	7.0
1	F	405	LYS	7.0
1	E	374	VAL	7.0
1	E	442	LEU	6.8
1	F	388	GLN	6.8
1	F	470	TYR	6.8
1	E	447	ALA	6.7
1	F	408	TYR	6.7
1	E	27	VAL	6.6
1	F	422	LYS	6.6
1	F	278	GLY	6.5
1	E	441	PHE	6.5
1	E	301	PHE	6.4
1	F	25	LEU	6.4
1	E	432	VAL	6.4
1	F	355	ALA	6.3
1	F	283	ASP	6.3
1	F	395	LEU	6.2
1	E	26	GLN	6.2
1	F	438	ALA	6.1
1	F	413	VAL	6.1
1	E	373	PHE	6.1
1	F	453	VAL	6.1
1	F	331	THR	6.1
1	F	406	ASP	6.1
1	F	350	MET	6.0
1	F	356	VAL	6.0
1	E	405	LYS	6.0
1	F	444	ILE	6.0
1	F	304	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	F	301	PHE	6.0
1	E	355	ALA	6.0
1	E	445	LEU	5.9
1	F	344	GLY	5.9
1	F	417	ALA	5.9
1	F	30	THR	5.8
1	C	417	ALA	5.8
1	E	450	PHE	5.8
1	F	337	TYR	5.8
1	F	441	PHE	5.8
1	E	454	ALA	5.8
1	F	401	ILE	5.7
1	F	291	VAL	5.7
1	E	470	TYR	5.7
1	F	339	ILE	5.6
1	E	354	GLU	5.6
1	E	392	ILE	5.6
1	E	65	HIS	5.5
1	F	371	TYR	5.5
1	F	427	LEU	5.5
1	E	456	ALA	5.5
1	F	456	ALA	5.5
1	F	440	SER	5.4
1	E	371	TYR	5.4
1	F	327	ASP	5.4
1	F	457	GLU	5.4
1	F	426	GLY	5.4
1	A	344	GLY	5.4
1	F	400	LYS	5.4
1	F	71	GLU	5.4
1	F	442	LEU	5.3
1	E	462	ILE	5.3
1	E	394	ILE	5.3
1	F	333	HIS	5.3
1	E	74	VAL	5.3
1	E	453	VAL	5.3
1	F	69	PHE	5.2
1	E	30	THR	5.2
1	F	349	GLU	5.2
1	E	410	GLY	5.2
1	E	409	PRO	5.2
1	F	407	CYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	440	SER	5.2
1	E	418	PRO	5.2
1	E	77	ALA	5.1
1	E	280	TYR	5.1
1	F	448	THR	5.1
1	F	436	THR	5.1
1	E	341	LEU	5.1
1	F	431	ALA	5.1
1	F	377	ILE	5.1
1	E	406	ASP	5.0
1	E	338	ARG	5.0
1	F	268	ILE	5.0
1	F	302	VAL	5.0
1	F	449	THR	5.0
1	F	300	ILE	4.9
1	F	429	LEU	4.9
1	F	276	LEU	4.9
1	F	70	LYS	4.9
1	E	414	PHE	4.9
1	E	438	ALA	4.8
1	E	393	ASP	4.8
1	E	389	LEU	4.8
1	F	452	GLU	4.8
1	E	278	GLY	4.8
1	F	390	VAL	4.7
1	E	390	VAL	4.7
1	F	280	TYR	4.7
1	F	328	THR	4.7
1	E	346	VAL	4.7
1	F	464	PHE	4.6
1	E	451	GLU	4.5
1	F	76	TYR	4.5
1	F	450	PHE	4.5
1	F	410	GLY	4.5
1	D	51	LYS	4.5
1	F	348	TYR	4.5
