



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:24 PM UTC

PDB ID : 6VCG / pdb_00006vcg
Title : Crystal structure of Nitrosotalea devanaterrea carotenoid cleavage dioxygenase, cobalt form
Authors : Daruwalla, A.; Shi, W.; Kiser, P.D.
Deposited on : 2019-12-20
Resolution : 2.30 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:

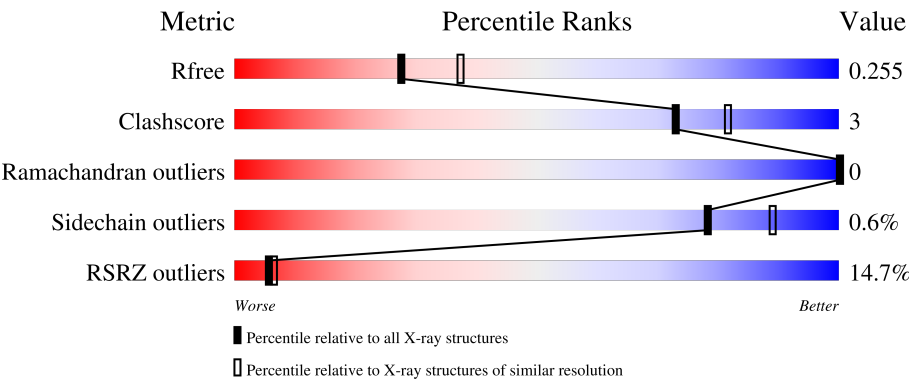
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	8% 88%8% .
1	B	472	2% 88%7% .
1	C	472	6% 89%7% .
1	D	472	5% 88%8% .
1	E	472	38% 79%10%10% .

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Mol	Chain	Length	Quality of chain
1	F	472	24% 83% 7% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21658 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	2	0
			3624	2335	589	693	7			
1	B	453	Total	C	N	O	S	0	2	0
			3643	2351	595	690	7			
1	C	453	Total	C	N	O	S	0	1	0
			3604	2326	588	683	7			
1	D	453	Total	C	N	O	S	0	0	0
			3597	2320	586	684	7			
1	E	423	Total	C	N	O	S	0	0	0
			3348	2161	541	639	7			
1	F	430	Total	C	N	O	S	0	0	0
			3372	2179	551	634	8			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

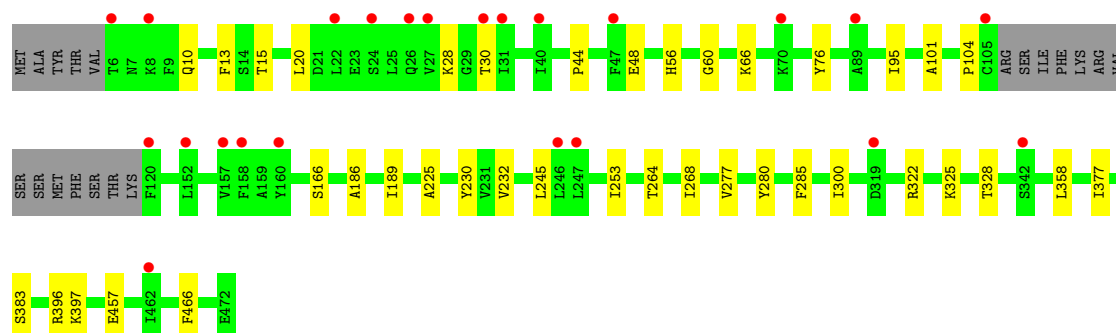
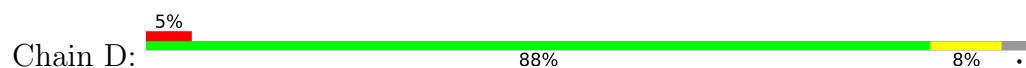
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	0	0
5	B	135	Total 135	O 135	0	0
5	C	89	Total 89	O 89	0	0
5	D	84	Total 84	O 84	0	0
5	E	21	Total 21	O 21	0	0
5	F	21	Total 21	O 21	0	0

- Molecule 1: carotenoid cleavage dioxygenase

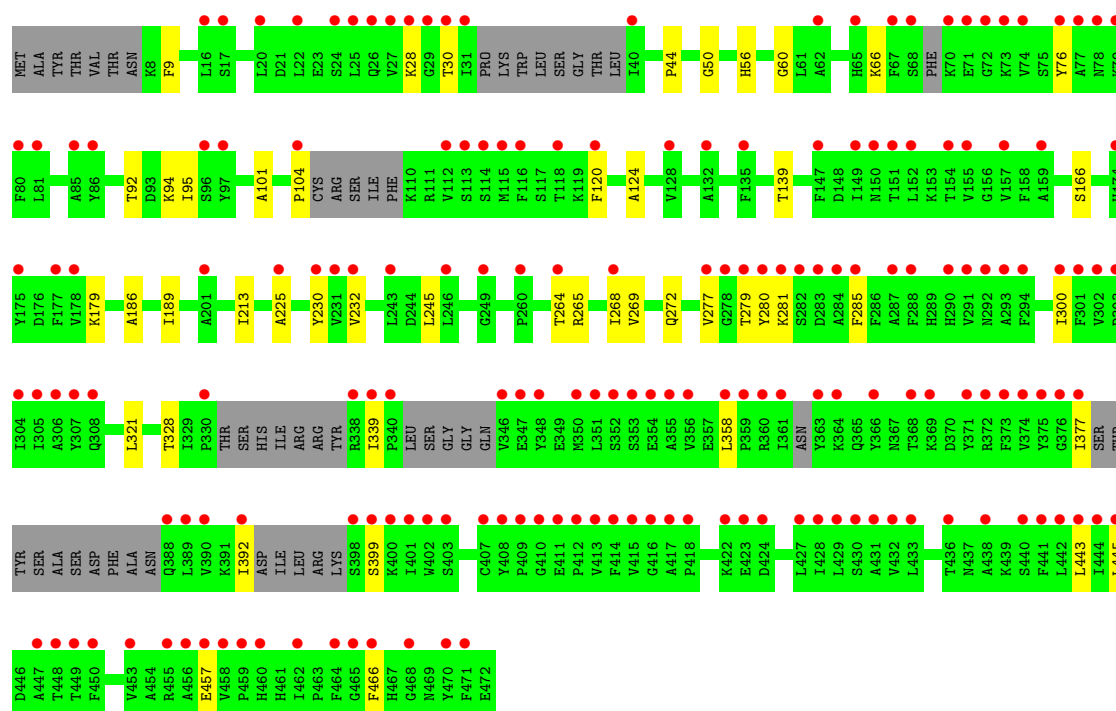
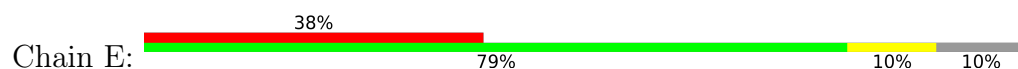




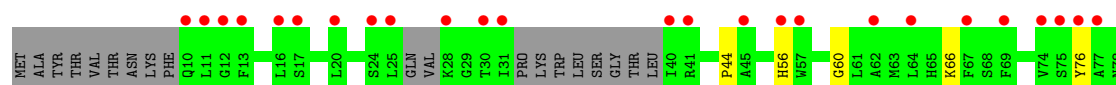
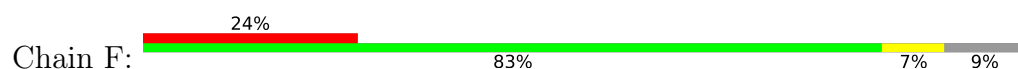
- Molecule 1: carotenoid cleavage dioxygenase

