



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:13 PM JST

PDB ID : 7VPN
Title : Crystal Structure of the dioxygenase CcTet from Coprinopsis cinereain in complex with Mn(II) and N-Oxalylglycine
Authors : Mu, Y.J.; Zhang, L.; Zhang, L.
Deposited on : 2021-10-17
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

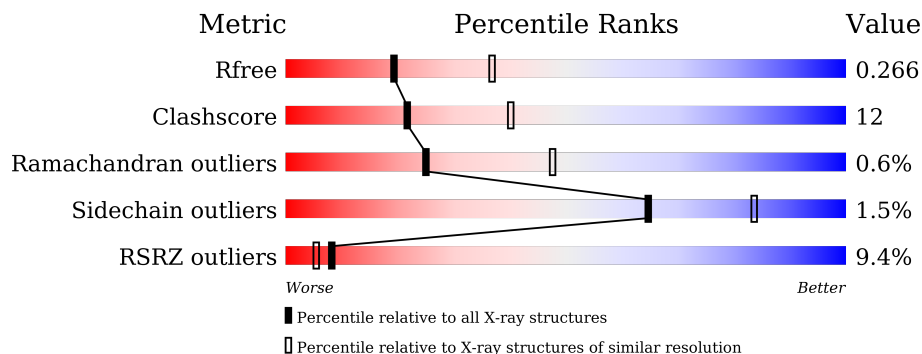
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	430	 69% 12% 19%
1	B	430	 66% 14% 18%
1	C	430	 63% 18% 17%
1	D	430	 43% 32% 22%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OGA	A	1002	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11103 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.

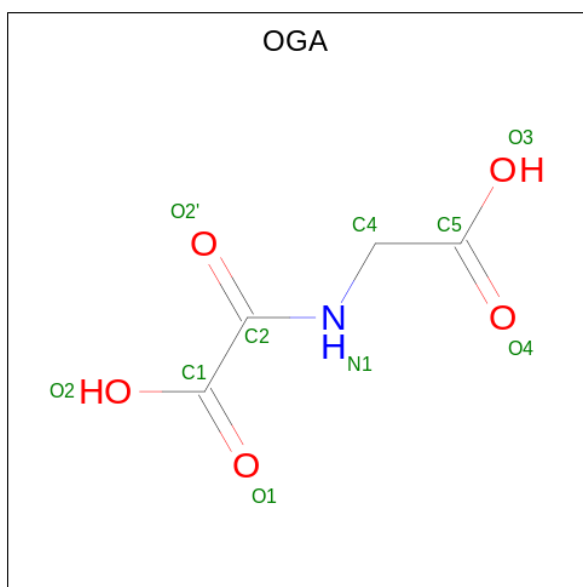
- Molecule 1 is a protein called CcTet molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2715	1743	471	487	14	0	0	0
1	B	351	2746	1764	474	495	13	0	0	0
1	C	356	2797	1795	487	502	13	0	0	0
1	D	334	2626	1689	456	469	12	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

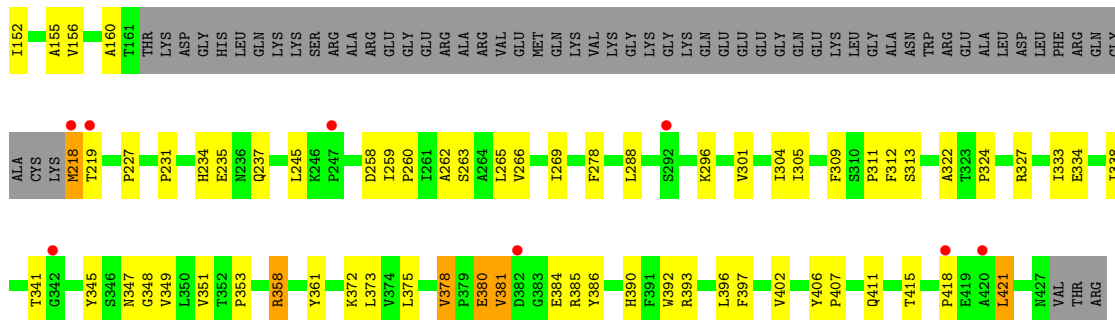
- Molecule 3 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C₄H₅NO₅) (labeled as "Ligand of Interest" by depositor).



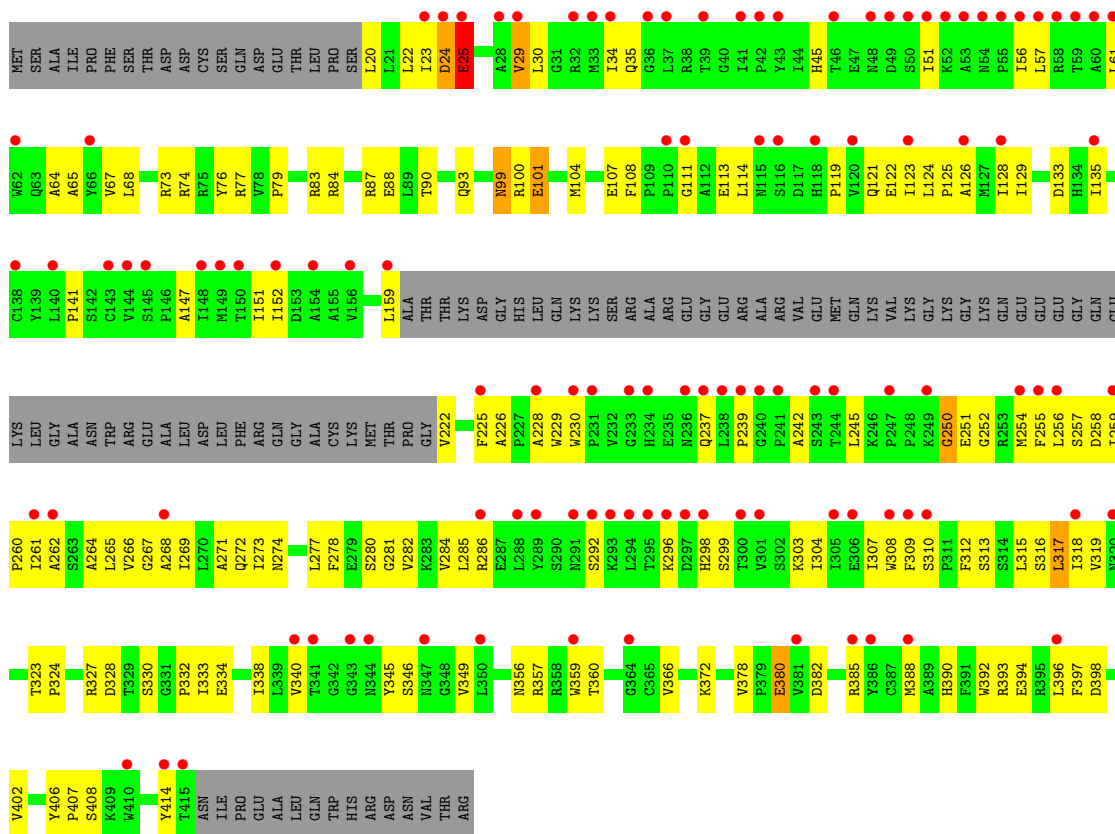
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	A	1	10	4	1	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	97	Total	O	0	0
			97	97		
4	C	31	Total	O	0	0
			31	31		
4	D	4	Total	O	0	0
			4	4		



• Molecule 1: CcTet molecule



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 219.80Å 77.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.16 – 2.60 49.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.3 (49.16-2.60) 91.3 (49.16-2.60)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217 , 0.266 0.220 , 0.266	Depositor DCC
R_{free} test set	3120 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11103	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: MN, OGA