1	E	325	LYS	4.5
1	F	297	GLN	4.4
1	D	386	ALA	4.4
1	E	388	GLN	4.4
1	E	408	TYR	4.4
1	E	425	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	300	ILE	4.3
1	F	28	LYS	4.3
1	F	421	THR	4.3
1	F	451	GLU	4.3
1	E	399	SER	4.3
1	F	353	SER	4.2
1	E	67	PHE	4.2
1	F	177	PHE	4.2
1	F	396	ARG	4.2
1	E	339	ILE	4.2
1	F	354	GLU	4.2
1	F	415	VAL	4.2
1	F	430	SER	4.2
1	F	277	VAL	4.1
1	E	299	GLU	4.1
1	E	416	GLY	4.1
1	F	432	VAL	4.1
1	F	332	SER	4.1
1	F	29	GLY	4.0
1	E	413	VAL	4.0
1	F	65	HIS	4.0
1	F	362	ASN	4.0
1	F	434	ASP	4.0
1	E	398	SER	4.0
1	F	419	ASP	4.0
1	F	424	ASP	4.0
1	F	447	ALA	3.9
1	F	247	LEU	3.9
1	F	455	ARG	3.9
1	F	370	ASP	3.9
1	E	424	ASP	3.9
1	F	420	ALA	3.8
1	F	435	ALA	3.8
1	E	294	PHE	3.8
1	E	362	ASN	3.8
1	B	25	LEU	3.7
1	F	73	LYS	3.7
1	E	324	GLN	3.7
1	D	120	PHE	3.7
1	E	431	ALA	3.7
1	F	402	TRP	3.7
1	E	351	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	416	GLY	3.7
1	F	178	VAL	3.6
1	F	428	ILE	3.6
1	C	120	PHE	3.6
1	E	356	VAL	3.6
1	E	433	LEU	3.6
1	E	435	ALA	3.6
1	E	428	ILE	3.6
1	F	338	ARG	3.5
1	F	393	ASP	3.5
1	E	302	VAL	3.5
1	F	330	PRO	3.5
1	E	458	VAL	3.5
1	D	25	LEU	3.5
1	D	97	TYR	3.5
1	D	419	ASP	3.5
1	F	75	SER	3.5
1	F	403	SER	3.5
1	E	397	LYS	3.5
1	F	460	HIS	3.5
1	E	415	VAL	3.5
1	E	402	TRP	3.5
1	F	418	PRO	3.4
1	E	372	ARG	3.4
1	F	462	ILE	3.4
1	E	353	SER	3.4
1	E	417	ALA	3.3
1	B	51	LYS	3.3
1	F	343	GLY	3.3
1	E	40	ILE	3.3
1	F	10	GLN	3.3
1	F	232	VAL	3.3
1	E	8	LYS	3.2
1	F	361	ILE	3.2
1	A	396	ARG	3.2
1	C	70	LYS	3.1
1	E	429	LEU	3.1
1	E	439	LYS	3.1
1	E	444	ILE	3.1
1	F	313	VAL	3.1
1	F	369	LYS	3.1
1	C	437	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	33	LYS	3.1
1	E	326	THR	3.1
1	F	23	GLU	3.0
1	E	150	ASN	3.0
1	B	342	SER	3.0
1	F	472	GLU	3.0
1	D	23	GLU	3.0
1	E	421	THR	3.0
1	E	296	LYS	3.0
1	E	323	GLY	3.0
1	F	372	ARG	3.0
1	E	366	TYR	3.0
1	E	230	TYR	3.0
1	F	411	GLU	3.0
1	E	22	LEU	2.9
