Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 01:20 PM JST

PDB ID	:	8Z29
Title	:	Crystal structure of apo Aspergillus terreus glutamate dehydrogenase (At-GDH) deletion mutant (T262-A263)
Authors	:	Godsora, B.K.J.; Bhaumik, P.
Deposited on	:	2024-04-12
Resolution	:	2.85 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:

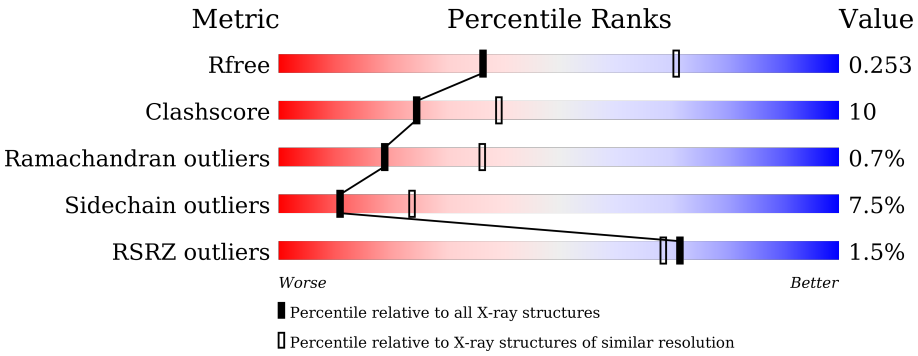
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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

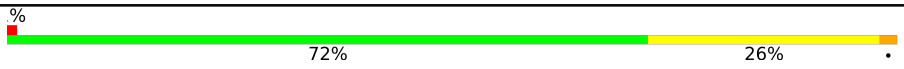
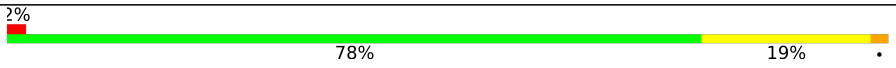
The reported resolution of this entry is 2.85 Å.

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}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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 <=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	458	
1	B	458	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7034 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total 3499	C 2206	N 608	O 671	S 14	0	7	0
1	B	456	Total 3460	C 2183	N 604	O 661	S 12	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP T2D1F5
A	?	-	ALA	deletion	UNP T2D1F5
B	?	-	THR	deletion	UNP T2D1F5
B	?	-	ALA	deletion	UNP T2D1F5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cl 2	0	0
2	B	3	Total 3	Cl 3	0	0

- Molecule 3 is water.

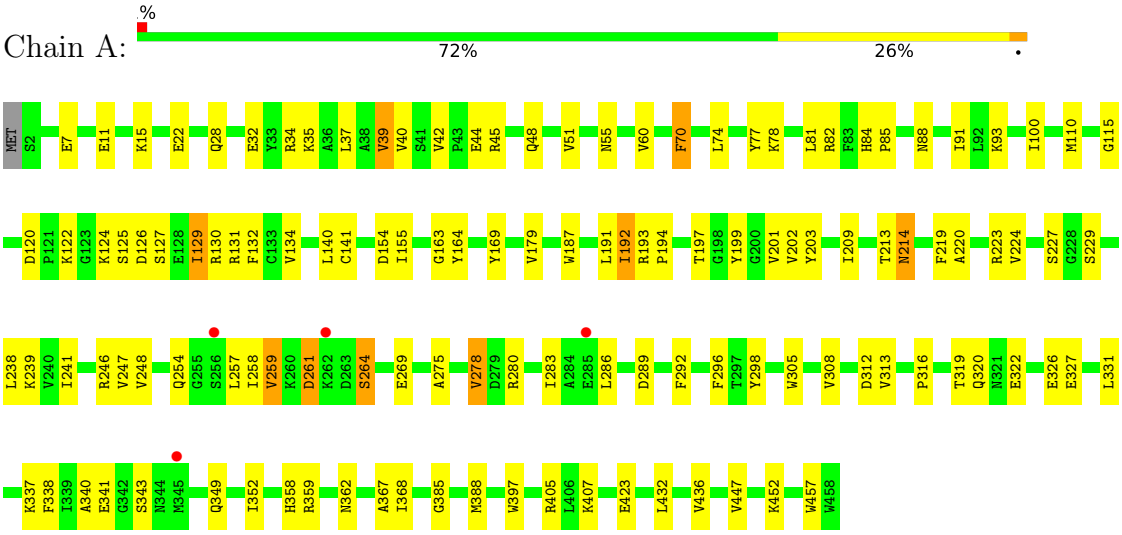
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	33	Total 33	O 33	0	0

