



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 6VCF / pdb_00006vcf
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 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

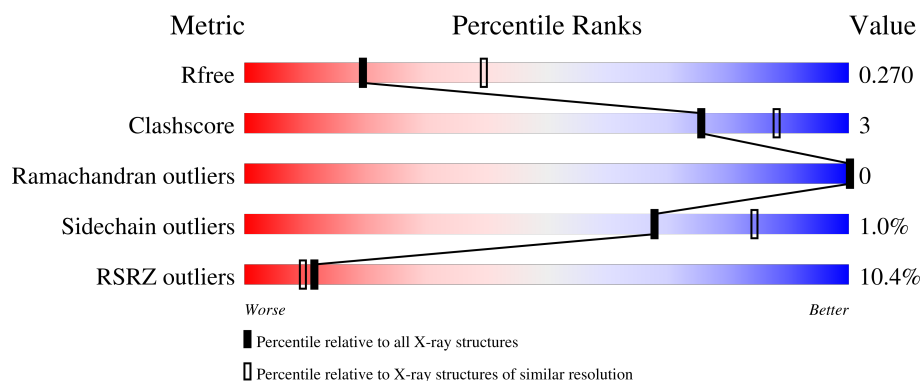
1 Overall quality at a glance

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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	472	3% 87% 9% .
1	B	472	% 88% 8% .
1	C	472	% 88% 8% .
1	D	472	4% 87% 8% .
1	E	472	23% 84% 7% 8%

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Mol	Chain	Length	Quality of chain
1	F	472	26% 84% 7% 8%

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 (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		

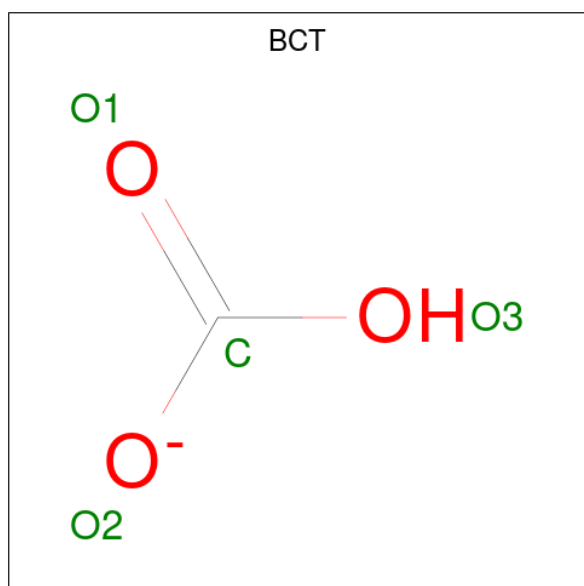
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is BICARBONATE ION (CCD ID: 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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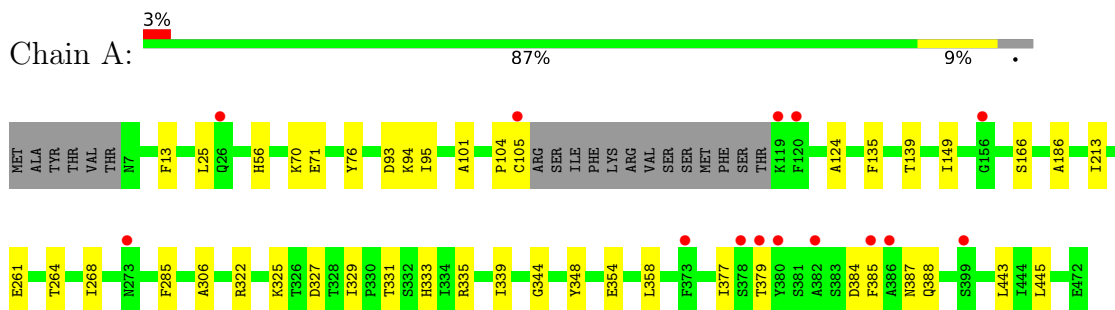
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	42	Total 42	O 42	0	0
6	D	45	Total 45	O 45	0	0
6	E	12	Total 12	O 12	0	0
6	F	9	Total 9	O 9	0	0

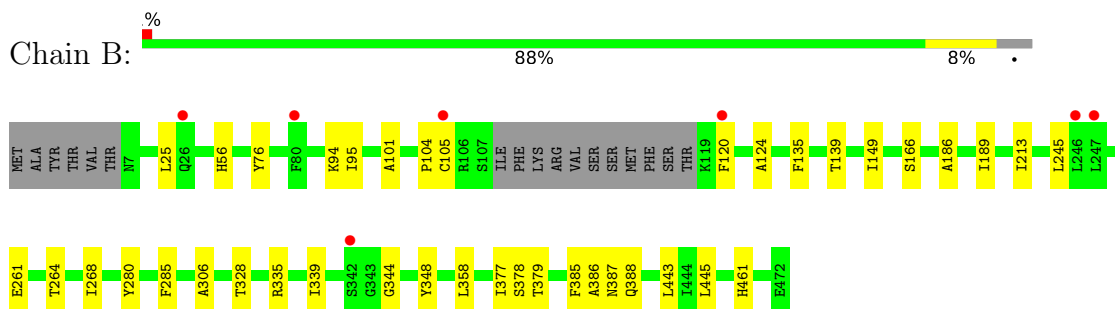
3 Residue-property plots [i](#)

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.