1	E	291	VAL	2.9
1	F	368	THR	2.9
1	E	21	ASP	2.9
1	E	327	ASP	2.9
1	A	76	TYR	2.9
1	F	12	GLY	2.9
1	D	71	GLU	2.9
1	F	227	THR	2.9
1	F	24	SER	2.9
1	F	334	ILE	2.9
1	F	286	PHE	2.9
1	F	13	PHE	2.8
1	A	381	SER	2.8
1	F	352	SER	2.8
1	F	335	ARG	2.8
1	F	341	LEU	2.8
1	E	452	GLU	2.8
1	E	434	ASP	2.8
1	F	461	HIS	2.8
1	A	25	LEU	2.8
1	F	439	LYS	2.8
1	E	330	PRO	2.8
1	E	12	GLY	2.8
1	E	29	GLY	2.8
1	A	373	PHE	2.7
1	D	24	SER	2.7
1	F	21	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	35	LEU	2.7
1	F	120	PHE	2.7
1	F	471	PHE	2.7
1	C	51	LYS	2.7
1	F	340	PRO	2.7
1	C	277	VAL	2.7
1	E	178	VAL	2.7
1	D	460	HIS	2.7
1	E	411	GLU	2.7
1	F	149	ILE	2.7
1	F	398	SER	2.7
1	A	297	GLN	2.6
1	E	297	GLN	2.6
1	E	19	GLU	2.6
1	F	336	ARG	2.6
1	B	421	THR	2.6
1	F	68	SER	2.6
1	B	417	ALA	2.6
1	D	247	LEU	2.6
1	A	342	SER	2.6
1	C	444	ILE	2.6
1	E	348	TYR	2.6
1	E	403	SER	2.6
1	F	175	TYR	2.6
1	F	346	VAL	2.6
1	D	385	PHE	2.6
1	A	395	LEU	2.6
1	E	298	GLU	2.6
1	C	453	VAL	2.6
1	F	269	VAL	2.6
1	D	387	ASN	2.6
1	E	70	LYS	2.6
1	E	426	GLY	2.6
1	E	391	LYS	2.6
1	C	419	ASP	2.6
1	F	446	ASP	2.6
1	F	267	ILE	2.5
1	F	412	PRO	2.5
1	B	120	PHE	2.5
1	E	120	PHE	2.5
1	E	448	THR	2.5
1	F	303	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	436	THR	2.5
1	B	341	LEU	2.5
1	F	230	TYR	2.5
1	F	299	GLU	2.5
1	E	369	LYS	2.5
1	F	433	LEU	2.5
1	F	264	THR	2.5
1	E	149	ILE	2.5
1	E	71	GLU	2.4
1	F	281	LYS	2.4
1	F	404	GLU	2.4
1	A	17	SER	2.4
1	E	430	SER	2.4
1	D	80	PHE	2.4
1	E	283	ASP	2.4
1	D	298	GLU	2.4
1	C	341	LEU	2.4
1	F	11	LEU	2.4
1	F	279	THR	2.4
1	E	68	SER	2.4
1	E	268	ILE	2.4
1	E	400	LYS	2.4
1	D	89	ALA	2.4
1	E	464	PHE	2.4
1	C	26	GLN	2.3
1	E	16	LEU	2.3
1	E	177	PHE	2.3
1	F	237	PRO	2.3
1	C	383	SER	2.3
1	E	443	LEU	2.3
1	E	370	ASP	2.3
1	B	23	GLU	2.3
1	E	80	PHE	2.3
1	F	296	LYS	2.3
1	F	111	ARG	2.3
1	E	18	GLU	2.3
1	D	96	SER	2.3
1	D	383	SER	2.3
1	F	358	LEU	2.3
1	A	385	PHE	2.3