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.

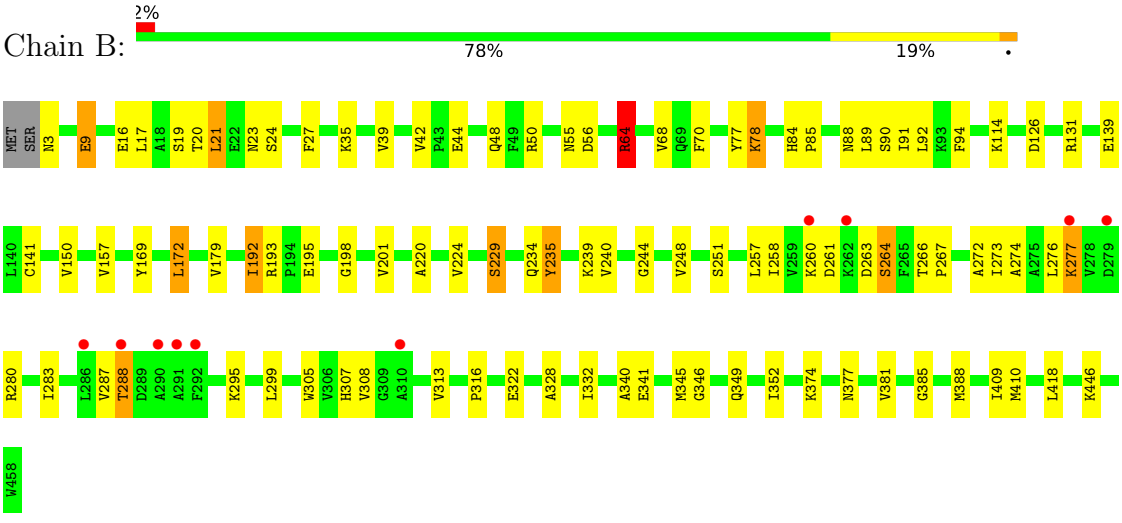
• Molecule 1: Glutamate dehydrogenase

Chain A:



• Molecule 1: Glutamate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	157.55Å 157.55Å 106.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.85) 99.8 (30.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.85Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.190 , 0.230 0.206 , 0.253	Depositor DCC
R_{free} test set	1777 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/3569	0.86	1/4827 (0.0%)
1	B	0.43	0/3530	0.84	2/4775 (0.0%)
All	All	0.43	0/7099	0.85	3/9602 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	235	TYR	CB-CA-C	5.10	120.59	110.40
1	B	64	ARG	CD-NE-CZ	5.09	130.73	123.60

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	3499	0	3430	72	0
1	B	3460	0	3399	63	0
2	A	2	0	0	1	0
2	B	3	0	0	0	0
3	A	37	0	0	6	0
3	B	33	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7034	0	6829	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 10.