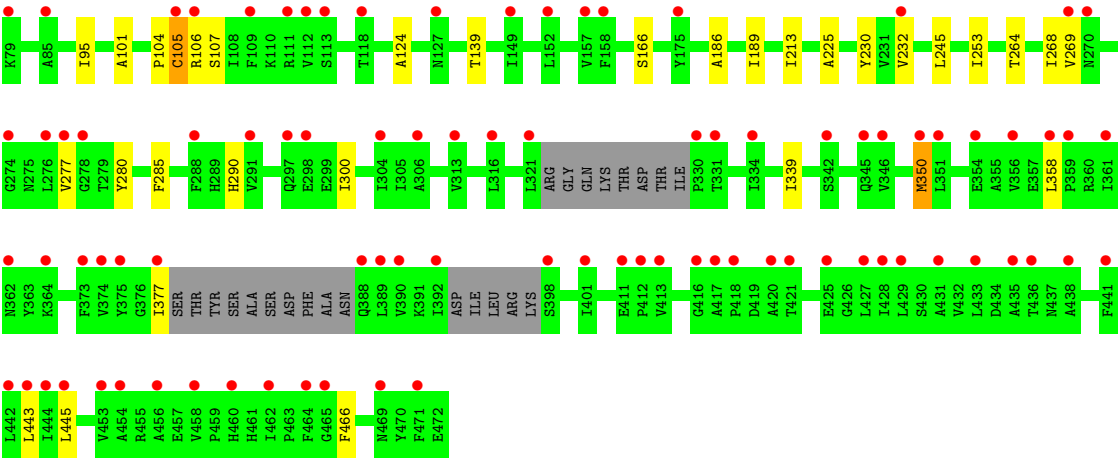


- Molecule 1: carotenoid cleavage dioxygenase



- 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	108.01Å 108.01Å 491.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.44 – 2.30 49.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.44-2.30) 99.8 (49.44-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.254 0.241 , 0.255	Depositor DCC
R_{free} test set	7076 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21658	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: NA, CO, 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	1.00	0/3717	1.28	4/5049 (0.1%)
1	B	1.01	1/3736 (0.0%)	1.28	3/5066 (0.1%)
1	C	1.01	1/3697 (0.0%)	1.27	2/5021 (0.0%)
1	D	1.02	0/3690	1.28	2/5015 (0.0%)
1	E	1.01	0/3426	1.28	1/4644 (0.0%)
1	F	1.02	0/3456	1.28	1/4691 (0.0%)
All	All	1.01	2/21722 (0.0%)	1.28	13/29486 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	329	ILE	N-CA	5.24	1.50	1.46
1	B	329	ILE	N-CA	5.16	1.50	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	105	CYS	CB-CA-C	-7.78	107.60	116.54
1	D	30	THR	CA-C-N	6.19	127.05	122.59
1	D	30	THR	C-N-CA	6.19	127.05	122.59
1	B	30	THR	CA-C-N	5.94	126.87	122.59
1	B	30	THR	C-N-CA	5.94	126.87	122.59
1	E	120	PHE	CA-C-O	-5.64	114.78	121.16
1	A	30	THR	CA-C-N	5.57	126.60	122.59
1	A	30	THR	C-N-CA	5.57	126.60	122.59
1	C	30	THR	CA-C-N	5.50	126.55	122.59
1	C	30	THR	C-N-CA	5.50	126.55	122.59
1	A	221	MET	CA-C-N	5.37	128.01	120.28
1	A	221	MET	C-N-CA	5.37	128.01	120.28
1	B	344	GLY	CA-C-O	-5.01	118.27	122.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3461	24	0
1	B	3643	0	3526	19	0
1	C	3604	0	3448	21	0
1	D	3597	0	3433	21	0
1	E	3348	0	3183	30	0
1	F	3372	0	3181	23	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	B	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	110	0	0	2	0
5	B	135	0	0	2	0
5	C	89	0	0	4	0
5	D	84	0	0	0	0
5	E	21	0	0	0	0
5	F	21	0	0	1	0
All	All	21658	0	20232	134	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 (134) 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:D:358:LEU:HD12	1:D:377:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD12	1:A:377:ILE:HD12	1.73	0.71
1:E:358:LEU:HD12	1:E:377:ILE:HD12	1.72	0.70
1:B:166:SER:HB2	1:B:186:ALA:HB1	1.75	0.69
1:D:358:LEU:HD12	1:D:377:ILE:CD1	2.23	0.69
1:B:30:THR:OG1	1:E:50:GLY:HA2	1.93	0.69
1:F:358:LEU:HD12	1:F:377:ILE:HD12	1.74	0.68
1:E:358:LEU:HD12	1:E:377:ILE:CD1	2.24	0.67
1:A:358:LEU:HD12	1:A:377:ILE:CD1	2.24	0.67
1:E:166:SER:HB2	1:E:186:ALA:HB1	1.77	0.67
1:F:358:LEU:HD12	1:F:377:ILE:CD1	2.25	0.67
1:C:166:SER:HB2	1:C:186:ALA:HB1	1.77	0.66
1:A:166:SER:HB2	1:A:186:ALA:HB1	1.78	0.65
1:F:166:SER:HB2	1:F:186:ALA:HB1	1.79	0.65
1:F:105:CYS:SG	1:F:106:ARG:N	2.71	0.62
1:A:325:LYS:O	1:A:328:THR:HG22	2.00	0.62
1:D:166:SER:HB2	1:D:186:ALA:HB1	1.80	0.62
1:D:325:LYS:O	1:D:328:THR:HG22	2.00	0.61
1:B:166:SER:CB	1:B:186:ALA:HB1	2.30	0.61
1:C:213:ILE:HD11	1:C:269:VAL:HG21	1.83	0.61
1:D:13:PHE:O	1:D:322:ARG:NH1	2.33	0.61
1:A:13:PHE:O	1:A:322:ARG:NH1	2.35	0.60
1:B:28:LYS:NZ	1:B:457:GLU:OE2	2.27	0.60
1:C:166:SER:CB	1:C:186:ALA:HB1	2.33	0.58
1:D:166:SER:CB	1:D:186:ALA:HB1	2.33	0.58
1:A:28:LYS:NZ	1:A:457:GLU:OE2	2.30	0.58
1:A:166:SER:CB	1:A:186:ALA:HB1	2.35	0.56
1:E:166:SER:CB	1:E:186:ALA:HB1	2.36	0.55
1:E:213:ILE:HD11	1:E:269:VAL:HG21	1.88	0.55
1:A:95:ILE:O	1:A:104:PRO:HB3	2.06	0.55
1:E:28:LYS:NZ	1:E:457:GLU:OE2	2.33	0.54
1:B:95:ILE:O	1:B:104:PRO:HB3	2.08	0.53
1:E:189:ILE:HG21	1:E:245:LEU:HD23	1.91	0.53
1:F:189:ILE:HG21	1:F:245:LEU:HD23	1.90	0.53
1:E:92:THR:O	1:E:94:LYS:HG2	2.09	0.53
1:E:265:ARG:HD2	1:E:279:THR:OG1	2.09	0.53
1:F:166:SER:CB	1:F:186:ALA:HB1	2.38	0.53
1:B:213:ILE:HD11	1:B:269:VAL:HG21	1.91	0.53
1:E:95:ILE:O	1:E:104:PRO:HB3	2.09	0.52
1:C:95:ILE:O	1:C:104:PRO:HB3	2.09	0.52
1:D:95:ILE:O	1:D:104:PRO:HB3	2.09	0.52
1:F:230:TYR:CE1	1:F:277:VAL:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:HIS:HB2	1:B:101:ALA:HB3	1.93	0.50
1:C:230:TYR:CE1	1:C:277:VAL:HG21	2.46	0.50
1:C:290:HIS:HE1	5:C:659:HOH:O	1.94	0.50
1:D:230:TYR:CE1	1:D:277:VAL:HG21	2.46	0.50
1:B:230:TYR:CE1	1:B:277:VAL:HG21	2.47	0.50
1:A:230:TYR:CE1	1:A:277:VAL:HG21	2.46	0.49
1:E:56:HIS:HB2	1:E:101:ALA:HB3	1.94	0.49
1:E:230:TYR:CE1	1:E:277:VAL:HG21	2.46	0.49
1:F:95:ILE:O	1:F:104:PRO:HB3	2.12	0.49
1:E:44:PRO:HD3	1:E:466:PHE:CE2	2.48	0.49
1:F:56:HIS:HB2	1:F:101:ALA:HB3	1.95	0.49
1:A:66:LYS:O	1:A:76:TYR:HA	2.14	0.48
1:C:56:HIS:HB2	1:C:101:ALA:HB3	1.96	0.48