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	0.52	0/2789	0.73	3/3805 (0.1%)
1	B	0.67	7/2821 (0.2%)	0.77	5/3851 (0.1%)
1	C	0.55	0/2875	0.83	6/3925 (0.2%)
1	D	0.53	5/2698 (0.2%)	0.76	5/3680 (0.1%)
All	All	0.57	12/11183 (0.1%)	0.77	19/15261 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	GLU	CG-CD	-7.76	1.40	1.51
1	D	101	GLU	CD-OE2	-7.24	1.17	1.25
1	D	25	GLU	CD-OE2	7.13	1.33	1.25
1	B	332	PRO	C-O	-6.29	1.10	1.23
1	B	331	GLY	C-O	-6.09	1.14	1.23
1	B	334	GLU	CD-OE2	-5.57	1.19	1.25
1	B	334	GLU	CD-OE1	-5.44	1.19	1.25
1	B	330	SER	CA-CB	-5.32	1.45	1.52
1	D	101	GLU	CD-OE1	-5.32	1.19	1.25
1	B	18	PRO	C-O	-5.13	1.12	1.23
1	D	35	GLN	CG-CD	5.13	1.62	1.51
1	B	18	PRO	N-CD	-5.07	1.40	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ARG	NE-CZ-NH1	-23.54	108.53	120.30
1	C	96	ARG	CD-NE-CZ	12.26	140.77	123.60
1	B	70	LYS	CD-CE-NZ	-9.46	89.94	111.70
1	D	25	GLU	CA-CB-CG	8.89	132.96	113.40
1	B	238	LEU	CA-CB-CG	8.63	135.14	115.30
1	A	83	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	D	25	GLU	CG-CD-OE2	-7.00	104.30	118.30
1	C	421	LEU	CA-CB-CG	6.97	131.34	115.30
1	D	317	LEU	CB-CG-CD2	6.64	122.29	111.00
1	C	41	ILE	CG1-CB-CG2	-6.28	97.59	111.40
1	C	17	LEU	N-CA-CB	-5.68	99.05	110.40
1	B	88	GLU	N-CA-CB	-5.51	100.67	110.60
1	A	83	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	21	LEU	CB-CG-CD1	-5.33	101.95	111.00
1	B	16	THR	CA-CB-OG1	-5.31	97.86	109.00
1	C	96	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	D	25	GLU	N-CA-CB	5.10	119.78	110.60
1	D	24	ASP	C-N-CA	-5.08	109.00	121.70
1	B	223	LEU	CB-CG-CD1	-5.06	102.40	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	96	ARG	Sidechain
1	D	25	GLU	Sidechain
1	D	250	GLY	Peptide

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	2715	0	2725	34	0
1	B	2746	0	2753	47	0
1	C	2797	0	2795	69	0
1	D	2626	0	2633	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	10	0	3	4	0
4	A	73	0	0	1	0
4	B	97	0	0	3	0
4	C	31	0	0	1	0
4	D	4	0	0	2	0
All	All	11103	0	10909	259	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 12.