1	D	433	LEU	2.3
1	F	295	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	328	THR	2.3
1	E	437	ASN	2.2
1	F	257	SER	2.2
1	E	363	TYR	2.2
1	E	75	SER	2.2
1	A	151	THR	2.2
1	C	396	ARG	2.2
1	B	249	GLY	2.2
1	E	305	ILE	2.2
1	B	70	LYS	2.2
1	C	7	ASN	2.2
1	F	366	TYR	2.2
1	B	107	SER	2.2
1	C	246	LEU	2.2
1	C	418	PRO	2.2
1	D	248	SER	2.2
1	B	422	LYS	2.2
1	F	459	PRO	2.2
1	A	90	ARG	2.2
1	D	381	SER	2.1
1	A	386	ALA	2.1
1	C	425	GLU	2.1
1	D	388	GLN	2.1
1	D	28	LYS	2.1
1	C	69	PHE	2.1
1	C	356	VAL	2.1
1	E	460	HIS	2.1
1	F	18	GLU	2.1
1	D	30	THR	2.1
1	F	135	PHE	2.1
1	F	437	ASN	2.1
1	C	247	LEU	2.1
1	D	409	PRO	2.1
1	F	292	ASN	2.1
1	A	301	PHE	2.1
1	F	117	SER	2.1
1	F	397	LYS	2.1
1	F	399	SER	2.1
1	F	176	ASP	2.1
1	D	20	LEU	2.1
1	D	10	GLN	2.1
1	C	71	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	74	VAL	2.1
1	D	90	ARG	2.1
1	C	300	ILE	2.1
1	F	345	GLN	2.1
1	E	461	HIS	2.0
1	E	304	ILE	2.0
1	C	386	ALA	2.0
1	C	34	TRP	2.0
1	C	421	THR	2.0
1	E	449	THR	2.0
1	F	266	PHE	2.0
1	E	347	GLU	2.0
1	D	417	ALA	2.0
1	E	24	SER	2.0
1	A	134	ARG	2.0
1	C	153	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	502	1/1	0.79	0.25	88,88,88,88	0
2	FE2	F	1000	1/1	0.87	0.16	93,93,93,93	0
5	BCT	C	502	4/4	0.91	0.33	71,71,72,73	0
5	BCT	B	502	4/4	0.92	0.24	58,59,59,60	0
4	NA	A	503	1/1	0.93	0.09	70,70,70,70	0
2	FE2	E	1000	1/1	0.94	0.22	73,73,73,73	0
4	NA	B	503	1/1	0.95	0.14	80,80,80,80	0

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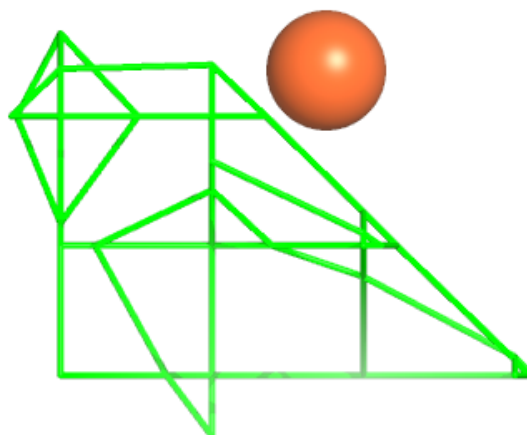
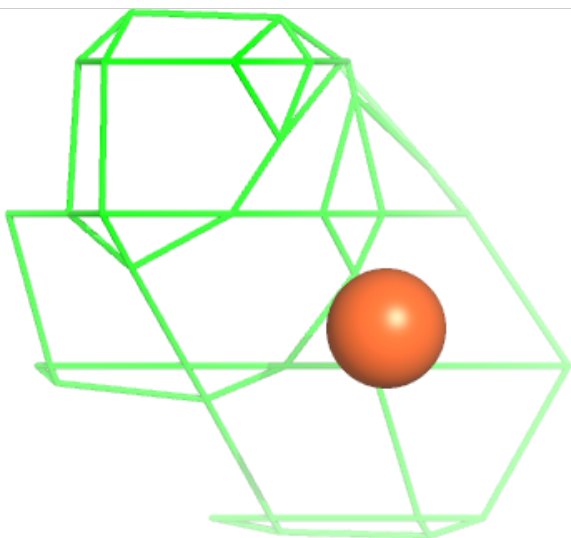
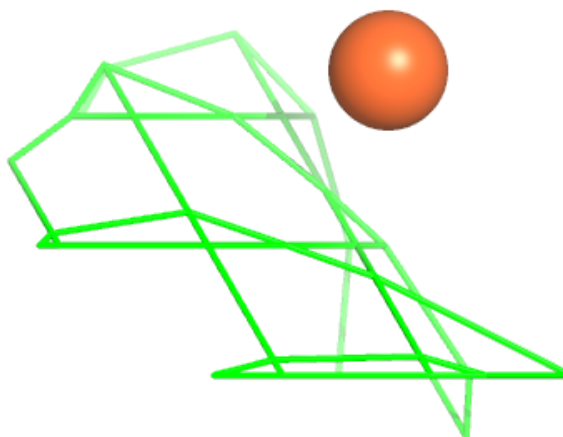
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	B	501	1/1	0.97	0.14	45,45,45,45	0
2	FE2	A	501	1/1	0.98	0.12	53,53,53,53	0
2	FE2	D	1000	1/1	0.98	0.18	61,61,61,61	0
2	FE2	C	501	1/1	0.99	0.16	54,54,54,54	0

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.