1:D:44:PRO:HD3	1:D:466:PHE:CE2	2.49	0.48
1:B:189:ILE:HG21	1:B:245:LEU:HD23	1.95	0.48
1:E:66:LYS:O	1:E:76:TYR:HA	2.13	0.48
1:F:66:LYS:O	1:F:76:TYR:HA	2.14	0.47
1:C:66:LYS:O	1:C:76:TYR:HA	2.13	0.47
1:A:56:HIS:HB2	1:A:101:ALA:HB3	1.95	0.47
1:C:44:PRO:HD3	1:C:466:PHE:CE2	2.50	0.47
1:C:28:LYS:NZ	1:C:457:GLU:OE2	2.33	0.47
1:F:213:ILE:HD11	1:F:269:VAL:HG21	1.97	0.47
1:A:44:PRO:HD3	1:A:466:PHE:CE2	2.49	0.47
1:C:189:ILE:HG21	1:C:245:LEU:HD23	1.97	0.47
1:D:56:HIS:HB2	1:D:101:ALA:HB3	1.95	0.47
1:C:268:ILE:HD12	1:C:280:TYR:CE2	2.51	0.46
1:D:66:LYS:O	1:D:76:TYR:HA	2.14	0.46
1:D:189:ILE:HG21	1:D:245:LEU:HD23	1.97	0.46
1:C:290:HIS:HD2	5:C:675:HOH:O	1.96	0.46
1:D:268:ILE:HD12	1:D:280:TYR:CE2	2.51	0.46
1:B:44:PRO:HD3	1:B:466:PHE:CE2	2.51	0.46
1:B:66:LYS:O	1:B:76:TYR:HA	2.14	0.46
1:E:9:PHE:HE1	1:E:321:LEU:O	1.99	0.46
1:A:324:GLN:OE1	1:C:397:LYS:NZ	2.47	0.46
1:B:268:ILE:HD12	1:B:280:TYR:CE2	2.51	0.46
1:F:44:PRO:HD3	1:F:466:PHE:CE2	2.50	0.46
1:A:268:ILE:HD12	1:A:280:TYR:CE2	2.51	0.46
1:C:324:GLN:OE1	5:C:601:HOH:O	2.21	0.46
1:C:44:PRO:HB2	1:C:60:GLY:HA3	1.98	0.46
1:E:268:ILE:HD12	1:E:280:TYR:CE2	2.51	0.46
1:C:225:ALA:HA	5:C:686:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:HIS:HE1	5:F:1114:HOH:O	1.98	0.45
1:A:44:PRO:HB2	1:A:60:GLY:HA3	1.98	0.45
1:F:268:ILE:HD12	1:F:280:TYR:CE2	2.52	0.44
1:A:93:ASP:CG	1:E:30:THR:HG21	2.42	0.44
1:D:225:ALA:HB3	1:D:232:VAL:HB	2.00	0.44
1:E:268:ILE:HD13	1:E:300:ILE:HD12	1.98	0.44
1:C:268:ILE:HD13	1:C:300:ILE:HD12	2.00	0.44
1:B:44:PRO:HB2	1:B:60:GLY:HA3	2.00	0.44
1:C:225:ALA:HB3	1:C:232:VAL:HB	2.00	0.43
1:D:44:PRO:HB2	1:D:60:GLY:HA3	1.99	0.43
1:E:328:THR:N	1:F:350:MET:HE1	2.33	0.43
1:E:443:LEU:HD21	1:E:445:LEU:HD21	2.01	0.43
1:B:216:GLU:HG2	5:B:734:HOH:O	2.18	0.43
1:F:44:PRO:HB2	1:F:60:GLY:HA3	1.99	0.43
1:B:225:ALA:HB3	1:B:232:VAL:HB	2.01	0.43
1:A:325:LYS:NZ	5:A:1114:HOH:O	2.52	0.43
1:E:44:PRO:HB2	1:E:60:GLY:HA3	2.00	0.43
1:F:253:ILE:HD12	1:F:253:ILE:HA	1.93	0.42
1:F:225:ALA:HB3	1:F:232:VAL:HB	2.00	0.42
1:B:202:ASP:O	5:B:601:HOH:O	2.21	0.42
1:A:268:ILE:HD13	1:A:300:ILE:HD12	2.01	0.42
1:D:268:ILE:HD13	1:D:300:ILE:HD12	2.01	0.42
1:B:268:ILE:HD13	1:B:300:ILE:HD12	2.02	0.42
1:E:225:ALA:HB3	1:E:232:VAL:HB	2.00	0.42
1:E:392:ILE:HD13	1:E:399:SER:HB2	2.01	0.42
1:F:264:THR:HG21	1:F:285:PHE:CE1	2.55	0.42
1:B:396:ARG:O	1:B:397:LYS:C	2.63	0.41
1:E:268:ILE:HD11	1:E:339:ILE:HG21	2.02	0.41
1:F:268:ILE:HD11	1:F:339:ILE:HG21	2.02	0.41
1:A:443:LEU:HD21	1:A:445:LEU:HD21	2.01	0.41
1:D:253:ILE:HD12	1:D:253:ILE:HA	1.91	0.41
1:E:268:ILE:HD12	1:E:280:TYR:HE2	1.86	0.41
1:F:124:ALA:HA	1:F:139:THR:HB	2.03	0.41
1:C:396:ARG:O	1:C:397:LYS:C	2.62	0.41
1:A:225:ALA:HB3	1:A:232:VAL:HB	2.03	0.41
1:A:290:HIS:HD2	5:A:1183:HOH:O	2.03	0.41
1:F:268:ILE:HD13	1:F:300:ILE:HD12	2.03	0.41
1:F:443:LEU:HD21	1:F:445:LEU:HD21	2.03	0.41
1:D:264:THR:HG21	1:D:285:PHE:CE1	2.56	0.41
1:E:124:ALA:HA	1:E:139:THR:HB	2.03	0.41
1:A:264:THR:HG21	1:A:285:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HD11	1:B:339:ILE:HG21	2.03	0.40
1:E:264:THR:HG21	1:E:285:PHE:CE1	2.56	0.40
1:E:392:ILE:HD13	1:E:399:SER:CB	2.51	0.40
1:A:396:ARG:O	1:A:397:LYS:C	2.64	0.40
1:D:28:LYS:NZ	1:D:457:GLU:OE2	2.35	0.40
1:A:253:ILE:HD12	1:A:253:ILE:HA	1.92	0.40
1:C:264:THR:HG21	1:C:285:PHE:CE1	2.56	0.40
1:D:15:THR:OG1	1:D:48:GLU:OE2	2.32	0.40
1:D:396:ARG:O	1:D:397:LYS:C	2.64	0.40
1:E:179:LYS:HE3	1:E:272:GLN:OE1	2.21	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	451/472 (96%)	432 (96%)	19 (4%)	0	100	100
1	B	451/472 (96%)	432 (96%)	19 (4%)	0	100	100
1	C	450/472 (95%)	431 (96%)	19 (4%)	0	100	100
1	D	449/472 (95%)	430 (96%)	19 (4%)	0	100	100
1	E	405/472 (86%)	392 (97%)	13 (3%)	0	100	100
1	F	418/472 (89%)	400 (96%)	18 (4%)	0	100	100
All	All	2624/2832 (93%)	2517 (96%)	107 (4%)	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	387/417 (93%)	385 (100%)	2 (0%)	81	90
1	B	392/417 (94%)	387 (99%)	5 (1%)	61	77
1	C	382/417 (92%)	381 (100%)	1 (0%)	86	93
1	D	382/417 (92%)	379 (99%)	3 (1%)	73	86
1	E	355/417 (85%)	354 (100%)	1 (0%)	86	93
1	F	350/417 (84%)	348 (99%)	2 (1%)	78	89
All	All	2248/2502 (90%)	2234 (99%)	14 (1%)	78	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	383	SER
1	B	20	LEU
1	B	24	SER
1	B	149	ILE
1	B	216	GLU
1	B	297	GLN
1	C	20	LEU
1	D	10	GLN
1	D	20	LEU
1	D	383	SER
1	E	281	LYS
1	F	107	SER
1	F	350	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	C	180	ASN
1	E	461	HIS