All (259) 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:C:334:GLU:HB2	1:C:407:PRO:HD3	1.32	1.05
1:D:274:ASN:HD22	1:D:277:LEU:HB2	1.28	0.95
1:A:232:VAL:HB	1:B:97:ASN:HD22	1.32	0.92
1:C:349:VAL:O	1:C:378:VAL:HG23	1.71	0.90
1:B:86:MET:HE1	1:B:373:LEU:HD12	1.55	0.87
1:B:404:PHE:O	1:D:84:ARG:NH2	2.10	0.84
1:D:129:ILE:HG22	1:D:135:ILE:HA	1.57	0.84
1:C:86:MET:SD	1:C:333:ILE:HD11	2.17	0.83
1:D:312:PHE:HZ	1:D:338:ILE:HD12	1.42	0.83
1:D:99:ASN:OD1	1:D:99:ASN:N	2.13	0.81
1:C:96:ARG:HH12	1:C:324:PRO:HG2	1.46	0.79
1:D:77:ARG:HG3	1:D:129:ILE:HG13	1.67	0.77
1:D:274:ASN:ND2	1:D:277:LEU:HB2	2.00	0.76
1:D:317:LEU:HD22	1:D:319:VAL:HG13	1.66	0.76
1:B:84:ARG:HH22	1:D:394:GLU:HG2	1.52	0.74
1:A:74:ARG:NH2	4:A:1101:HOH:O	2.21	0.73
1:C:333:ILE:HG23	1:C:334:GLU:OE1	1.87	0.73
1:D:312:PHE:CZ	1:D:338:ILE:HD12	2.24	0.73
1:B:332:PRO:HG3	1:B:394:GLU:HB2	1.70	0.72
1:C:122:GLU:OE1	4:C:1101:HOH:O	2.06	0.72
1:D:334:GLU:HB2	1:D:407:PRO:HD3	1.72	0.70
1:D:346:SER:OG	4:D:1101:HOH:O	2.10	0.70
1:D:225:PHE:HD1	1:D:245:LEU:HD21	1.58	0.68
1:B:120:VAL:O	4:B:1101:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:O	1:B:15:GLU:HG3	1.92	0.67
1:B:83:ARG:NH1	1:B:132:GLU:OE1	2.29	0.66
1:D:274:ASN:HD22	1:D:277:LEU:CB	2.07	0.66
1:A:316:SER:HB2	1:A:391:PHE:HE2	1.60	0.65
1:D:255:PHE:O	1:D:259:ILE:HG12	1.96	0.65
1:D:265:LEU:O	1:D:269:ILE:HG13	1.97	0.64
1:D:119:PRO:HG3	1:D:356:ASN:O	1.98	0.64
1:D:281:GLY:O	1:D:285:LEU:HD12	1.96	0.64
1:A:332:PRO:HG3	1:A:394:GLU:HB2	1.79	0.64
1:D:242:ALA:HB3	1:D:245:LEU:HD23	1.79	0.64
1:C:17:LEU:C	1:C:17:LEU:HD23	2.18	0.64
1:A:334:GLU:HB2	1:A:407:PRO:HD3	1.78	0.63
1:D:230:TRP:CZ2	1:D:239:PRO:HG3	2.33	0.63
1:D:30:LEU:O	1:D:34:ILE:HG12	1.99	0.63
1:B:154:ALA:O	1:B:158:THR:HG23	1.99	0.63
1:B:323:THR:HB	1:B:378:VAL:HG12	1.80	0.63
1:D:76:TYR:HB2	1:D:128:ILE:HG12	1.80	0.62
1:D:68:LEU:HD21	1:D:269:ILE:HG23	1.82	0.62
1:D:84:ARG:O	1:D:87:ARG:HG2	1.99	0.62
1:A:246:LYS:O	1:A:248:PRO:HD3	1.99	0.62
1:C:96:ARG:HH12	1:C:324:PRO:CG	2.12	0.61
1:B:74:ARG:NH2	1:B:122:GLU:OE2	2.32	0.61
1:A:398:ASP:OD2	1:C:84:ARG:NH2	2.33	0.61
1:C:45:HIS:HE1	1:C:49:ASP:OD1	1.84	0.61
1:D:313:SER:HB2	1:D:396:LEU:HD12	1.81	0.61
1:D:125:PRO:HB3	1:D:141:PRO:HD2	1.82	0.60
1:C:160:ALA:HB1	1:C:218:MET:HG3	1.82	0.60
1:D:29:VAL:HG21	1:D:51:ILE:HG13	1.82	0.60
1:D:340:VAL:HG22	1:D:366:VAL:HG22	1.83	0.60
1:B:16:THR:O	1:B:16:THR:HG22	2.02	0.59
1:D:73:ARG:NH1	1:D:414:TYR:OH	2.35	0.59
1:D:378:VAL:HG13	1:D:378:VAL:O	2.02	0.59
1:B:417:ILE:O	1:B:417:ILE:HG13	2.03	0.59
1:D:20:LEU:N	4:D:1102:HOH:O	2.35	0.59
1:D:222:VAL:HG23	1:D:318:ILE:HG13	1.85	0.59
1:D:225:PHE:CD1	1:D:245:LEU:HD21	2.38	0.59
1:C:406:TYR:CG	1:C:407:PRO:HD2	2.38	0.59
1:D:266:VAL:HG21	1:D:390:HIS:CE1	2.37	0.58
1:D:292:SER:HA	1:D:298:HIS:ND1	2.18	0.58
1:A:230:TRP:CE2	1:A:239:PRO:HB3	2.39	0.58
1:D:250:GLY:O	1:D:252:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HD12	1:A:372:LYS:HG2	1.85	0.58
1:B:43:TYR:OH	1:B:45:HIS:ND1	2.23	0.57
1:D:147:ALA:O	1:D:151:ILE:HG12	2.05	0.57
1:D:333:ILE:H	1:D:333:ILE:HD12	1.69	0.57
1:D:101:GLU:OE1	1:D:101:GLU:HA	2.03	0.57
1:D:330:SER:HB3	1:D:393:ARG:HH12	1.70	0.57
1:C:90:THR:H	1:C:93:GLN:HE21	1.51	0.56
1:D:123:ILE:HG23	1:D:124:LEU:HD12	1.87	0.56
1:C:353:PRO:HD2	1:C:375:LEU:HB3	1.85	0.56
1:D:284:VAL:HG21	1:D:397:PHE:CD1	2.40	0.56
1:C:418:PRO:HA	1:C:421:LEU:HD23	1.87	0.56
1:D:30:LEU:HD13	1:D:61:LEU:HB3	1.87	0.56
1:D:20:LEU:HD12	1:D:22:LEU:H	1.69	0.56
1:D:332:PRO:HB3	1:D:394:GLU:HB2	1.88	0.56
1:A:378:VAL:HG11	3:A:1002:OGA:O4	2.06	0.56
1:D:83:ARG:HG3	1:D:406:TYR:OH	2.06	0.55
1:A:291:ASN:OD1	1:A:293:LYS:HG2	2.05	0.55
1:C:90:THR:H	1:C:93:GLN:NE2	2.04	0.55
1:C:288:LEU:HD11	1:C:396:LEU:HD22	1.88	0.55
1:B:316:SER:HB2	1:B:391:PHE:HE1	1.71	0.55
1:A:159:LEU:HD21	1:A:223:LEU:HD23	1.88	0.55
1:D:304:ILE:O	1:D:308:TRP:N	2.39	0.55
1:B:84:ARG:NH2	1:D:398:ASP:OD1	2.40	0.55
1:B:17:LEU:HD22	1:B:17:LEU:H	1.73	0.54
1:D:255:PHE:CZ	1:D:317:LEU:HD12	2.43	0.54
1:B:260:PRO:HB3	1:B:309:PHE:CD1	2.43	0.54
1:C:334:GLU:HB2	1:C:407:PRO:CD	2.23	0.54
1:D:254:MET:O	1:D:258:ASP:N	2.37	0.53