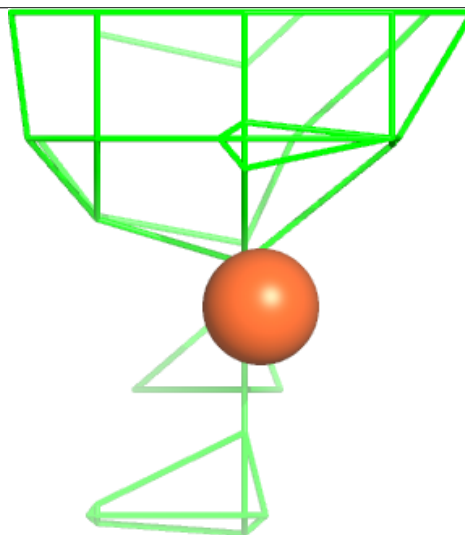
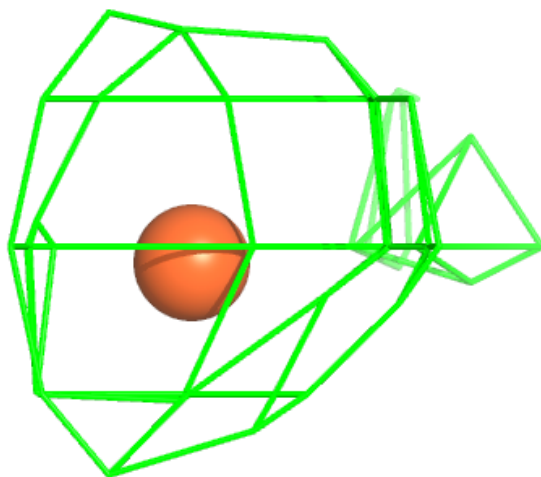
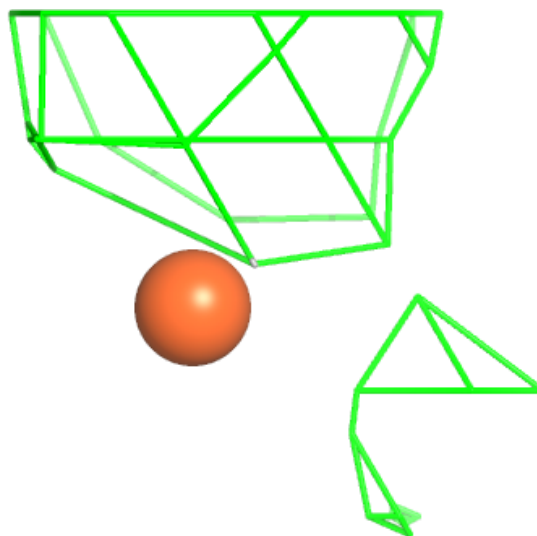
Electron density around FE2 F 1000:

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



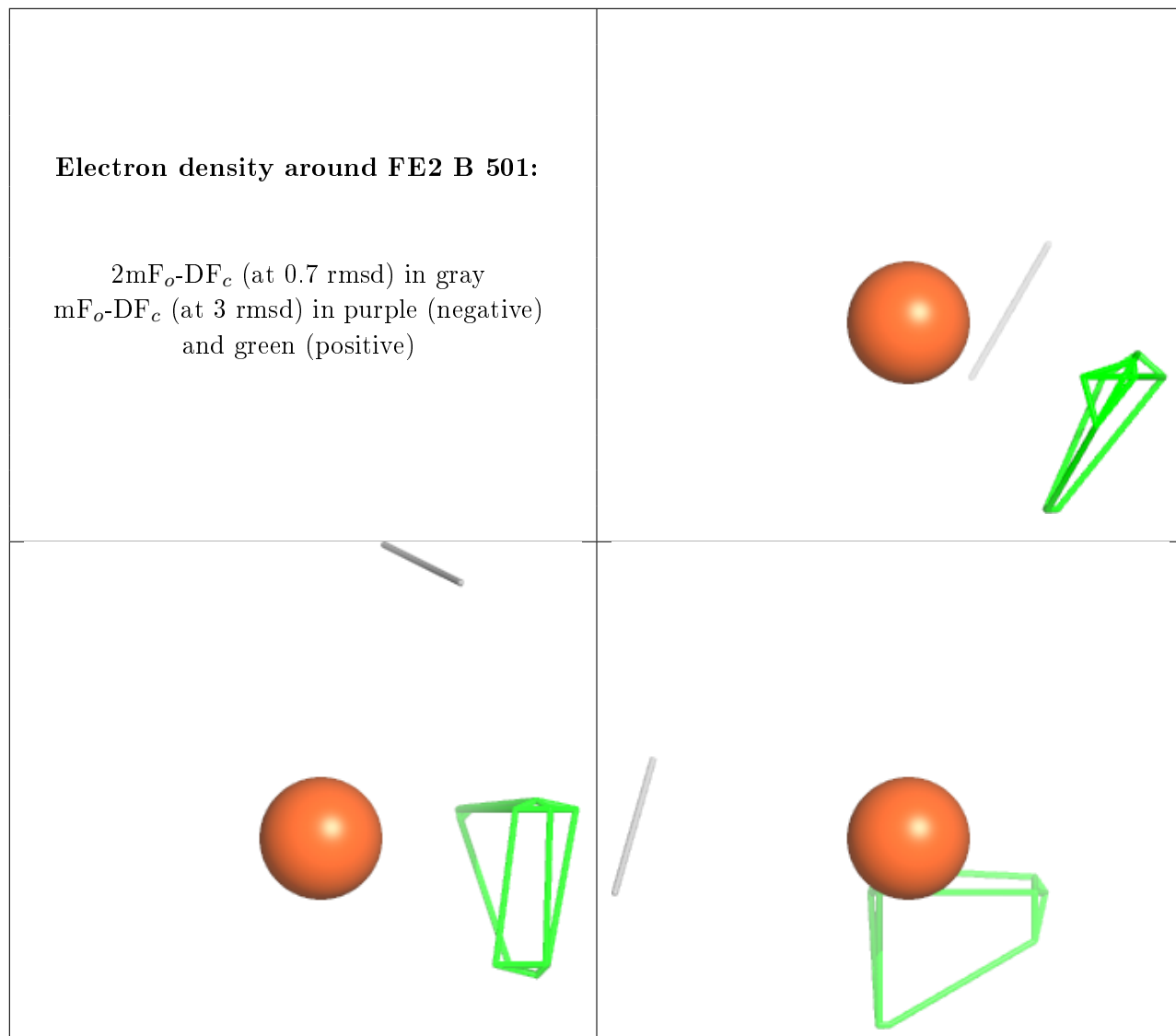
Electron density around FE2 E 1000:

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