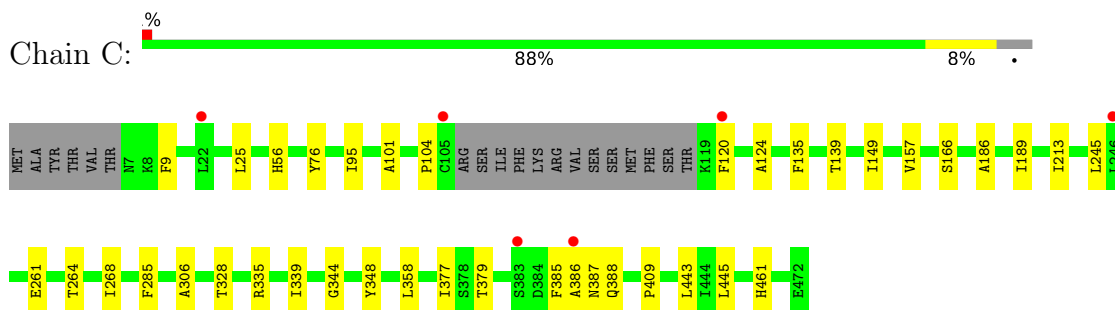
- Molecule 1: carotenoid cleavage dioxygenase



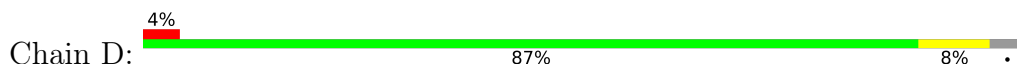
- Molecule 1: carotenoid cleavage dioxygenase

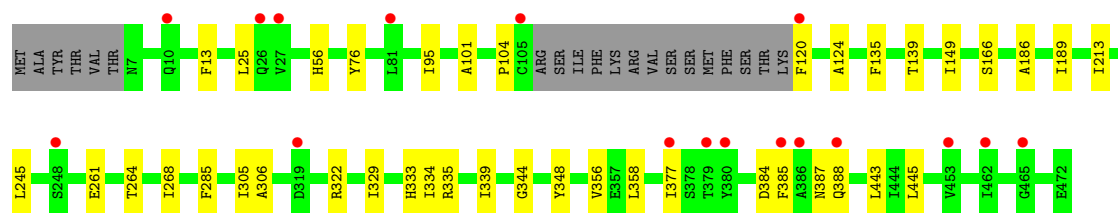


- Molecule 1: carotenoid cleavage dioxygenase

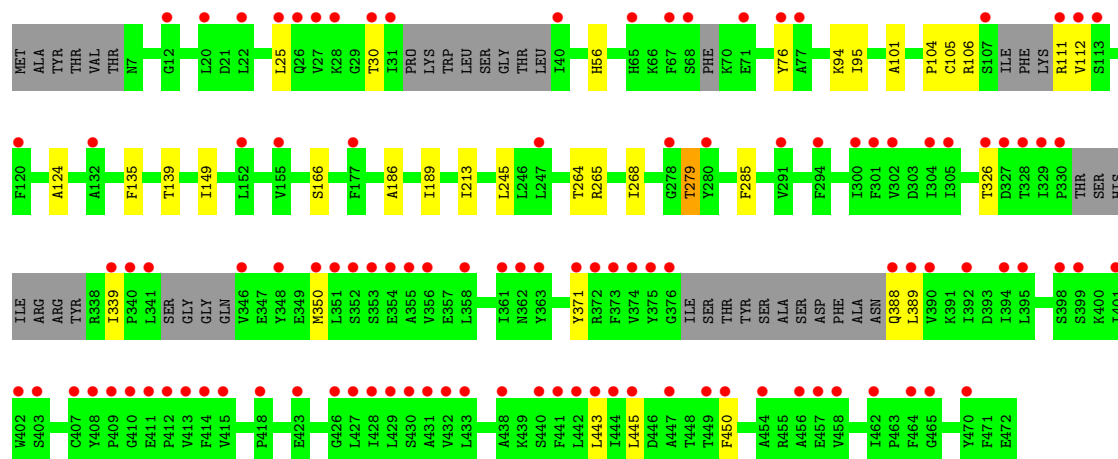
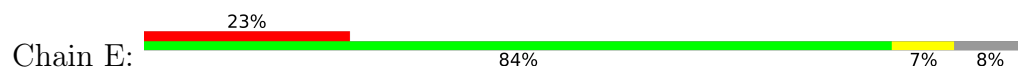


- Molecule 1: carotenoid cleavage dioxygenase

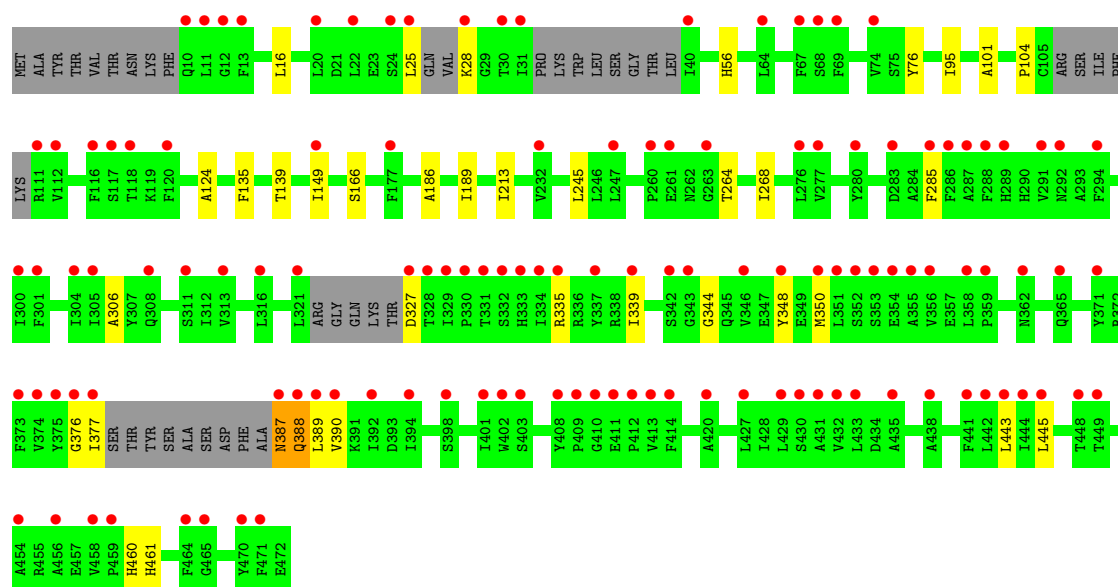
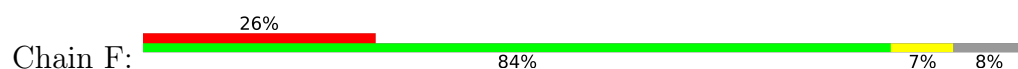