1:D:261:ILE:HD12	1:D:261:ILE:H	1.73	0.53
1:C:90:THR:OG1	1:C:93:GLN:HB2	2.08	0.53
1:C:160:ALA:CB	1:C:218:MET:HG3	2.38	0.53
1:D:397:PHE:HB3	1:D:402:VAL:O	2.09	0.53
1:C:406:TYR:CD2	1:C:407:PRO:HD2	2.43	0.53
1:B:86:MET:HE1	1:B:373:LEU:HB2	1.91	0.53
1:B:349:VAL:O	1:B:378:VAL:HG23	2.09	0.53
1:C:278:PHE:CD2	1:C:311:PRO:HG3	2.43	0.53
1:C:235:GLU:OE2	1:D:324:PRO:HB3	2.09	0.52
1:D:83:ARG:HH12	1:D:84:ARG:NH2	2.07	0.52
1:B:99:ASN:O	1:B:103:VAL:HG23	2.09	0.52
1:C:231:PRO:HD2	1:C:234:HIS:HB2	1.91	0.52
1:D:23:ILE:HG22	1:D:264:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:GLU:HA	1:D:380:GLU:OE1	2.09	0.51
1:D:345:TYR:CE1	1:D:385:ARG:HG3	2.45	0.51
1:C:29:VAL:HG21	1:C:51:ILE:HG13	1.92	0.51
1:C:99:ASN:O	1:C:103:VAL:HG23	2.09	0.51
1:C:43:TYR:OH	1:C:45:HIS:HD2	1.94	0.51
1:C:86:MET:HE3	1:C:373:LEU:HD12	1.93	0.51
1:C:334:GLU:OE1	1:C:334:GLU:N	2.40	0.51
1:B:53:ALA:O	1:B:55:PRO:HD3	2.11	0.51
1:C:341:THR:HB	1:C:361:TYR:CZ	2.46	0.51
1:D:64:ALA:O	1:D:67:VAL:HG12	2.11	0.51
1:B:160:ALA:HB1	1:B:218:MET:HB3	1.93	0.50
1:D:135:ILE:HD13	1:D:273:ILE:HG23	1.92	0.50
1:D:312:PHE:CG	1:D:390:HIS:HB3	2.46	0.50
1:D:74:ARG:HD3	1:D:126:ALA:HB2	1.93	0.50
1:D:159:LEU:HD12	1:D:255:PHE:HB2	1.94	0.50
1:A:225:PHE:HB3	1:A:245:LEU:HD11	1.94	0.49
1:C:86:MET:HE3	1:C:373:LEU:CG	2.42	0.49
1:D:274:ASN:OD1	1:D:408:SER:CB	2.60	0.49
1:B:259:ILE:N	1:B:260:PRO:HD3	2.26	0.49
1:C:266:VAL:HG13	1:C:338:ILE:HG21	1.94	0.49
1:D:122:GLU:HB2	1:D:359:TRP:CE3	2.46	0.49
1:D:245:LEU:HD11	1:D:256:LEU:HD13	1.93	0.49
1:D:271:ALA:HB2	1:D:278:PHE:CD2	2.47	0.49
1:C:411:GLN:HB3	1:C:421:LEU:HB2	1.93	0.49
1:D:260:PRO:HD2	1:D:261:ILE:HD12	1.93	0.49
1:D:282:VAL:O	1:D:286:ARG:HB2	2.13	0.49
1:A:406:TYR:CD1	1:A:407:PRO:HD2	2.47	0.49
1:A:129:ILE:HA	1:A:134:HIS:O	2.12	0.48
1:D:274:ASN:OD1	1:D:408:SER:OG	2.22	0.48
1:B:86:MET:CE	1:B:373:LEU:HB2	2.43	0.48
1:D:90:THR:OG1	1:D:93:GLN:HB2	2.13	0.48
1:A:231:PRO:HD2	1:A:234:HIS:HB2	1.95	0.48
1:D:79:PRO:HD3	1:D:111:GLY:HA3	1.95	0.48
1:D:267:GLY:O	1:D:278:PHE:HE2	1.95	0.48
1:C:349:VAL:O	1:C:378:VAL:CG2	2.53	0.48
1:C:17:LEU:HD11	1:C:305:ILE:HG22	1.96	0.48
1:B:246:LYS:HB3	1:B:247:PRO:HD3	1.96	0.48
1:D:77:ARG:N	1:D:113:GLU:OE1	2.36	0.48
1:C:327:ARG:HD3	1:C:372:LYS:O	2.13	0.48
1:C:345:TYR:HE2	1:C:348:GLY:HA3	1.78	0.48
1:C:265:LEU:O	1:C:269:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:HIS:HD2	1:D:45:HIS:O	1.97	0.47
1:D:310:SER:HB3	1:D:312:PHE:HD1	1.79	0.47
1:B:83:ARG:NH1	1:D:406:TYR:HB2	2.29	0.47
1:C:313:SER:HB2	1:C:392:TRP:HA	1.97	0.47
1:B:333:ILE:HA	1:B:372:LYS:HG3	1.97	0.47
1:D:77:ARG:NH1	1:D:133:ASP:OD1	2.47	0.47
1:C:322:ALA:N	1:C:380:GLU:OE1	2.48	0.47
1:D:388:MET:SD	1:D:390:HIS:CE1	3.08	0.47
1:C:312:PHE:CG	1:C:390:HIS:HB3	2.50	0.47
1:B:17:LEU:HD21	1:B:289:TYR:CD2	2.50	0.47
1:C:260:PRO:HB3	1:C:309:PHE:CD1	2.49	0.47
1:A:46:THR:HG21	1:A:51:ILE:HB	1.97	0.46
1:B:87:ARG:HH11	1:B:87:ARG:CG	2.28	0.46
1:C:86:MET:HE3	1:C:373:LEU:HG	1.97	0.46
1:D:87:ARG:HG3	1:D:88:GLU:N	2.29	0.46
1:B:416:ASN:HB2	4:B:1120:HOH:O	2.14	0.46
1:D:315:LEU:HD21	1:D:388:MET:HG3	1.97	0.46
1:D:56:ILE:HG13	1:D:57:LEU:N	2.30	0.46
1:A:76:TYR:HB2	1:A:128:ILE:HG12	1.98	0.46
1:D:121:GLN:OE1	1:D:349:VAL:HG22	2.16	0.46
1:A:246:LYS:HD2	1:A:300:THR:HG21	1.97	0.46
1:D:123:ILE:HD13	1:D:360:THR:HG21	1.98	0.46
1:B:406:TYR:CD1	1:B:407:PRO:HD2	2.51	0.46
1:C:237:GLN:HE21	1:C:296:LYS:NZ	2.14	0.46
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.51	0.45
1:B:406:TYR:CG	1:B:407:PRO:HD2	2.50	0.45
1:C:393:ARG:HA	1:C:393:ARG:HD3	1.75	0.45
1:D:254:MET:HA	1:D:257:SER:HB2	1.97	0.45
1:C:351:VAL:HG22	1:C:358:ARG:HG3	1.96	0.45
1:B:17:LEU:HG	1:B:20:LEU:HD23	1.98	0.45
1:B:393:ARG:HD3	1:B:393:ARG:HA	1.65	0.45
1:C:41:ILE:O	1:C:41:ILE:HG13	2.17	0.45
1:D:45:HIS:O	1:D:45:HIS:CD2	2.69	0.45
1:C:155:ALA:HB2	1:C:258:ASP:HB3	1.99	0.45
1:C:245:LEU:HD23	1:C:304:ILE:HG21	1.98	0.45
1:A:245:LEU:HD21	1:A:256:LEU:HD13	1.99	0.44
1:D:152:ILE:HD11	1:D:262:ALA:HB2	1.99	0.44
1:D:328:ASP:O	1:D:372:LYS:HG3	2.17	0.44
1:B:29:VAL:HG11	1:B:51:ILE:HG21	1.98	0.44
1:B:96:ARG:HA	1:B:96:ARG:HD3	1.83	0.44