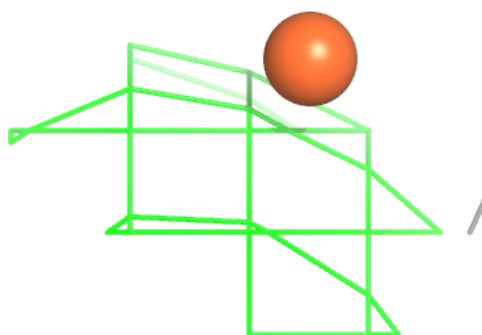
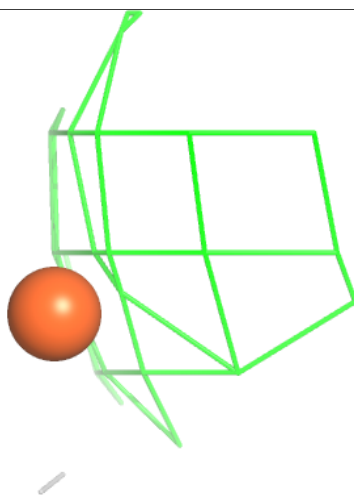
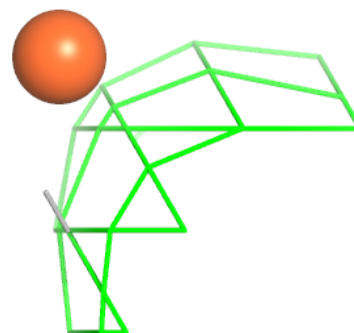
Electron density around FE2 B 501:

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



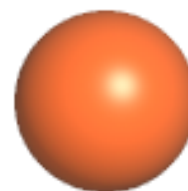
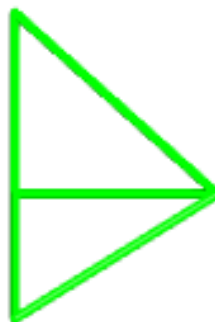