● Molecule 1: carotenoid cleavage dioxygenase



● 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) 99.7 (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)	0.33 , 69.5	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	0.93	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, CL, FE2, NA

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	1.01	0/3729	1.30	1/5061 (0.0%)
1	B	1.00	0/3748	1.29	1/5080 (0.0%)
1	C	1.01	0/3723	1.29	1/5050 (0.0%)
1	D	1.01	0/3710	1.29	1/5034 (0.0%)
1	E	1.01	0/3502	1.28	0/4747
1	F	1.02	0/3518	1.29	1/4771 (0.0%)
All	All	1.01	0/21930	1.29	5/29743 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	GLY	CA-C-O	-5.75	118.26	122.23
1	A	344	GLY	CA-C-O	-5.69	118.31	122.23
1	D	344	GLY	CA-C-O	-5.67	118.32	122.23
1	B	344	GLY	CA-C-O	-5.67	118.32	122.23
1	F	344	GLY	CA-C-O	-5.63	118.34	122.23

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
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:OE1	1:A:354[B]:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:95:ILE:O	1:B:104:PRO:HB3	2.09	0.52
1:B:213:ILE:HD12	1:B:213:ILE:N	2.25	0.52
1:E:105:CYS:SG	1:E:106:ARG:N	2.82	0.52
1:C:213:ILE:N	1:C:213:ILE:HD12	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:HD12	1:D:213:ILE:N	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:A:93:ASP:CG	1:E:30:THR:HB	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:94:LYS:NZ	1:A:105:CYS:SG	2.83	0.48
1:F:95:ILE:O	1:F:104:PRO:HB3	2.13	0.48
1:D:166:SER:CB	1:D:186:ALA:HB1	2.43	0.47
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:A:70:LYS:C	1:A:71:GLU:HG2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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	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%)	81	91
1	B	397/417 (95%)	392 (99%)	5 (1%)	61	81
1	C	392/417 (94%)	387 (99%)	5 (1%)	61	81
1	D	390/417 (94%)	387 (99%)	3 (1%)	73	87
1	E	365/417 (88%)	362 (99%)	3 (1%)	73	87
1	F	363/417 (87%)	359 (99%)	4 (1%)	65	83
All	All	2299/2502 (92%)	2277 (99%)	22 (1%)	68	84

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
1	A	388	GLN
1	B	120	PHE
1	B	261	GLU
1	B	385	PHE
1	B	388	GLN
1	B	461	HIS
1	C	120	PHE
1	C	157	VAL
1	C	261	GLU
1	C	388	GLN
1	C	461	HIS
1	D	120	PHE
1	D	261	GLU
1	D	388	GLN
1	E	279	THR
1	E	371	TYR
1	E	388	GLN
1	F	28	LYS
1	F	387	ASN
1	F	388	GLN
1	F	461	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	180	ASN
1	A	208	ASN
1	A	461	HIS
1	C	208	ASN
1	C	367	ASN
1	D	10	GLN
1	D	208	ASN
1	D	461	HIS
1	E	208	ASN
1	E	367	ASN
1	E	461	HIS
1	F	180	ASN
1	F	208	ASN
1	F	367	ASN

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Mol	Chain	Res	Type
1	F	460	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	502	2	3,3,3	0.98	0	2,3,3	1.66	1 (50%)
5	BCT	C	502	2	3,3,3	1.04	0	2,3,3	1.58	1 (50%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	BCT	O2-C-O1	2.18	125.25	119.68
5	C	502	BCT	O2-C-O1	2.05	124.93	119.68

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%)	0.30	14 (3%)	51	47	32, 74, 105, 127	1 (0%)
1	B	455/472 (96%)	0.17	7 (1%)	72	69	38, 70, 107, 126	0
1	C	453/472 (95%)	0.24	6 (1%)	75	73	47, 79, 115, 138	0
1	D	452/472 (95%)	0.44	17 (3%)	44	39	47, 87, 133, 168	0
1	E	432/472 (91%)	1.31	110 (25%)	1	1	49, 101, 203, 246	0
1	F	434/472 (91%)	1.45	124 (28%)	1	1	61, 114, 215, 244	0
All	All	2679/2832 (94%)	0.64	278 (10%)	11	10	32, 84, 175, 246	1 (0%)