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Mol	Chain	Res	Type
1	F	333	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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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%)	0.81	40 (8%)	15 17	29, 67, 99, 126	2 (0%)
1	B	453/472 (95%)	0.22	9 (1%)	65 66	21, 56, 85, 105	2 (0%)
1	C	453/472 (95%)	0.69	27 (5%)	27 29	24, 73, 110, 133	1 (0%)
1	D	453/472 (95%)	0.57	23 (5%)	33 35	43, 69, 103, 132	0
1	E	423/472 (89%)	2.04	180 (42%)	0 0	44, 88, 165, 198	0
1	F	430/472 (91%)	1.42	113 (26%)	1 2	51, 87, 136, 148	0
All	All	2665/2832 (94%)	0.94	392 (14%)	6 6	21, 72, 128, 198	5 (0%)

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	374	VAL	7.0
1	E	31	ILE	6.9
1	E	373	PHE	6.7
1	E	355	ALA	6.2
1	E	375	TYR	6.1
1	E	291	VAL	6.0
1	E	68	SER	6.0
1	E	427	LEU	5.7
1	E	429	LEU	5.6
1	E	376	GLY	5.6
1	E	351	LEU	5.3
1	E	470	TYR	5.3
1	E	361	ILE	5.2
1	E	414	PHE	5.2
1	E	76	TYR	5.2
1	E	428	ILE	5.2
1	E	177	PHE	5.1
1	E	389	LEU	5.0
1	F	31	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	301	PHE	4.8
1	E	25	LEU	4.8
1	E	431	ALA	4.8
1	E	392	ILE	4.7
1	E	340	PRO	4.7
1	E	460	HIS	4.7
1	E	413	VAL	4.7
1	E	26	GLN	4.6
1	F	374	VAL	4.6
1	E	444	ILE	4.6
1	F	392	ILE	4.6
1	E	67	PHE	4.6
1	E	371	TYR	4.6
1	E	462	ILE	4.6
1	E	278	GLY	4.5
1	E	40	ILE	4.5
1	E	390	VAL	4.5
1	E	71	GLU	4.5
1	E	410	GLY	4.4
1	E	22	LEU	4.4
1	E	453	VAL	4.4
1	E	442	LEU	4.3
1	C	385	PHE	4.3
1	E	305	ILE	4.3
1	E	356	VAL	4.3
1	E	377	ILE	4.3
1	E	27	VAL	4.2
1	E	450	PHE	4.2
1	E	443	LEU	4.2
1	E	300	ILE	4.2
1	F	40	ILE	4.2
1	B	384	ASP	4.2
1	E	70	LYS	4.2
1	E	112	VAL	4.1
1	F	149	ILE	4.1
1	E	363	TYR	4.1
1	F	377	ILE	4.1
1	E	438	ALA	4.1
1	E	366	TYR	4.1
1	F	465	GLY	4.1
1	F	390	VAL	4.1
1	E	447	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	25	LEU	4.0
1	E	292	ASN	4.0
1	C	120	PHE	4.0
1	C	275	ASN	4.0
1	E	24	SER	3.9
1	E	346	VAL	3.9
1	E	471	PHE	3.9
1	F	67	PHE	3.9
1	E	280	TYR	3.9
1	E	388	GLN	3.9
1	E	350	MET	3.9
1	E	458	VAL	3.9
1	E	73	LYS	3.8
1	E	408	TYR	3.8
1	E	20	LEU	3.8
1	C	7	ASN	3.8
1	E	306	ALA	3.7
1	E	339	ILE	3.7
1	E	65	HIS	3.7
1	C	167	GLY	3.7
1	E	293	ALA	3.7
1	E	441	PHE	3.7
1	F	428	ILE	3.7
1	E	155	VAL	3.7
1	E	432	VAL	3.7
1	E	348	TYR	3.7
1	A	342	SER	3.7
1	F	10	GLN	3.7
1	F	11	LEU	3.7
1	F	351	LEU	3.7
1	E	415	VAL	3.7
1	E	364	LYS	3.7
1	D	120	PHE	3.6
1	E	294	PHE	3.6
1	E	449	THR	3.6
1	E	412	PRO	3.6
1	E	150	ASN	3.6
1	F	342	SER	3.6
1	A	373	PHE	3.6
1	F	330	PRO	3.6
1	D	105	CYS	3.5
1	A	230	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	249	GLY	3.5
1	D	6	THR	3.5
1	E	411	GLU	3.5
1	E	302	VAL	3.5
1	F	74	VAL	3.5
1	E	113	SER	3.5
1	F	429	LEU	3.5
1	E	74	VAL	3.4
1	F	158	PHE	3.4
1	F	413	VAL	3.4
1	D	26	GLN	3.4
1	E	116	PHE	3.4
1	E	352	SER	3.4
1	E	416	GLY	3.4
1	E	402	TRP	3.4
1	B	385	PHE	3.4
1	E	28	LYS	3.4
1	E	359	PRO	3.3
1	E	347	GLU	3.3
1	E	304	ILE	3.3
1	E	401	ILE	3.3
1	E	279	THR	3.3
1	F	375	TYR	3.3
1	E	243	LEU	3.3
1	E	372	ARG	3.3
1	F	464	PHE	3.3
1	F	443	LEU	3.2
1	A	120	PHE	3.2
1	B	7	ASN	3.2
1	C	246	LEU	3.2
1	F	444	ILE	3.2
1	F	13	PHE	3.2
1	E	115	MET	3.2
1	B	79[A]	LYS	3.2
1	A	105	CYS	3.2
1	C	342	SER	3.2
1	A	268	ILE	3.2
1	F	152	LEU	3.1
1	F	321	LEU	3.1
1	C	9	PHE	3.1
1	C	24	SER	3.1
1	E	417	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	157	VAL	3.1
1	A	229	ASN	3.1
1	F	431	ALA	3.1
1	F	334	ILE	3.1
1	F	288	PHE	3.1
1	A	280	TYR	3.0
1	C	71	GLU	3.0
1	D	462	ILE	3.0
1	E	29	GLY	3.0
1	F	12	GLY	3.0
1	F	418	PRO	3.0
1	F	276	LEU	3.0
1	F	277	VAL	3.0
1	A	277	VAL	3.0
1	F	442	LEU	3.0
1	F	453	VAL	3.0
1	D	160	TYR	3.0
1	E	30	THR	3.0
1	C	247	LEU	3.0
1	F	64	LEU	3.0
1	E	369	LYS	3.0
1	E	118	THR	3.0
1	E	368	THR	3.0
1	E	448	THR	3.0
1	B	249	GLY	3.0
1	E	418	PRO	3.0
1	E	225	ALA	2.9
1	E	456	ALA	2.9
1	F	460	HIS	2.9
1	F	28	LYS	2.9
1	E	459	PRO	2.9
1	C	453	VAL	2.9
1	F	345	GLN	2.9