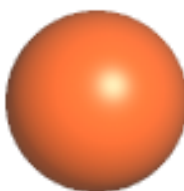
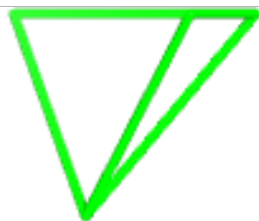
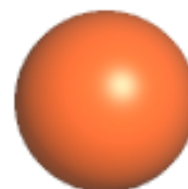
Electron density around FE2 A 501:

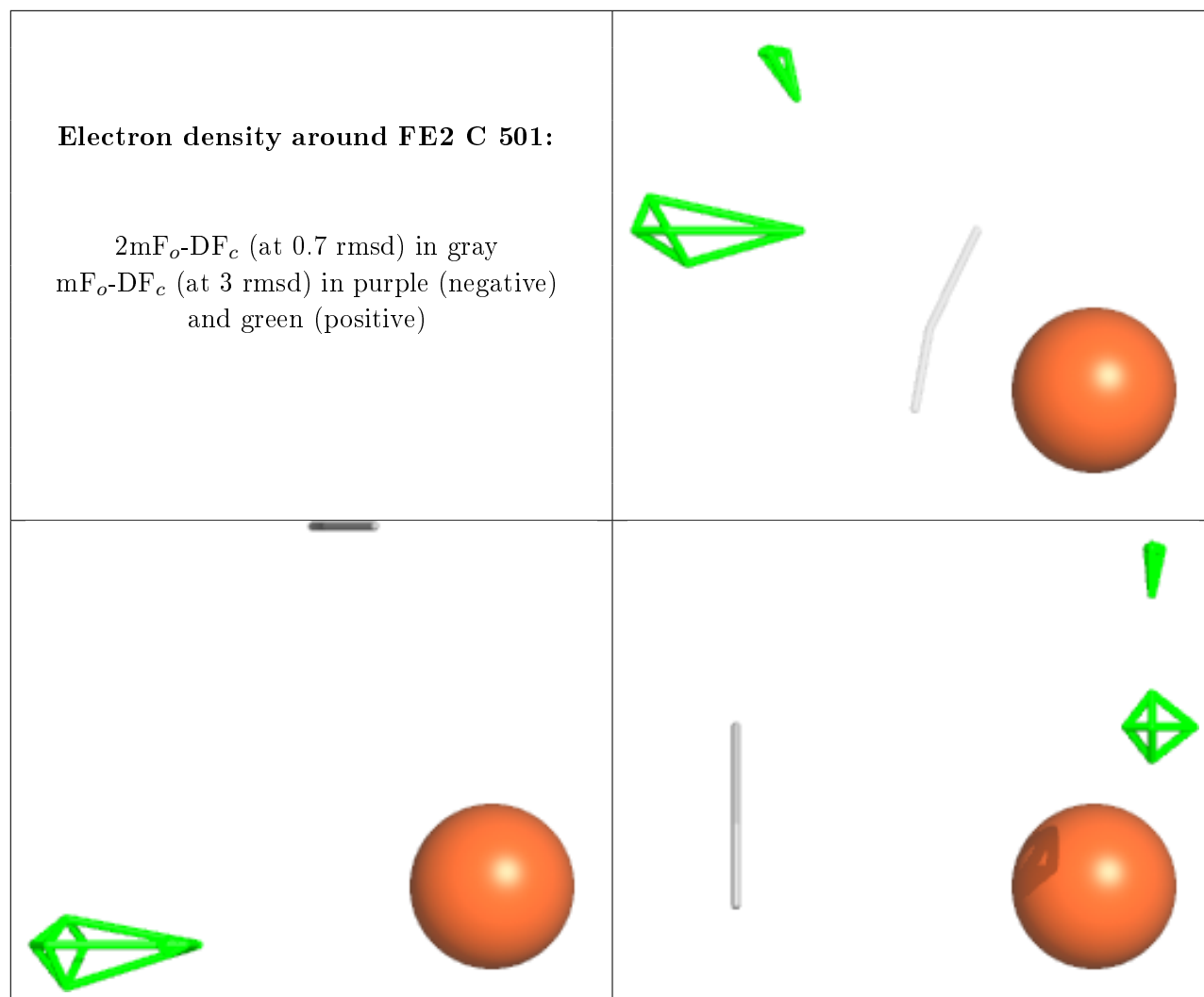
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE2 D 1000:

$2mF_o - DF_c$ (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.