1:D:88:GLU:HG3	1:D:104:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:HH12	1:C:324:PRO:CB	2.31	0.44
1:C:347:ASN:OD1	1:C:381:VAL:HG12	2.18	0.44
1:C:17:LEU:C	1:C:17:LEU:CD2	2.85	0.44
1:D:56:ILE:HG13	1:D:57:LEU:H	1.83	0.44
1:D:226:ALA:HB3	1:D:229:TRP:HB2	1.99	0.44
1:D:237:GLN:OE1	1:D:296:LYS:NZ	2.26	0.44
1:D:245:LEU:HB3	1:D:304:ILE:HD11	2.00	0.43
1:C:218:MET:N	1:C:384:GLU:OE1	2.52	0.43
1:A:117:ASP:OD1	1:A:118:HIS:N	2.51	0.43
1:D:307:ILE:O	1:D:309:PHE:HD1	2.01	0.43
1:C:86:MET:HE2	1:C:86:MET:HA	2.00	0.43
1:C:152:ILE:HD11	1:C:262:ALA:HB1	2.01	0.43
1:D:388:MET:SD	1:D:390:HIS:NE2	2.91	0.43
1:A:339:LEU:HD13	3:A:1002:OGA:C4	2.48	0.43
1:B:29:VAL:O	1:B:33:MET:HG3	2.18	0.43
1:C:96:ARG:HH12	1:C:324:PRO:HB2	1.84	0.43
1:D:267:GLY:O	1:D:278:PHE:CE2	2.71	0.43
1:B:278:PHE:O	1:B:282:VAL:HG23	2.19	0.42
1:C:156:VAL:HG21	1:C:386:TYR:CE2	2.54	0.42
1:D:34:ILE:CD1	1:D:65:ALA:HA	2.48	0.42
1:B:87:ARG:HH11	1:B:87:ARG:HG2	1.84	0.42
1:D:304:ILE:HA	1:D:307:ILE:CG2	2.49	0.42
1:D:228:ALA:HB1	1:D:239:PRO:HB2	1.99	0.42
1:D:114:LEU:O	1:D:357:ARG:NH1	2.52	0.42
1:C:79:PRO:HD3	1:C:111:GLY:HA3	2.01	0.42
1:C:235:GLU:OE1	1:C:235:GLU:N	2.33	0.42
1:B:88:GLU:O	1:B:100:ARG:NH2	2.52	0.42
1:D:45:HIS:HE1	1:D:51:ILE:HB	1.85	0.42
1:D:101:GLU:OE2	1:D:327:ARG:NH1	2.46	0.42
1:C:345:TYR:CE1	1:C:385:ARG:HG3	2.54	0.42
1:D:45:HIS:CE1	1:D:51:ILE:HB	2.55	0.42
1:D:280:SER:O	1:D:284:VAL:HG23	2.20	0.42
1:D:292:SER:HA	1:D:298:HIS:CE1	2.55	0.42
1:A:263:SER:HB3	1:A:309:PHE:O	2.20	0.42
1:A:393:ARG:HD3	1:A:393:ARG:HA	1.78	0.42
1:B:328:ASP:OD2	1:B:330:SER:O	2.37	0.42
1:B:96:ARG:HD3	4:B:1109:HOH:O	2.19	0.41
1:D:323:THR:HA	1:D:324:PRO:HD3	1.85	0.41
1:D:299:SER:O	1:D:303:LYS:HG2	2.19	0.41
1:D:313:SER:OG	1:D:392:TRP:HA	2.19	0.41
1:A:86:MET:HG2	1:A:333:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:HB	1:A:378:VAL:HG12	2.02	0.41
1:C:415:THR:HG23	1:C:421:LEU:HB3	2.02	0.41
1:C:263:SER:HB3	1:C:309:PHE:O	2.20	0.41
1:C:345:TYR:HB2	1:C:381:VAL:HB	2.01	0.41
1:C:378:VAL:O	1:C:378:VAL:HG13	2.21	0.41
1:B:17:LEU:CB	1:B:20:LEU:HD23	2.51	0.41
1:D:93:GLN:NE2	1:D:100:ARG:HG3	2.35	0.41
1:A:339:LEU:HD13	3:A:1002:OGA:H4C2	2.03	0.41
1:D:323:THR:OG1	1:D:378:VAL:HG12	2.21	0.41
1:A:110:PRO:HB2	1:A:115:ASN:HB3	2.03	0.41
1:C:397:PHE:HB3	1:C:402:VAL:O	2.20	0.41
1:D:20:LEU:CD1	1:D:22:LEU:H	2.34	0.41
1:D:285:LEU:HD21	1:D:308:TRP:CD1	2.55	0.41
1:D:315:LEU:HD23	1:D:316:SER:N	2.35	0.41
1:A:48:ASN:OD1	1:A:50:SER:HB2	2.20	0.41
1:C:20:LEU:HA	1:C:23:ILE:HG12	2.03	0.41
1:C:96:ARG:NH1	1:C:324:PRO:HB2	2.36	0.41
1:D:107:GLU:HG2	1:D:108:PHE:CE1	2.55	0.41
1:D:268:ALA:O	1:D:272:GLN:HG2	2.21	0.41
1:A:44:ILE:HA	1:A:44:ILE:HD13	1.82	0.40
1:A:266:VAL:HG21	1:A:390:HIS:NE2	2.35	0.40
1:A:333:ILE:CD1	1:A:372:LYS:HE3	2.51	0.40
1:C:227:PRO:O	1:C:301:VAL:HG13	2.21	0.40
1:D:64:ALA:O	1:D:67:VAL:N	2.54	0.40
1:B:218:MET:HG3	1:B:384:GLU:OE1	2.22	0.40
1:C:45:HIS:CE1	1:C:49:ASP:OD1	2.69	0.40
1:A:378:VAL:CG1	3:A:1002:OGA:O4	2.68	0.40
1:B:72:TYR:CE2	1:B:413:SER:HB2	2.56	0.40
1:B:343:GLY:HA3	1:B:384:GLU:O	2.22	0.40
1:D:278:PHE:O	1:D:282:VAL:HG23	2.20	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	343/430 (80%)	328 (96%)	14 (4%)	1 (0%)	41	64
1	B	347/430 (81%)	330 (95%)	14 (4%)	3 (1%)	17	35
1	C	352/430 (82%)	329 (94%)	22 (6%)	1 (0%)	41	64
1	D	330/430 (77%)	305 (92%)	22 (7%)	3 (1%)	17	35
All	All	1372/1720 (80%)	1292 (94%)	72 (5%)	8 (1%)	25	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	VAL
1	D	24	ASP
1	B	419	GLU
1	B	115	ASN
1	D	251	GLU
1	B	259	ILE
1	C	259	ILE
1	A	259	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/362 (81%)	293 (100%)	0	100	100
1	B	296/362 (82%)	291 (98%)	5 (2%)	60	81
1	C	301/362 (83%)	293 (97%)	8 (3%)	44	71
1	D	282/362 (78%)	278 (99%)	4 (1%)	67	85
All	All	1172/1448 (81%)	1155 (98%)	17 (2%)	65	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	PRO
1	B	21	LEU
1	B	87	ARG
1	B	330	SER
1	B	333	ILE
1	C	16	THR
1	C	17	LEU
1	C	218	MET
1	C	219	THR
1	C	358	ARG
1	C	378	VAL
1	C	380	GLU
1	C	381	VAL
1	D	25	GLU
1	D	99	ASN
1	D	380	GLU
1	D	382	ASP