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	376	GLY	6.6
1	F	374	VAL	6.1
1	E	374	VAL	5.8
1	F	351	LEU	5.7
1	F	376	GLY	5.3
1	F	355	ALA	5.1
1	F	356	VAL	5.1
1	E	355	ALA	5.1
1	F	328	THR	5.0
1	E	31	ILE	4.9
1	E	431	ALA	4.8
1	E	375	TYR	4.8
1	E	327	ASP	4.8
1	E	392	ILE	4.7
1	E	351	LEU	4.7
1	F	377	ILE	4.6
1	E	362	ASN	4.5
1	E	429	LEU	4.4
1	F	389	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	392	ILE	4.4
1	F	350	MET	4.3
1	F	358	LEU	4.3
1	F	388	GLN	4.3
1	F	354	GLU	4.3
1	E	68	SER	4.3
1	E	388	GLN	4.3
1	E	76	TYR	4.3
1	E	427	LEU	4.2
1	F	291	VAL	4.2
1	F	375	TYR	4.2
1	F	304	ILE	4.1
1	F	327	ASP	4.0
1	E	389	LEU	4.0
1	F	431	ALA	4.0
1	F	413	VAL	4.0
1	F	334	ILE	4.0
1	F	67	PHE	4.0
1	E	413	VAL	4.0
1	E	442	LEU	4.0
1	E	301	PHE	3.9
1	E	409	PRO	3.9
1	F	394	ILE	3.9
1	F	353	SER	3.9
1	F	429	LEU	3.9
1	E	410	GLY	3.9
1	C	120	PHE	3.8
1	F	348	TYR	3.8
1	F	333	HIS	3.8
1	E	356	VAL	3.8
1	E	353	SER	3.7
1	E	432	VAL	3.7
1	F	387	ASN	3.7
1	E	390	VAL	3.6
1	F	13	PHE	3.6
1	F	69	PHE	3.6
1	F	409	PRO	3.6
1	F	329	ILE	3.6
1	E	26	GLN	3.5
1	F	410	GLY	3.5
1	D	385	PHE	3.5
1	E	25	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	341	LEU	3.5
1	F	313	VAL	3.5
1	F	390	VAL	3.5
1	D	386	ALA	3.4
1	E	346	VAL	3.4
1	E	27	VAL	3.4
1	F	74	VAL	3.4
1	E	407	CYS	3.4
1	E	373	PHE	3.4
1	F	112	VAL	3.4
1	F	464	PHE	3.4
1	F	427	LEU	3.3
1	F	435	ALA	3.3
1	F	294	PHE	3.3
1	F	31	ILE	3.3
1	E	470	TYR	3.3
1	F	401	ILE	3.3
1	F	20	LEU	3.3
1	F	330	PRO	3.3
1	A	385	PHE	3.3
1	E	112	VAL	3.3
1	F	277	VAL	3.3
1	E	430	SER	3.2
1	E	408	TYR	3.2
1	E	401	ILE	3.2
1	E	444	ILE	3.2
1	F	359	PRO	3.2
1	E	440	SER	3.2
1	F	12	GLY	3.2
1	F	408	TYR	3.2
1	F	68	SER	3.2
1	F	352	SER	3.2
1	D	120	PHE	3.2
1	F	25	LEU	3.1
1	E	330	PRO	3.1
1	E	441	PHE	3.1
1	E	428	ILE	3.1
1	E	291	VAL	3.1
1	E	354	GLU	3.1
1	E	329	ILE	3.1
1	E	394	ILE	3.1
1	F	111	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	40	ILE	3.1
1	E	447	ALA	3.1
1	E	294	PHE	3.1
1	E	348	TYR	3.0
1	F	411	GLU	3.0
1	A	379	THR	3.0
1	E	326	THR	3.0
1	E	120	PHE	3.0
1	F	373	PHE	3.0
1	F	441	PHE	3.0
1	D	379	THR	3.0
1	B	120	PHE	3.0
1	E	411	GLU	3.0
1	E	462	ILE	2.9
1	F	331	THR	2.9
1	E	67	PHE	2.9
1	F	412	PRO	2.9
1	D	105	CYS	2.9
1	F	371	TYR	2.9
1	E	300	ILE	2.9
1	D	465	GLY	2.9
1	D	380	TYR	2.9
1	F	445	LEU	2.9
1	A	382	ALA	2.9
1	E	22	LEU	2.9
1	F	443	LEU	2.9
1	E	450	PHE	2.9
1	F	301	PHE	2.9
1	F	300	ILE	2.8
1	F	339	ILE	2.8
1	E	20	LEU	2.8
1	E	458	VAL	2.8
1	E	371	TYR	2.8
1	D	462	ILE	2.8
1	F	120	PHE	2.8
1	F	286	PHE	2.8
1	F	470	TYR	2.8
1	E	113	SER	2.8
1	B	247	LEU	2.8
1	F	432	VAL	2.7
1	F	308	GLN	2.7
1	F	22	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	414	PHE	2.7
1	E	339	ILE	2.7
1	E	403	SER	2.7
1	E	438	ALA	2.7
1	E	361	ILE	2.7
1	F	465	GLY	2.7
1	F	337	TYR	2.6
1	D	81	LEU	2.6
1	E	457	GLU	2.6
1	A	120	PHE	2.6
1	E	445	LEU	2.6
1	E	465	GLY	2.6
1	A	386	ALA	2.6
1	A	380	TYR	2.6
1	E	278	GLY	2.6
1	E	340	PRO	2.6
1	E	456	ALA	2.6
1	F	362	ASN	2.6
1	D	319	ASP	2.6
1	F	283	ASP	2.6
1	E	454	ALA	2.6
1	F	287	ALA	2.6
1	B	26	GLN	2.6
1	F	321	LEU	2.5
1	F	398	SER	2.5
1	E	65	HIS	2.5
1	E	412	PRO	2.5
1	E	132	ALA	2.5
1	F	118	THR	2.5
1	E	402	TRP	2.5
1	F	335	ARG	2.5
1	E	30	THR	2.5
1	F	343	GLY	2.5
1	D	388	GLN	2.5
1	F	64	LEU	2.4
1	E	352	SER	2.4
1	E	414	PHE	2.4
1	F	24	SER	2.4
1	F	332	SER	2.4
1	F	403	SER	2.4
1	F	280	TYR	2.4
1	F	433	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	289	HIS	2.4
1	F	430	SER	2.4
1	D	26	GLN	2.4
1	E	155	VAL	2.4
1	E	415	VAL	2.4
1	F	454	ALA	2.4
1	F	11	LEU	2.4
1	B	342	SER	2.4
1	F	342	SER	2.4
1	A	105	CYS	2.4
1	E	358	LEU	2.3
1	F	444	ILE	2.3
1	C	383	SER	2.3
1	F	402	TRP	2.3
1	C	105	CYS	2.3
1	F	346	VAL	2.3
1	F	458	VAL	2.3
1	E	328	THR	2.3
1	E	423	GLU	2.3
1	B	105	CYS	2.3
1	F	247	LEU	2.3
1	F	288	PHE	2.3
1	F	442	LEU	2.3
1	F	456	ALA	2.3
1	E	111	ARG	2.3
1	E	12	GLY	2.3
1	C	246	LEU	2.3
1	E	247	LEU	2.3
1	E	443	LEU	2.3
1	E	77	ALA	2.3
1	F	449	THR	2.3
1	A	378	SER	2.3
1	E	426	GLY	2.3
1	E	398	SER	2.2
1	F	305	ILE	2.2
1	F	438	ALA	2.2
1	F	292	ASN	2.2
1	F	260	PRO	2.2
1	A	399	SER	2.2
1	E	433	LEU	2.2
1	F	232	VAL	2.2
1	F	30	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	280	TYR	2.2
1	A	26	GLN	2.2
1	A	119	LYS	2.2
1	C	22	LEU	2.2
1	D	248	SER	2.2
1	F	117	SER	2.2
1	D	377	ILE	2.2
1	C	386	ALA	2.2
1	F	261	GLU	2.1
1	E	418	PRO	2.1
1	E	28	LYS	2.1
1	F	365	GLN	2.1
1	F	316	LEU	2.1
1	F	149	ILE	2.1
1	A	373	PHE	2.1
1	F	116	PHE	2.1
1	E	449	THR	2.1
1	A	156	GLY	2.1
1	B	80	PHE	2.1
1	E	107	SER	2.1
1	E	399	SER	2.1
1	F	471	PHE	2.1
1	F	420	ALA	2.1
1	F	276	LEU	2.1
1	E	305	ILE	2.1
1	F	40	ILE	2.1
1	E	464	PHE	2.1
1	E	372	ARG	2.1
1	F	263	GLY	2.1
1	E	304	ILE	2.1
1	E	177	PHE	2.1
1	F	285	PHE	2.1
1	E	71	GLU	2.0
1	F	311	SER	2.0
1	F	448	THR	2.0
1	E	350	MET	2.0
1	F	459	PRO	2.0
1	E	152	LEU	2.0
1	D	453	VAL	2.0
1	E	363	TYR	2.0
1	F	177	PHE	2.0
1	F	28	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	246	LEU	2.0
1	D	10	GLN	2.0
1	E	395	LEU	2.0
1	F	10	GLN	2.0
1	A	273	ASN	2.0
1	D	27	VAL	2.0
1	E	302	VAL	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](#)