1	E	230	TYR	2.9
1	F	427	LEU	2.9
1	E	424	ASP	2.9
1	E	132	ALA	2.9
1	E	407	CYS	2.9
1	F	106	ARG	2.8
1	E	285	PHE	2.8
1	F	401	ILE	2.8
1	F	462	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	353	SER	2.8
1	E	399	SER	2.8
1	E	358	LEU	2.8
1	E	120	PHE	2.8
1	E	457	GLU	2.8
1	F	112	VAL	2.8
1	C	105	CYS	2.8
1	F	274	GLY	2.8
1	E	423	GLU	2.8
1	C	33	LYS	2.8
1	D	31	ILE	2.8
1	A	274	GLY	2.8
1	E	409	PRO	2.8
1	D	22	LEU	2.8
1	E	152	LEU	2.8
1	E	466	PHE	2.8
1	A	272	GLN	2.7
1	E	17	SER	2.7
1	E	307	TYR	2.7
1	E	464	PHE	2.7
1	A	275	ASN	2.7
1	F	298	GLU	2.7
1	E	422	LYS	2.7
1	E	16	LEU	2.7
1	F	454	ALA	2.7
1	F	109	PHE	2.7
1	A	27	VAL	2.7
1	D	30	THR	2.7
1	F	421	THR	2.7
1	E	403	SER	2.7
1	A	382	ALA	2.7
1	F	354	GLU	2.7
1	A	210	ILE	2.7
1	E	440	SER	2.7
1	C	22	LEU	2.7
1	A	385	PHE	2.6
1	F	471	PHE	2.6
1	E	303	ASP	2.6
1	F	425	GLU	2.6
1	F	297	GLN	2.6
1	A	33	LYS	2.6
1	E	354	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	ASN	2.6
1	F	356	VAL	2.6
1	E	104	PRO	2.6
1	F	24	SER	2.6
1	C	386	ALA	2.6
1	F	85	ALA	2.6
1	F	157	VAL	2.6
1	F	412	PRO	2.6
1	D	40	ILE	2.6
1	F	433	LEU	2.6
1	F	350	MET	2.6
1	E	147	PHE	2.6
1	D	27	VAL	2.6
1	E	277	VAL	2.6
1	D	342	SER	2.6
1	E	86	TYR	2.6
1	E	268	ILE	2.6
1	F	56	HIS	2.6
1	F	389	LEU	2.5
1	F	445	LEU	2.5
1	E	78	ASN	2.5
1	F	57	TRP	2.5
1	E	465	GLY	2.5
1	E	149	ILE	2.5
1	F	361	ILE	2.5
1	A	246	LEU	2.5
1	E	433	LEU	2.5
1	F	362	ASN	2.5
1	E	114	SER	2.5
1	E	77	ALA	2.5
1	E	201	ALA	2.5
1	F	113	SER	2.5
1	F	364	LYS	2.5
1	D	319	ASP	2.5
1	F	469	ASN	2.5
1	B	386	ALA	2.5
1	A	156	GLY	2.5
1	F	388	GLN	2.5
1	C	30	THR	2.4
1	B	120	PHE	2.4
1	F	69	PHE	2.4
1	F	304	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	2.4
1	E	287	ALA	2.4
1	F	435	ALA	2.4
1	E	72	GLY	2.4
1	E	154	THR	2.4
1	F	118	THR	2.4
1	F	17	SER	2.4
1	A	149	ILE	2.4
1	D	246	LEU	2.4
1	F	20	LEU	2.4
1	F	358	LEU	2.4
1	F	411	GLU	2.4
1	C	417	ALA	2.4
1	F	30	THR	2.4
1	D	157	VAL	2.4
1	E	232	VAL	2.4
1	F	269	VAL	2.4
1	F	373	PHE	2.4
1	F	441	PHE	2.4
1	E	175	TYR	2.4
1	F	76	TYR	2.4
1	E	468	GLY	2.4
1	E	398	SER	2.4
1	A	26	GLN	2.4
1	F	438	ALA	2.3
1	E	178	VAL	2.3
1	E	97	TYR	2.3
1	E	260	PRO	2.3
1	F	278	GLY	2.3
1	F	420	ALA	2.3
1	E	264	THR	2.3
1	E	455	ARG	2.3
1	A	158	PHE	2.3
1	F	291	VAL	2.3
1	A	341	LEU	2.3
1	E	246	LEU	2.3
1	E	445	LEU	2.3
1	C	34	TRP	2.3
1	E	284	ALA	2.3
1	F	77	ALA	2.3
1	F	331	THR	2.3
1	E	282	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	80	PHE	2.3
1	F	346	VAL	2.3
1	E	81	LEU	2.3
1	D	89	ALA	2.3
1	F	306	ALA	2.3
1	A	24	SER	2.3
1	C	272	GLN	2.3
1	D	158	PHE	2.2
1	A	30	THR	2.2
1	E	151	THR	2.2
1	E	290	HIS	2.2
1	E	79	LYS	2.2
1	C	396	ARG	2.2
1	E	430	SER	2.2
1	F	75	SER	2.2
1	B	20	LEU	2.2
1	F	316	LEU	2.2
1	E	174	HIS	2.2
1	F	79	LYS	2.2
1	A	279	THR	2.2
1	E	159	ALA	2.2
1	F	436	THR	2.2
1	F	456	ALA	2.2
1	A	34	TRP	2.2
1	D	152	LEU	2.2
1	A	155	VAL	2.2
1	C	8	LYS	2.2
1	A	416	GLY	2.2
1	A	417	ALA	2.2
1	E	62	ALA	2.2
1	F	417	ALA	2.2
1	C	25	LEU	2.1
1	A	269	VAL	2.1
1	A	73	LYS	2.1
1	F	359	PRO	2.1
1	A	383	SER	2.1
1	E	85	ALA	2.1
1	F	398	SER	2.1
1	E	338	ARG	2.1
1	E	360	ARG	2.1
1	A	273	ASN	2.1
1	A	231	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	128	VAL	2.1
1	F	313	VAL	2.1
1	F	458	VAL	2.1
1	E	135	PHE	2.1
1	E	308	GLN	2.1
1	F	416	GLY	2.1
1	C	92	THR	2.1
1	F	45	ALA	2.1
1	D	70	LYS	2.1
1	A	76	TYR	2.1
1	B	387	ASN	2.1
1	C	470	TYR	2.1
1	F	41	ARG	2.1
1	E	436	THR	2.1
1	E	281	LYS	2.1
1	F	62	ALA	2.1
1	C	26	GLN	2.1
1	E	283	ASP	2.1
1	F	270	ASN	2.1
1	E	330	PRO	2.1
1	F	175	TYR	2.1
1	F	111	ARG	2.1
1	D	24	SER	2.0
1	F	105	CYS	2.0
1	D	247	LEU	2.0
1	F	16	LEU	2.0
1	E	231	VAL	2.0
1	F	232	VAL	2.0
1	D	47	PHE	2.0
1	E	288	PHE	2.0
1	D	8	LYS	2.0
1	C	298	GLU	2.0
1	E	96	SER	2.0
1	F	127	ASN	2.0
1	A	300	ILE	2.0
1	A	418	PRO	2.0
1	E	400	LYS	2.0

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

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](#)