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

Mol	Chain	Res	Type
1	C	45	HIS
1	C	93	GLN
1	C	237	GLN
1	D	45	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OGA	A	1002	2	9,9,9	2.97	5 (55%)	10,11,11	3.30	6 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OGA	A	1002	2	-	3/8/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	OGA	C4-C5	5.72	1.63	1.51
3	A	1002	OGA	C2-N1	4.61	1.41	1.33
3	A	1002	OGA	O3-C5	-3.04	1.20	1.30
3	A	1002	OGA	C4-N1	2.76	1.52	1.45
3	A	1002	OGA	O2-C1	-2.43	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1002	OGA	C4-N1-C2	5.12	129.27	121.25
3	A	1002	OGA	O2'-C2-C1	-5.05	114.20	121.32
3	A	1002	OGA	C5-C4-N1	4.70	127.55	113.06
3	A	1002	OGA	O2-C1-C2	3.55	123.61	113.15
3	A	1002	OGA	O2-C1-O1	-2.93	116.91	123.61
3	A	1002	OGA	O3-C5-O4	-2.71	116.55	123.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

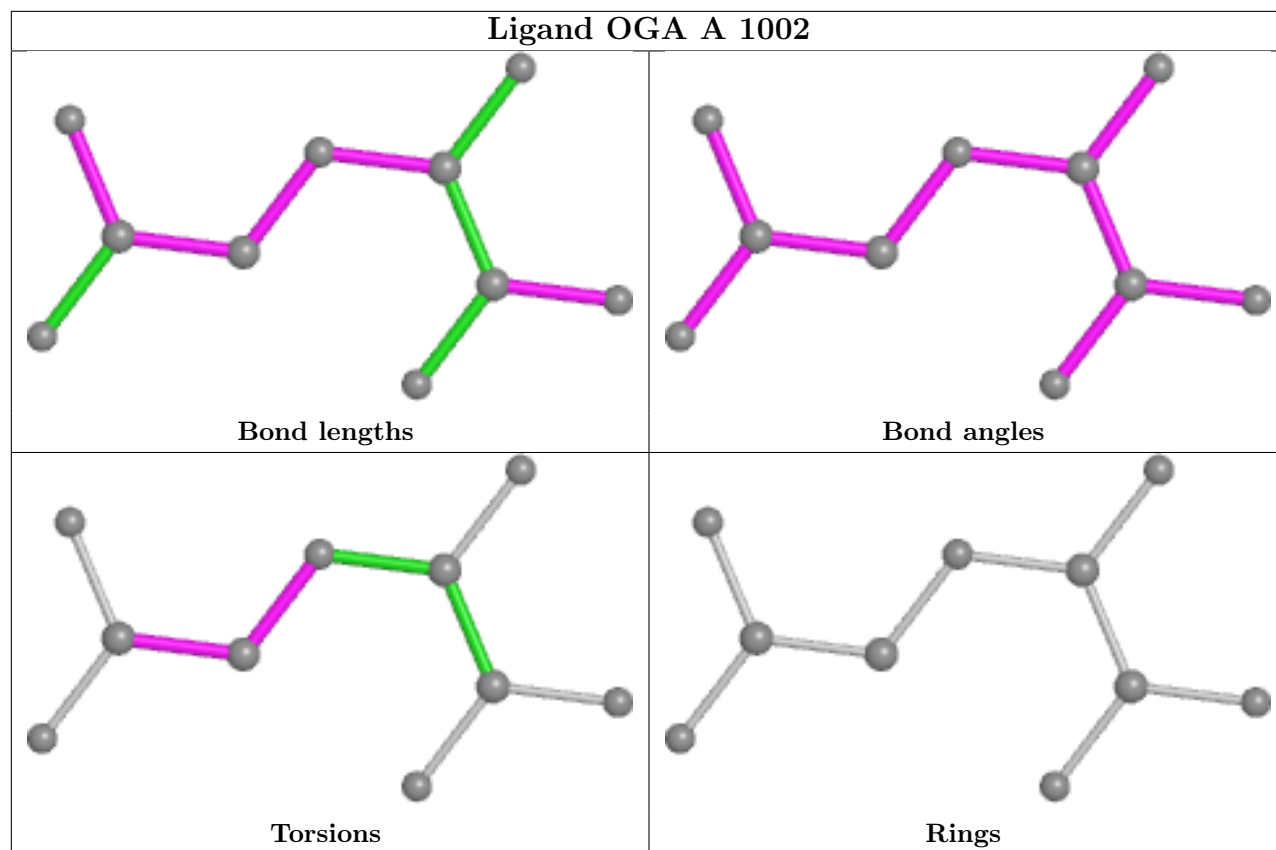
Mol	Chain	Res	Type	Atoms
3	A	1002	OGA	N1-C4-C5-O4
3	A	1002	OGA	N1-C4-C5-O3
3	A	1002	OGA	C5-C4-N1-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	OGA	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	347/430 (80%)	-0.35	0 100 100	20, 37, 67, 92	0
1	B	351/430 (81%)	-0.41	4 (1%) 80 78	21, 35, 75, 103	0
1	C	356/430 (82%)	0.00	14 (3%) 39 32	29, 58, 92, 156	0
1	D	334/430 (77%)	1.56	112 (33%) 0 0	65, 111, 139, 146	0
All	All	1388/1720 (80%)	0.18	130 (9%) 8 5	20, 50, 131, 156	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	GLY	8.1
1	D	60	ALA	7.8
1	D	144	VAL	7.4
1	D	52	LYS	5.9
1	D	53	ALA	5.4
1	D	57	LEU	5.3
1	D	295	THR	5.2
1	D	340	VAL	5.2
1	D	51	ILE	5.0
1	D	148	ILE	5.0
1	D	126	ALA	5.0
1	D	118	HIS	4.9
1	D	259	ILE	4.9
1	D	255	PHE	4.9
1	D	241	PRO	4.9
1	D	294	LEU	4.8
1	D	55	PRO	4.8
1	D	41	ILE	4.7
1	D	256	LEU	4.7
1	D	249	LYS	4.6
1	C	218	MET	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	296	LYS	4.5
1	D	261	ILE	4.5
1	D	150	THR	4.4
1	D	233	GLY	4.4
1	D	116	SER	4.2
1	D	23	ILE	4.2
1	D	386	TYR	4.1
1	B	15	GLU	4.1
1	D	61	LEU	4.1
1	D	300	THR	4.0
1	D	143	CYS	4.0
1	D	48	ASN	4.0
1	C	116	SER	3.9
1	D	49	ASP	3.9
1	D	36	GLY	3.8
1	D	247	PRO	3.8
1	D	292	SER	3.8
1	D	305	ILE	3.7
1	D	58	ARG	3.7
1	D	135	ILE	3.7
1	D	234	HIS	3.5
1	D	289	TYR	3.5
1	D	359	TRP	3.5
1	D	154	ALA	3.5
1	D	262	ALA	3.4
1	D	50	SER	3.3
1	D	56	ILE	3.3
1	D	293	LYS	3.3
1	D	236	ASN	3.3
1	D	62	TRP	3.3
1	D	385	ARG	3.3
1	D	268	ALA	3.2
1	D	39	THR	3.2
1	D	301	VAL	3.2
1	D	286	ARG	3.2
1	D	414	TYR	3.2
1	D	59	THR	3.1
1	D	239	PRO	3.1
1	D	145	SER	3.1
1	D	152	ILE	3.1
1	D	309	PHE	3.0
1	D	156	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	320	ASN	3.0
1	D	37	LEU	3.0
1	C	219	THR	2.9
1	C	16	THR	2.9
1	D	244	THR	2.9
1	D	341	THR	2.9
1	D	254	MET	2.9
1	D	115	ASN	2.8
1	D	388	MET	2.8
1	D	159	LEU	2.8
1	D	231	PRO	2.8
1	D	306	GLU	2.7
1	D	228	ALA	2.7
1	C	118	HIS	2.7
1	D	111	GLY	2.7
1	D	347	ASN	2.7
1	D	230	TRP	2.7
1	D	298	HIS	2.7
1	D	308	TRP	2.7
1	D	350	LEU	2.7
1	D	120	VAL	2.6
1	D	29	VAL	2.6
1	D	138	CYS	2.6
1	D	237	GLN	2.5
1	D	43	TYR	2.5
1	D	140	LEU	2.5
1	D	238	LEU	2.5
1	D	42	PRO	2.5
1	D	110	PRO	2.5
1	D	123	ILE	2.4
1	D	34	ILE	2.4
1	B	92	ARG	2.4
1	C	420	ALA	2.4
1	D	54	ASN	2.4
1	D	32	ARG	2.4
1	D	240	GLY	2.3
1	D	128	ILE	2.3
1	C	382	ASP	2.3
1	D	66	TYR	2.3
1	C	119	PRO	2.3
1	D	149	MET	2.3
1	C	117	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	297	ASP	2.3
1	D	396	LEU	2.3
1	D	310	SER	2.2
1	C	418	PRO	2.2
1	C	292	SER	2.2
1	D	291	ASN	2.2
1	B	93	GLN	2.2
1	D	25	GLU	2.2
1	D	364	GLY	2.2
1	D	243	SER	2.2
1	D	381	VAL	2.2
1	D	288	LEU	2.2
1	D	46	THR	2.2
1	C	247	PRO	2.1
1	D	410	TRP	2.1
1	D	33	MET	2.1
1	D	344	ASN	2.1
1	D	318	ILE	2.1
1	D	28	ALA	2.1
1	D	24	ASP	2.1
1	C	120	VAL	2.1
1	D	225	PHE	2.1
1	C	342	GLY	2.0
1	D	415	THR	2.0
1	B	96	ARG	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](#)

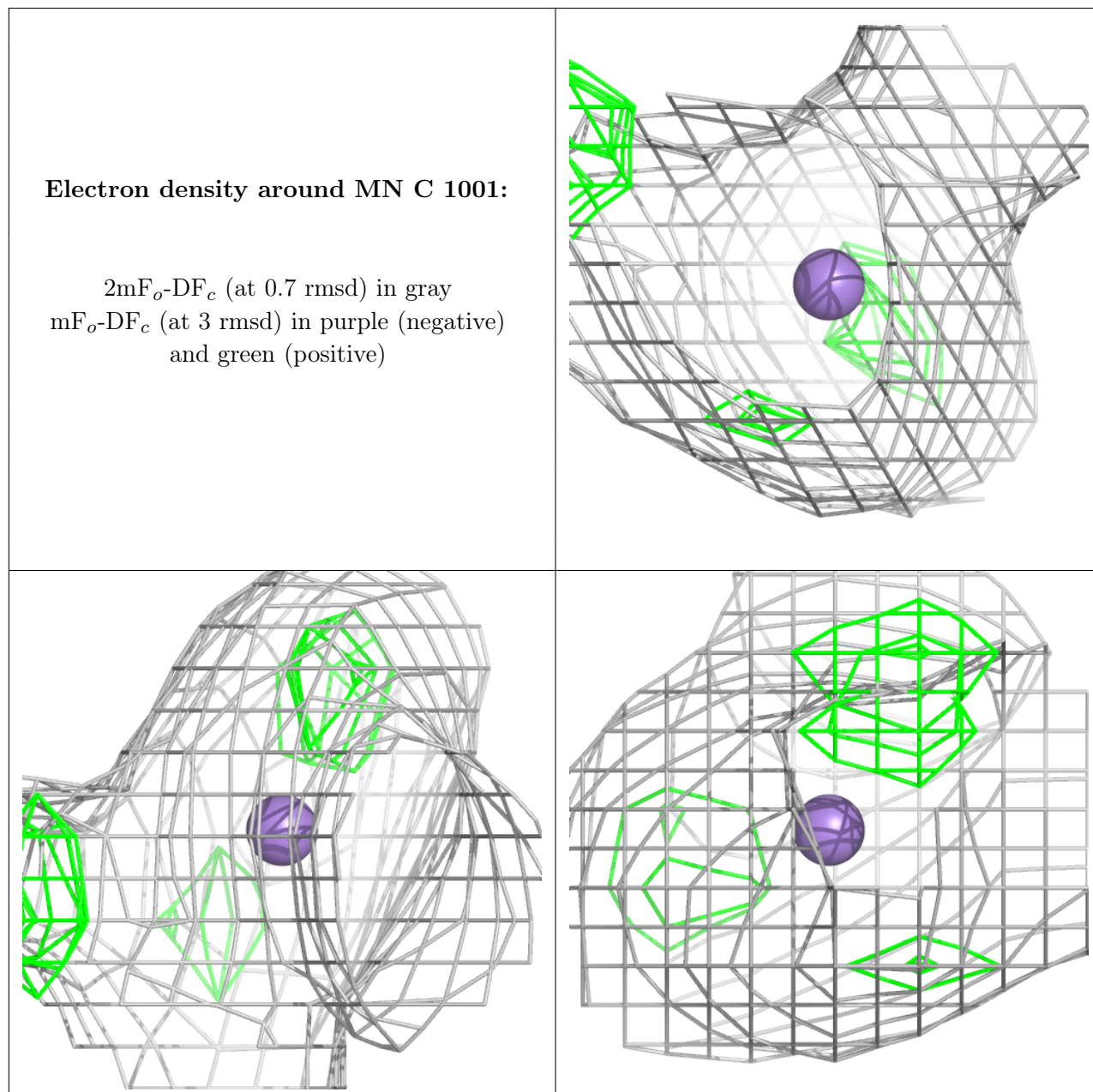
There are no monosaccharides in this entry.