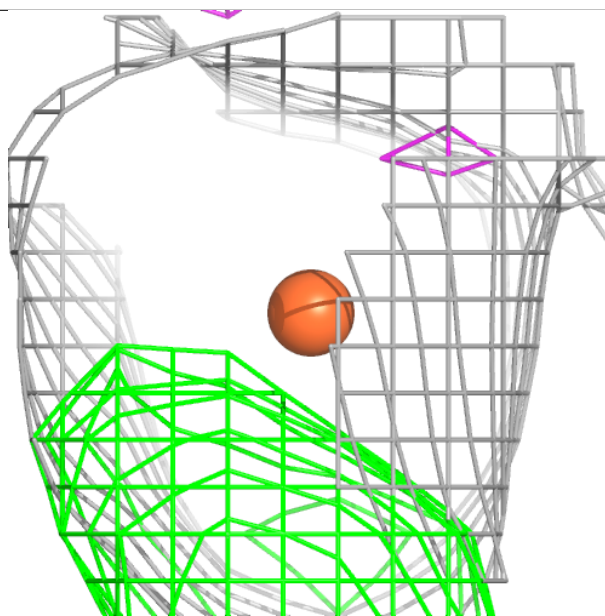
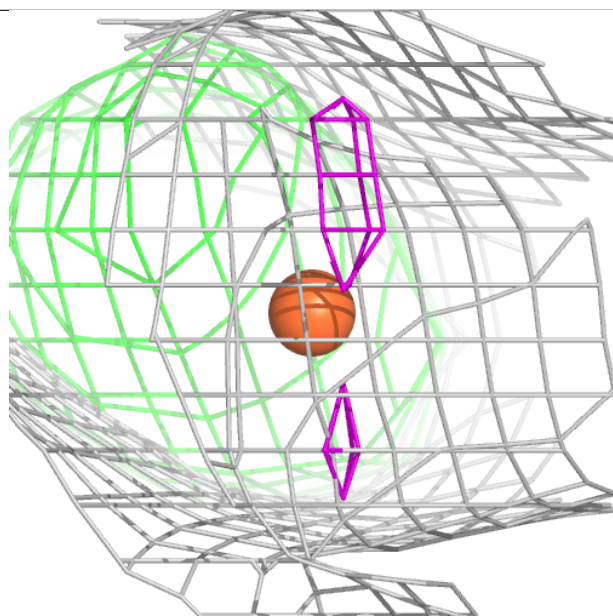
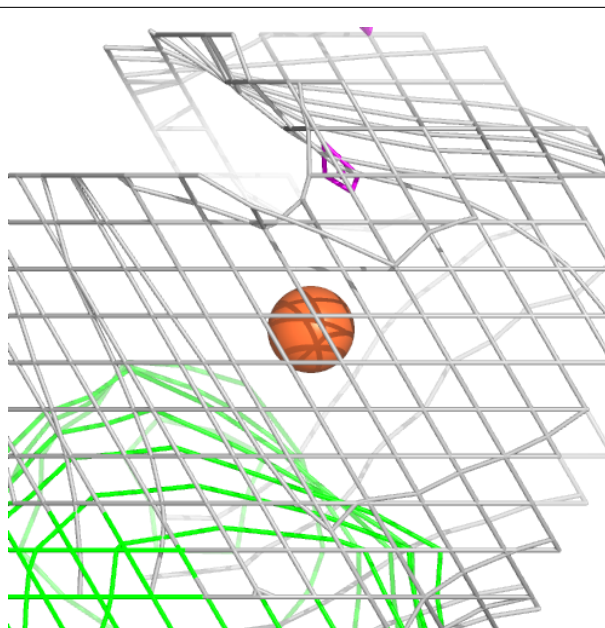
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE2	F	1000	1/1	0.85	0.09	93,93,93,93	0
4	NA	B	503	1/1	0.89	0.10	80,80,80,80	0
3	CL	A	502	1/1	0.91	0.09	88,88,88,88	0
5	BCT	C	502	4/4	0.91	0.14	71,71,72,73	0
2	FE2	A	501	1/1	0.93	0.05	53,53,53,53	0
4	NA	A	503	1/1	0.93	0.11	70,70,70,70	0
5	BCT	B	502	4/4	0.94	0.10	58,59,59,60	0
2	FE2	E	1000	1/1	0.95	0.05	73,73,73,73	0
2	FE2	C	501	1/1	0.99	0.02	54,54,54,54	0
2	FE2	D	1000	1/1	0.99	0.02	61,61,61,61	0
2	FE2	B	501	1/1	0.99	0.03	45,45,45,45	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.