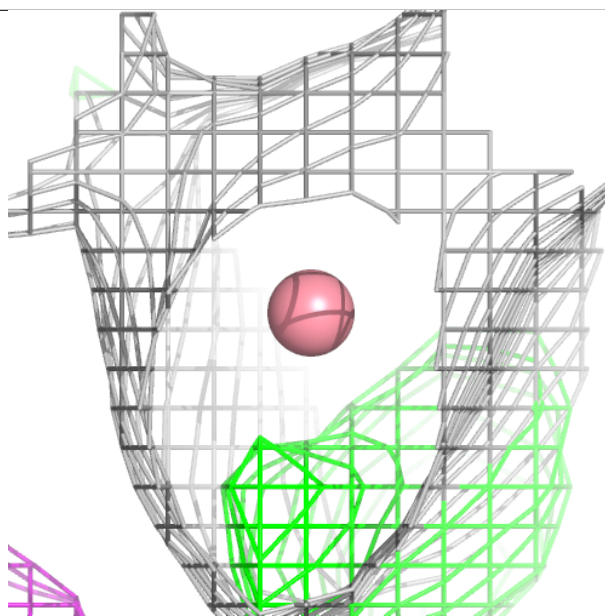
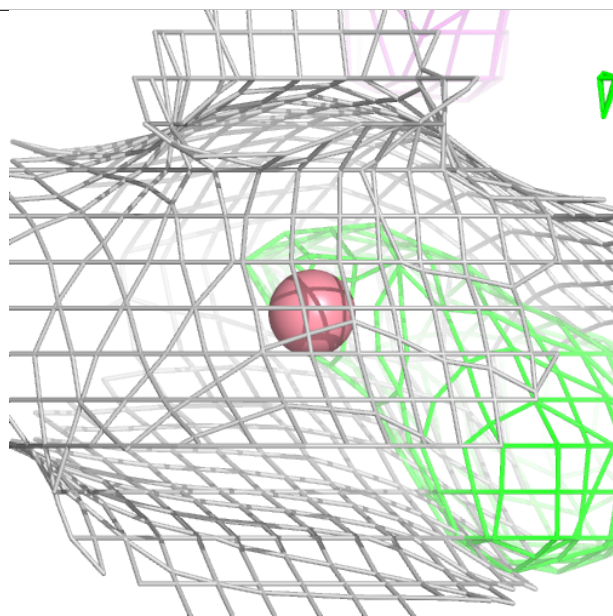
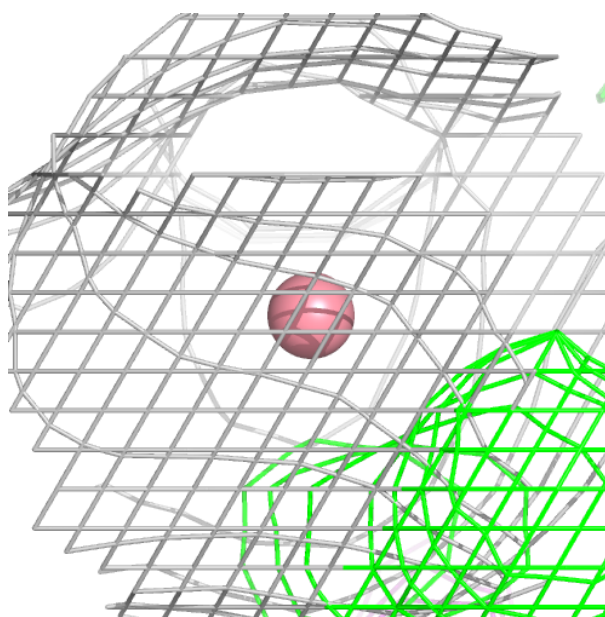
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	C	503	1/1	0.92	0.12	79,79,79,79	0
4	CL	E	502	1/1	0.95	0.18	60,60,60,60	0
2	CO	F	1000	1/1	0.97	0.05	71,71,71,71	0
3	NA	B	502	1/1	0.97	0.07	70,70,70,70	0
3	NA	C	502	1/1	0.98	0.09	67,67,67,67	0
2	CO	E	501	1/1	0.99	0.04	61,61,61,61	0
2	CO	C	501	1/1	1.00	0.02	54,54,54,54	0
2	CO	D	1000	1/1	1.00	0.02	53,53,53,53	0
2	CO	A	1000	1/1	1.00	0.02	42,42,42,42	0
2	CO	B	501	1/1	1.00	0.01	38,38,38,38	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.

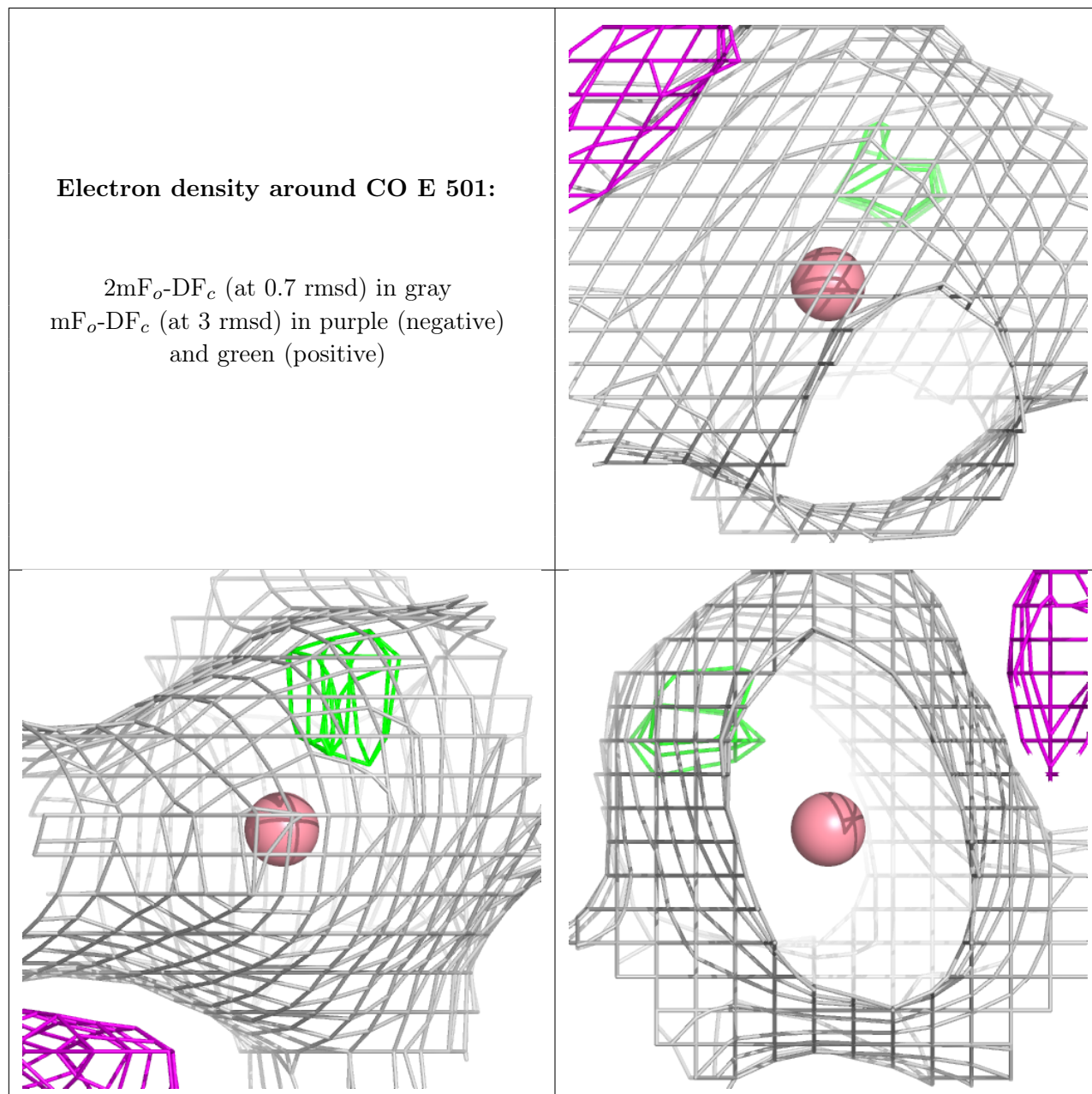
Electron density around CO F 1000:

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



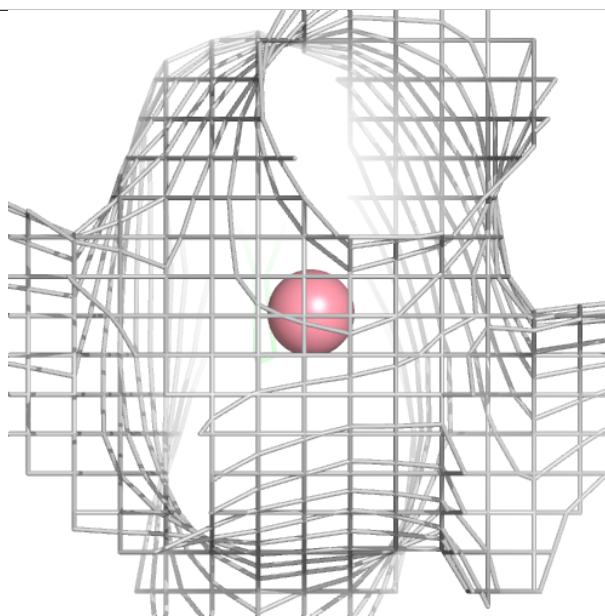
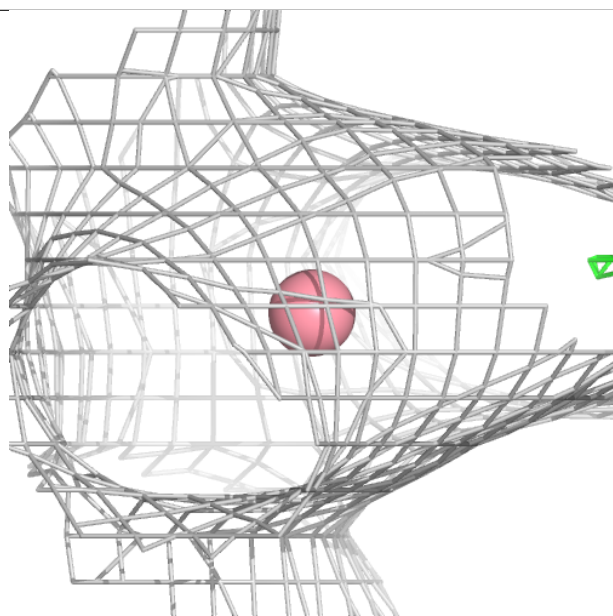
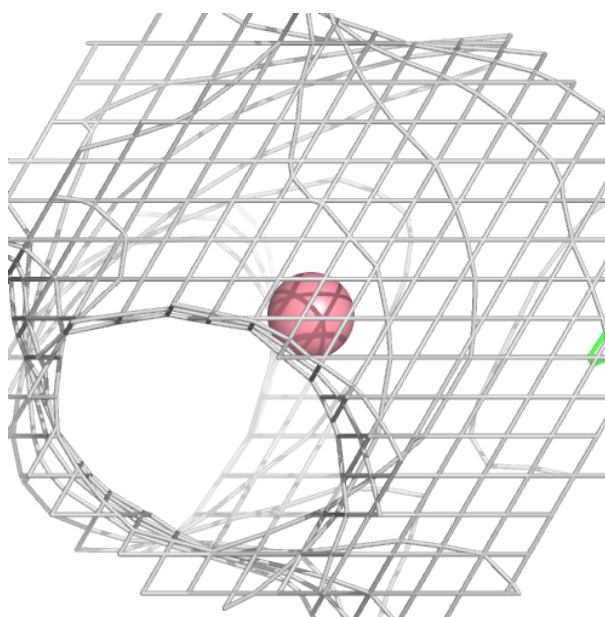
Electron density around CO E 501:

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



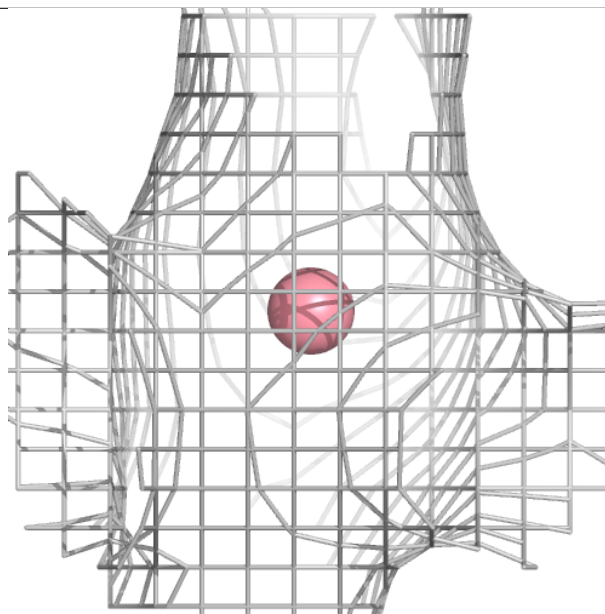
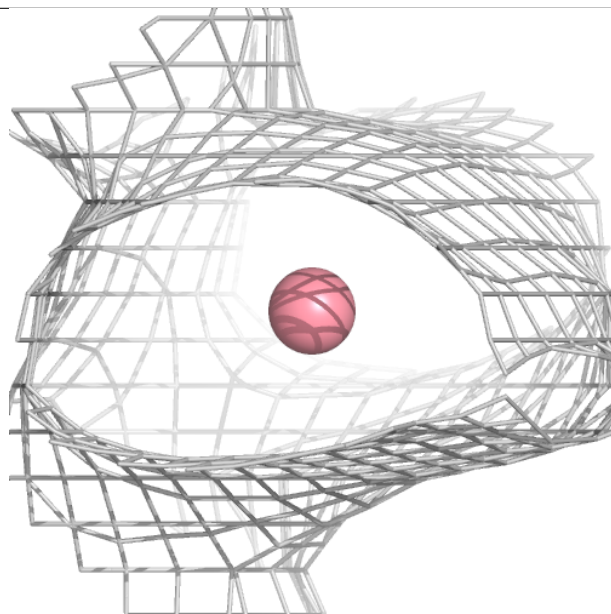
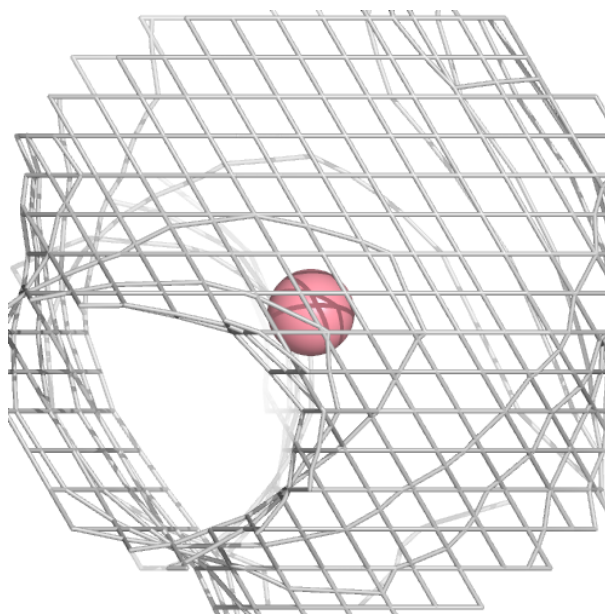
Electron density around CO C 501:

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



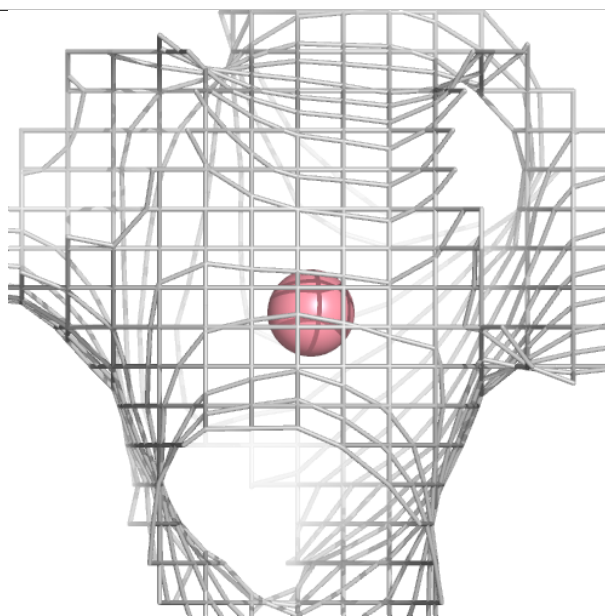
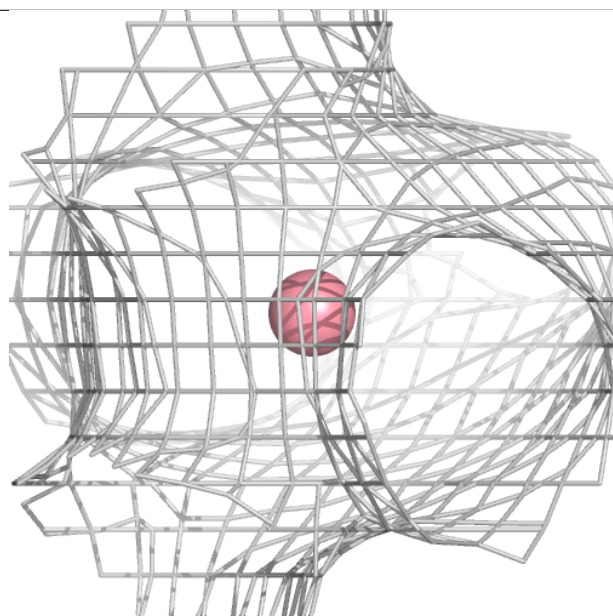
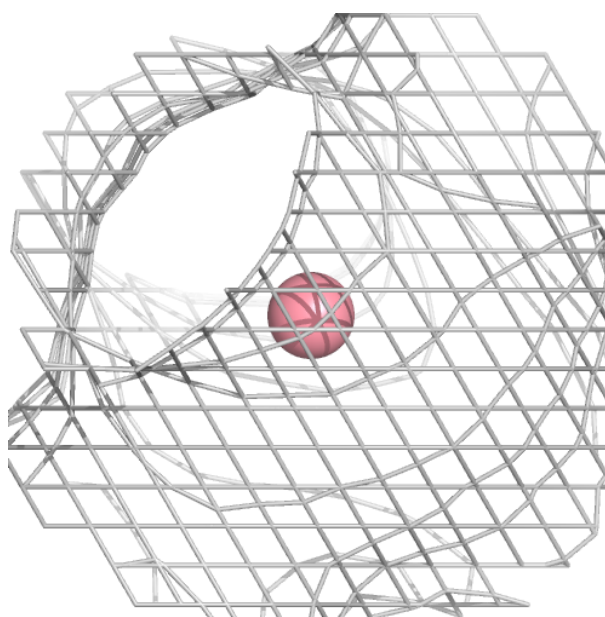
Electron density around CO D 1000:

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



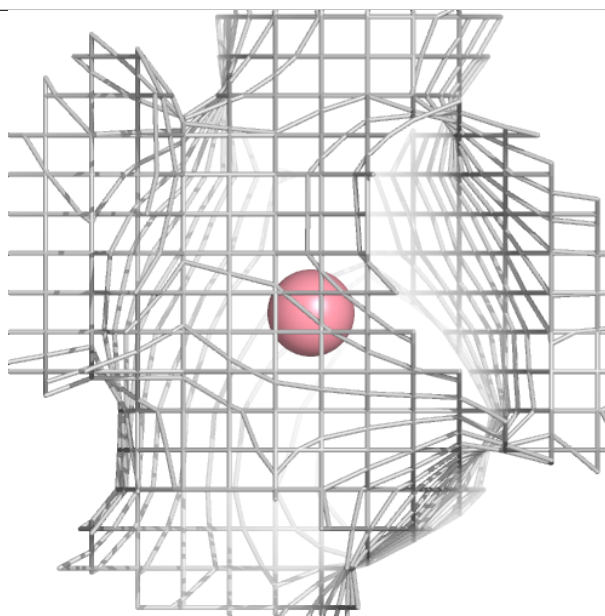
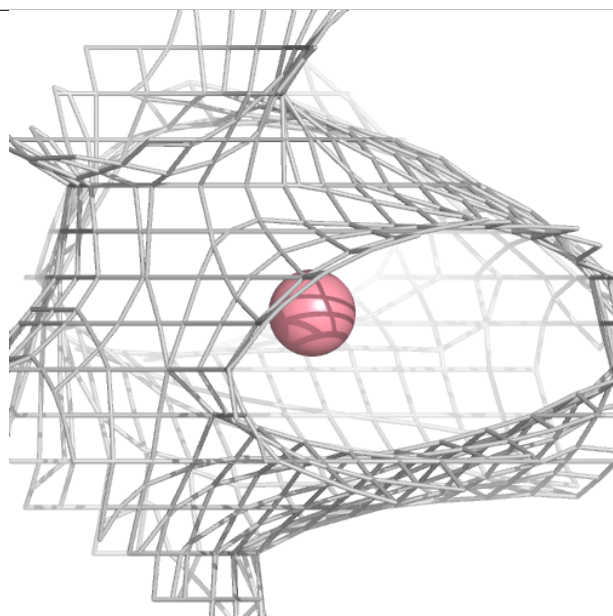
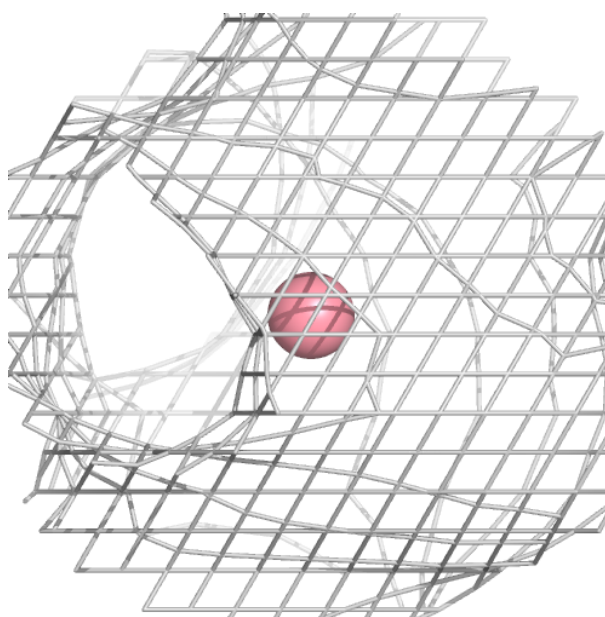
Electron density around CO A 1000:

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



Electron density around CO 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.