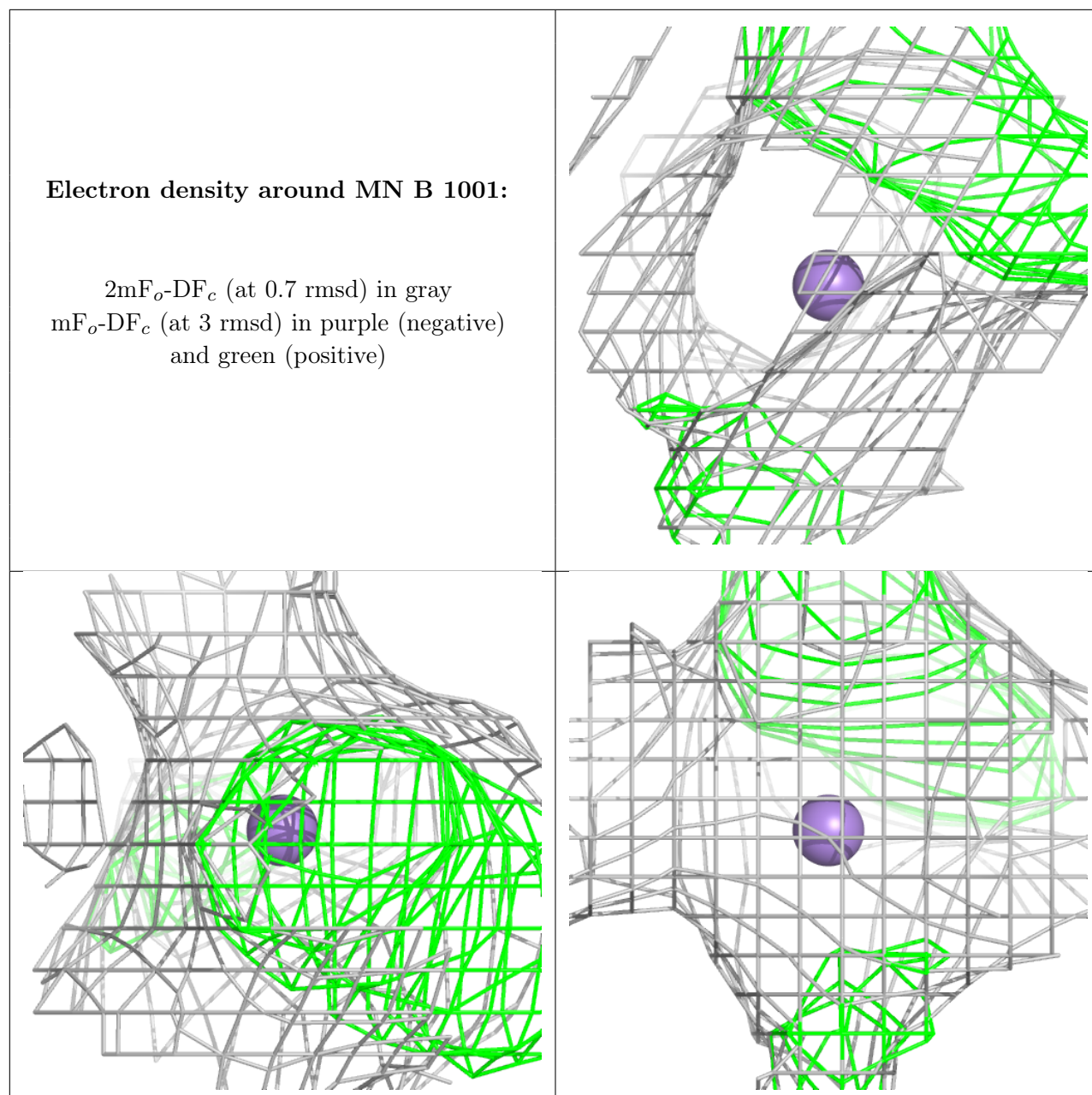
6.4 Ligands [i](#)

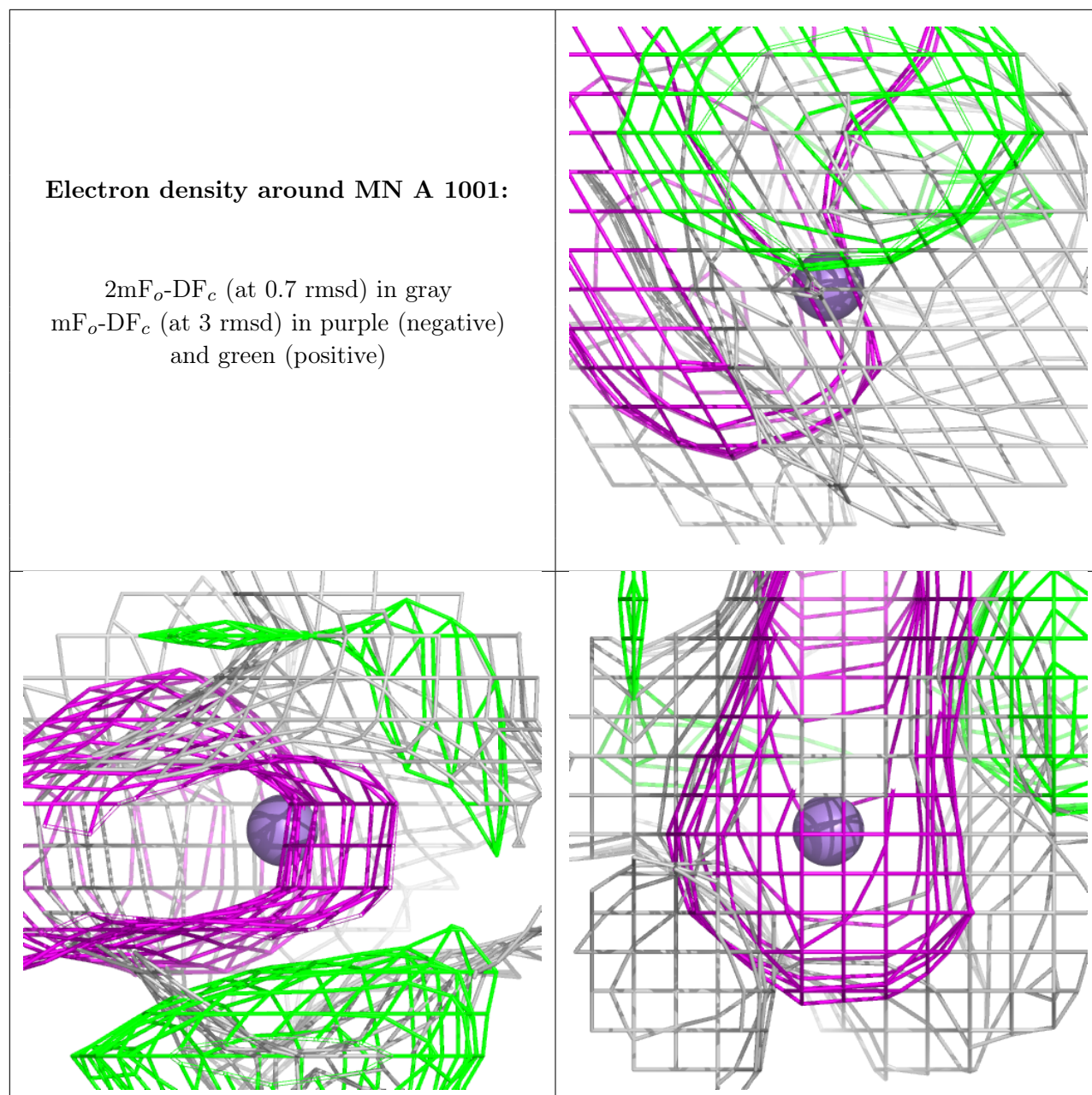
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	C	1001	1/1	0.32	0.17	114,114,114,114	0
2	MN	B	1001	1/1	0.72	0.10	89,89,89,89	0
2	MN	A	1001	1/1	0.81	0.16	59,59,59,59	0
3	OGA	A	1002	10/10	0.84	0.30	13,15,18,20	0
2	MN	D	1001	1/1	0.85	0.23	111,111,111,111	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.