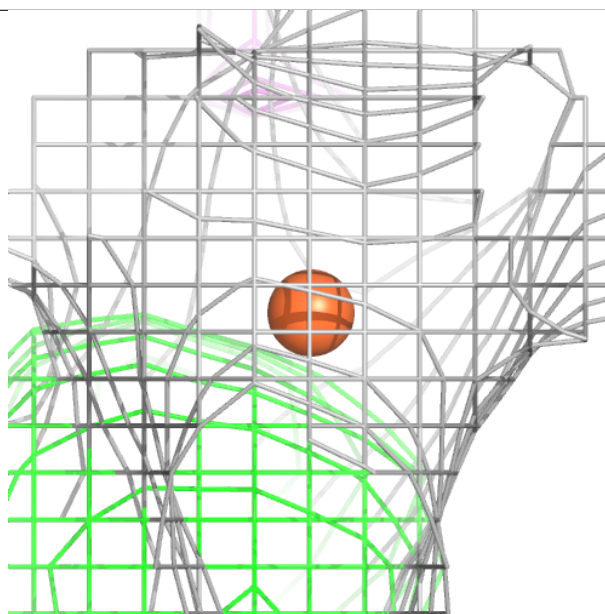
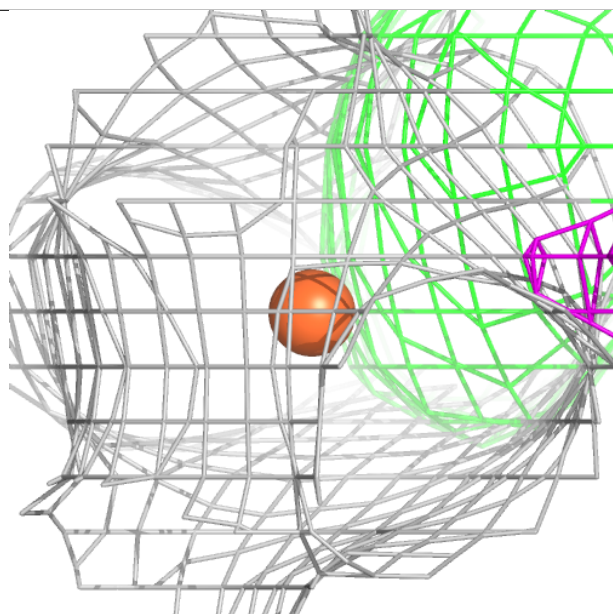
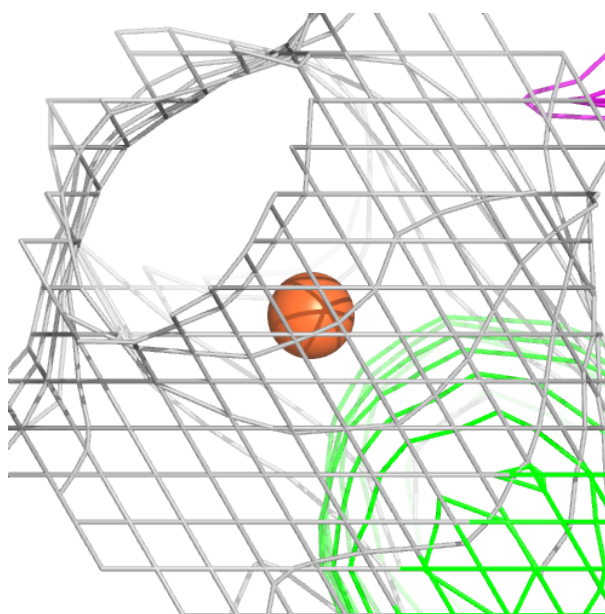
Electron density around FE2 F 1000:

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



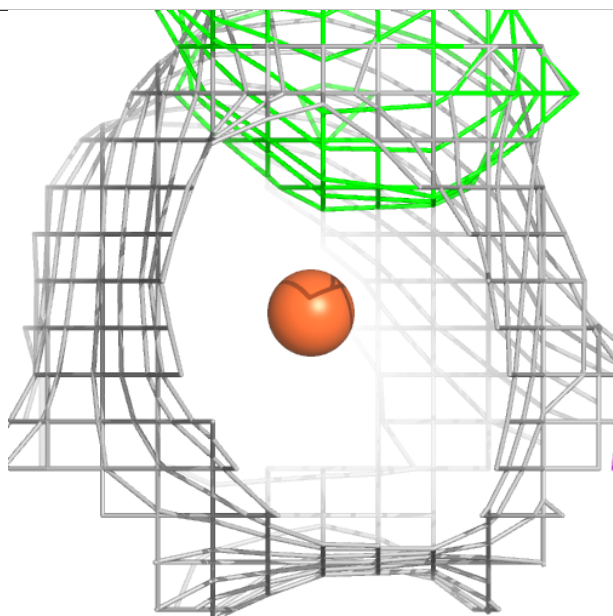
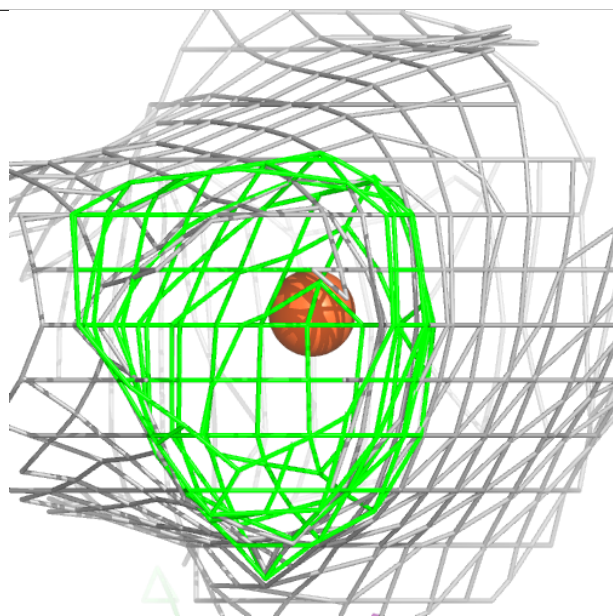
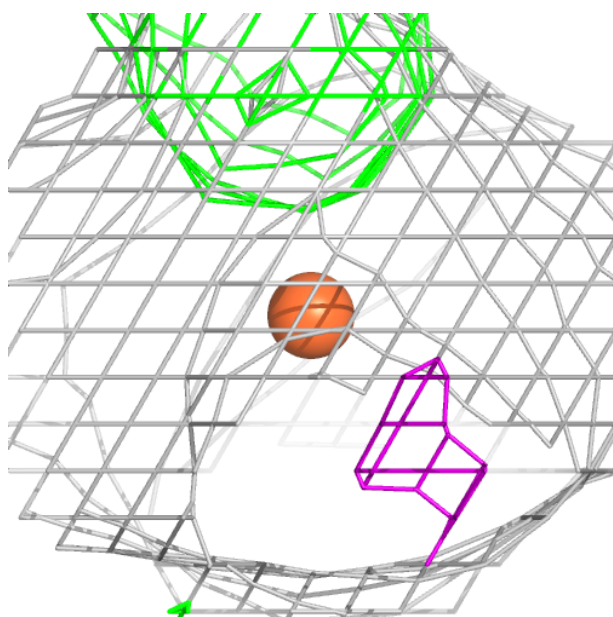
Electron density around FE2 A 501:

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



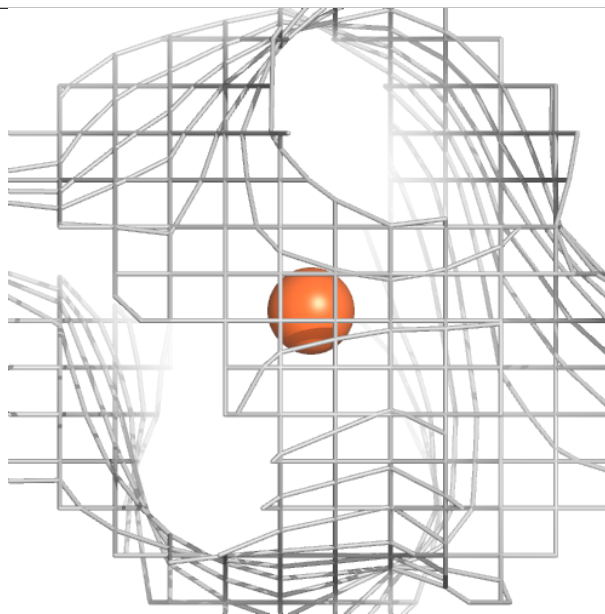
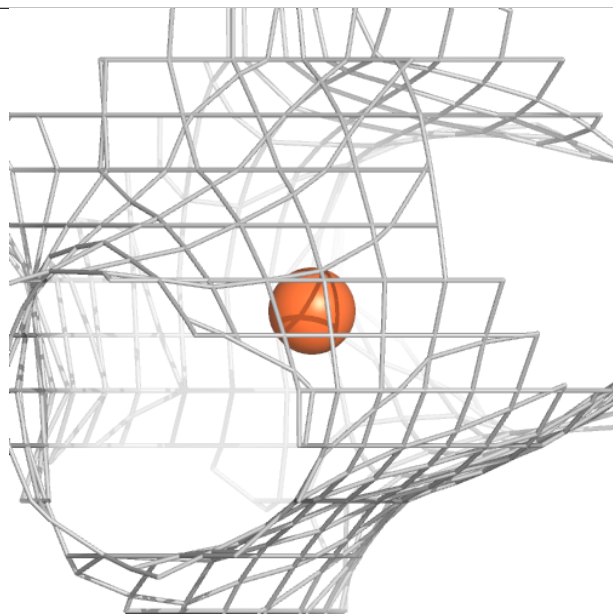
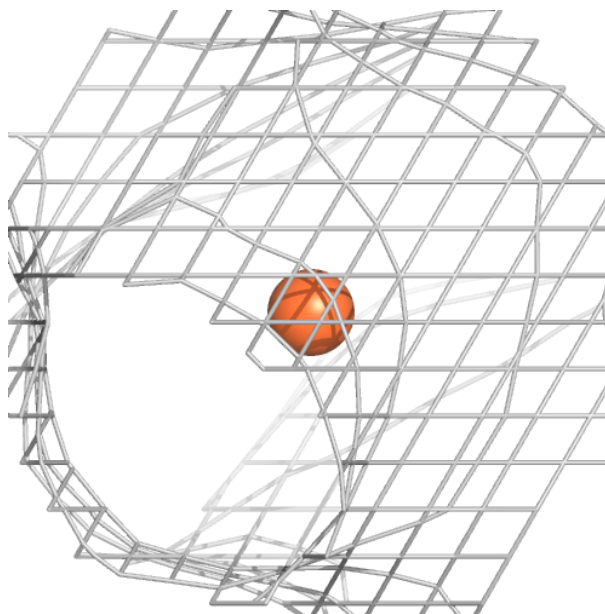
Electron density around FE2 E 1000:

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



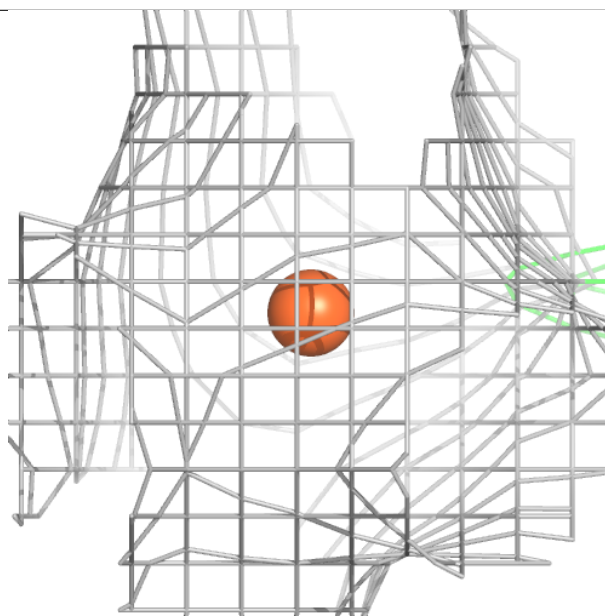
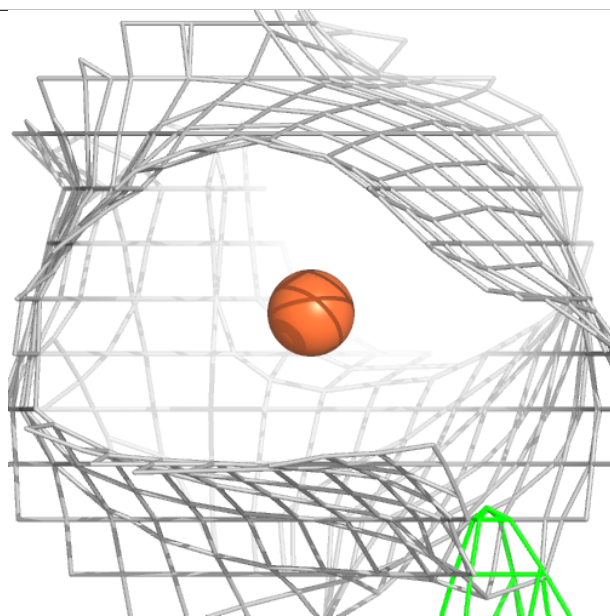
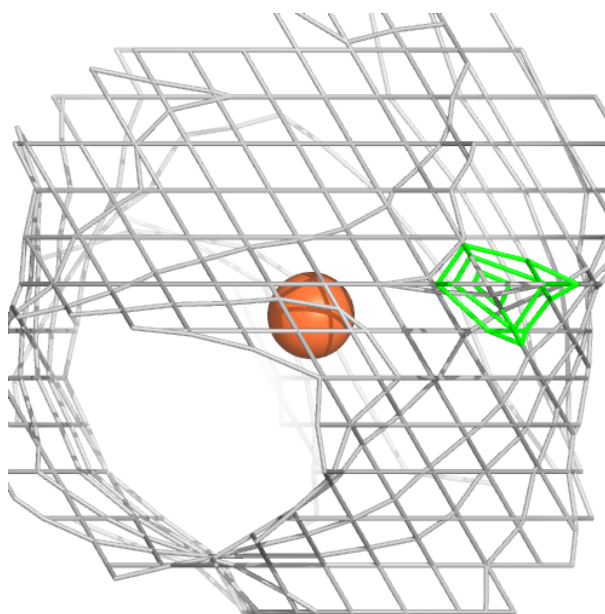
Electron density around FE2 C 501:

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



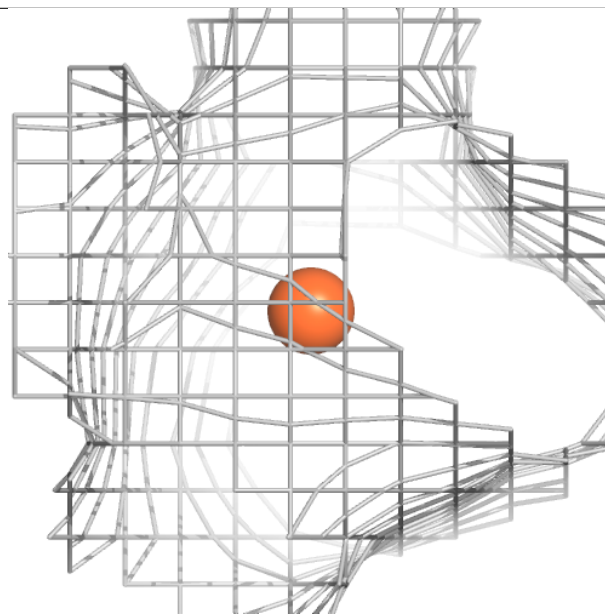
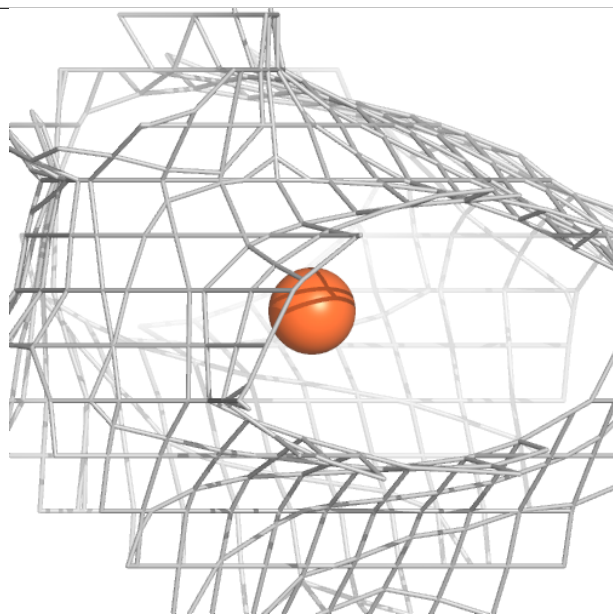
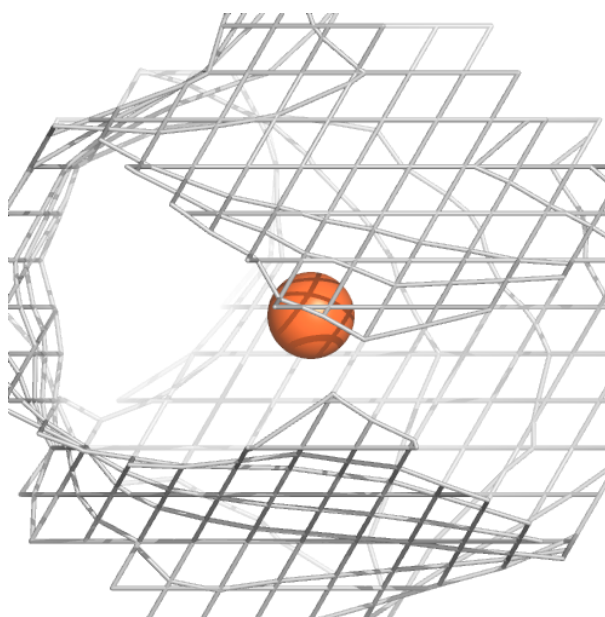
Electron density around FE2 D 1000:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.