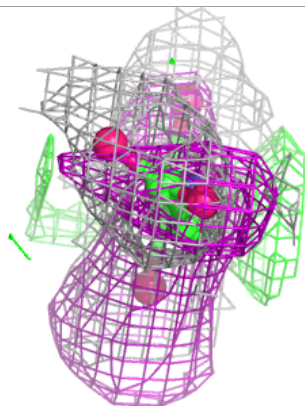
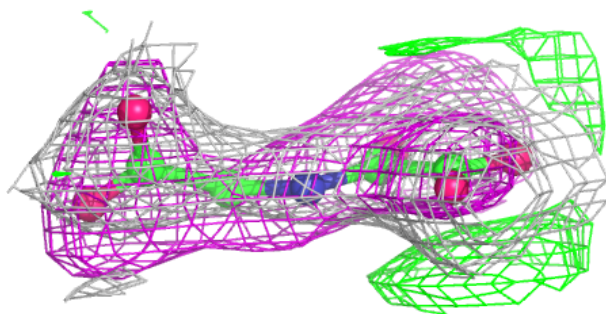
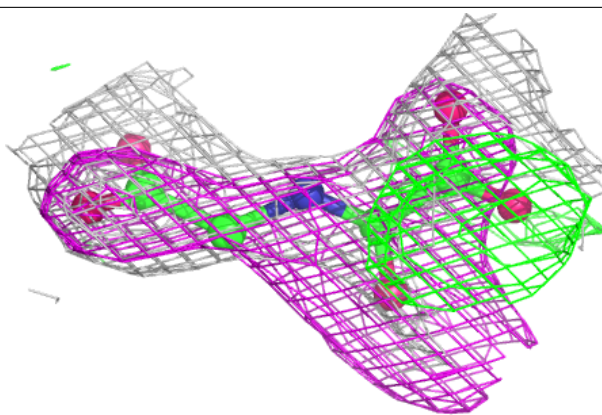


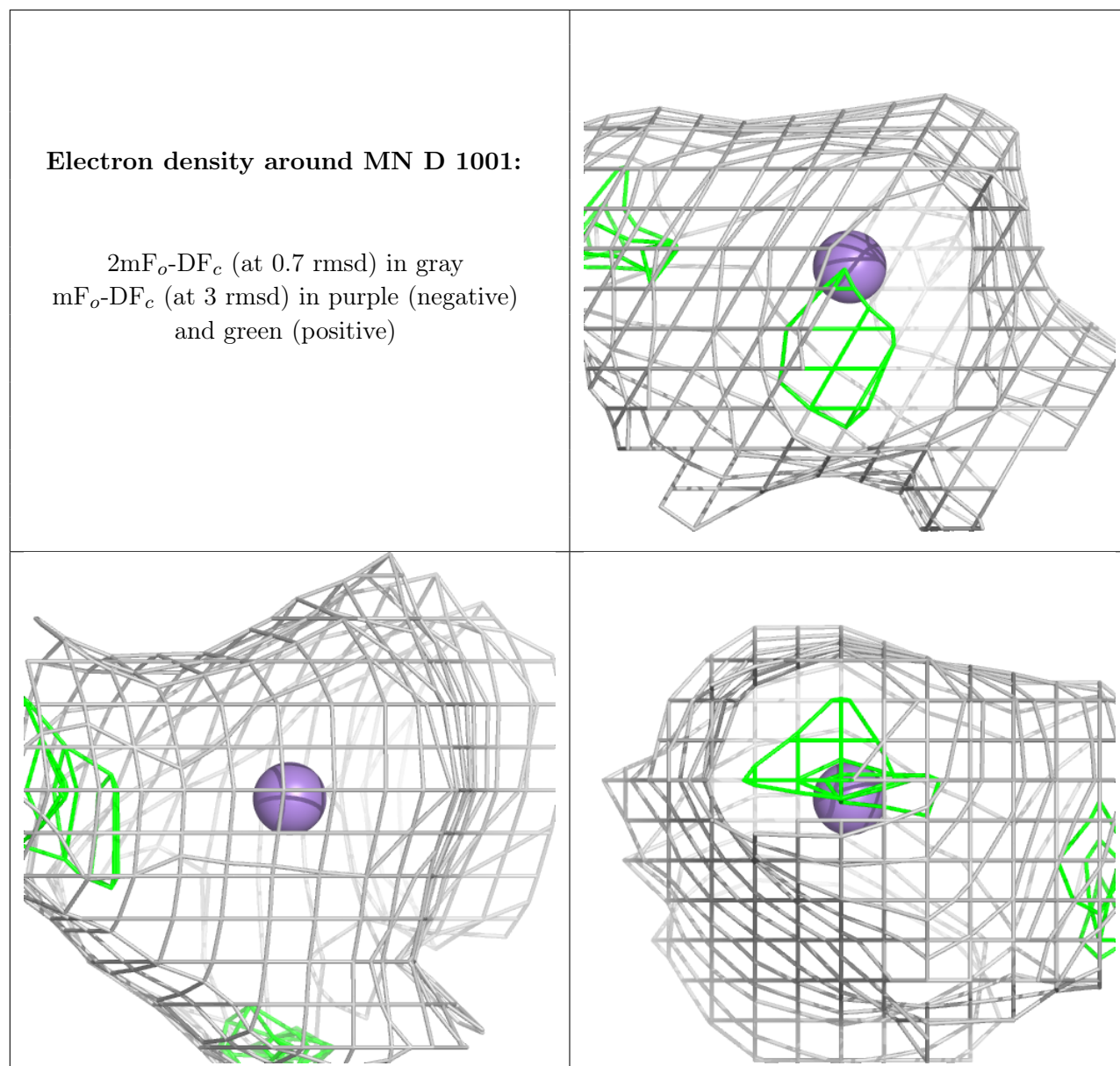




Electron density around OGA A 1002:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.