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:B:44:GLU:OE2	1:B:77:TYR:OH	1.99	0.81
1:B:224:VAL:HG11	1:B:240:VAL:HG11	1.64	0.79
2:A:501:CL:CL	3:A:625:HOH:O	2.41	0.76
1:A:259:VAL:HG13	1:A:261:ASP:H	1.51	0.75
1:B:257:LEU:HD12	1:B:283:ILE:HG12	1.71	0.72
1:B:381:VAL:HG13	3:B:607:HOH:O	1.90	0.70
1:A:359:ARG:NE	1:A:432:LEU:O	2.25	0.70
1:B:9:GLU:OE1	1:B:90:SER:OG	2.08	0.68
1:B:287:VAL:O	1:B:288:THR:HG22	1.96	0.65
1:B:9:GLU:H	1:B:9:GLU:CD	2.00	0.65
1:B:78:LYS:HG2	1:B:388:MET:HE1	1.79	0.65
1:A:124:LYS:HB2	1:A:129:ILE:HD11	1.79	0.64
1:A:385:GLY:HA2	1:A:388:MET:HE3	1.80	0.62
1:B:234:GLN:OE1	1:B:274:ALA:HB2	1.98	0.62
1:B:258:ILE:HG21	1:B:307:HIS:O	2.01	0.61
1:A:169:TYR:CD2	1:A:179:VAL:HG11	2.35	0.61
1:A:257:LEU:HD12	1:A:283:ILE:CG2	2.31	0.61
1:A:7:GLU:OE1	1:A:93:LYS:NZ	2.33	0.61
1:A:341:GLU:HB3	1:A:343:SER:O	2.00	0.61
1:A:35:LYS:O	1:A:39:VAL:HG13	2.01	0.60
1:A:220:ALA:HB3	3:A:612:HOH:O	2.02	0.59
1:B:261:ASP:HB3	1:B:295:LYS:HA	1.85	0.59
1:A:44:GLU:OE2	1:A:77:TYR:OH	2.11	0.58
1:A:193:ARG:HB3	1:A:194:PRO:HD3	1.87	0.56
1:B:84:HIS:CG	1:B:85:PRO:HD2	2.40	0.56
1:A:327:GLU:O	1:A:331:LEU:HG	2.07	0.55
1:A:192:ILE:O	1:A:192:ILE:HG22	2.05	0.55
1:A:124:LYS:HB2	1:A:129:ILE:CD1	2.36	0.55
1:A:22:GLU:CD	1:A:34:ARG:HH21	2.10	0.54
1:A:257:LEU:HD12	1:A:283:ILE:HG22	1.89	0.54
1:A:452:LYS:HD3	1:A:457:TRP:CH2	2.42	0.54
1:A:78:LYS:HE2	1:A:388:MET:CE	2.39	0.53
1:A:45:ARG:HD3	1:B:139:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.22	0.53
1:A:238:LEU:HA	1:A:241:ILE:HD12	1.92	0.52
1:A:55:ASN:OD1	1:A:55:ASN:C	2.47	0.52
1:A:84:HIS:CG	1:A:85:PRO:HD2	2.45	0.52
1:A:209:ILE:HA	1:A:338:PHE:CZ	2.44	0.52
1:B:78:LYS:HD3	1:B:150:VAL:O	2.10	0.52
1:A:22:GLU:OE2	1:A:34:ARG:NH2	2.43	0.52
1:A:423[A]:GLU:HA	1:A:423[A]:GLU:OE1	2.09	0.51
1:A:367:ALA:HB2	3:A:615:HOH:O	2.09	0.51
1:A:367:ALA:CB	3:A:615:HOH:O	2.58	0.51
1:B:21:LEU:HB3	1:B:27:PHE:CE2	2.46	0.51
1:B:56:ASP:OD2	1:B:131:ARG:NH2	2.40	0.51
1:A:275:ALA:O	1:A:278:VAL:O	2.29	0.51
1:B:195:GLU:HB3	1:B:235:TYR:CG	2.46	0.50
1:A:163:GLY:HA2	1:A:187:TRP:CH2	2.46	0.50
1:B:328:ALA:O	1:B:332:ILE:HG13	2.11	0.50
1:A:42:VAL:O	1:B:50:ARG:HD3	2.10	0.50
1:B:374:LYS:NZ	3:B:601:HOH:O	2.34	0.50
1:B:229:SER:HB2	1:B:277:LYS:HD3	1.91	0.50
1:A:88:ASN:OD1	1:A:91:ILE:HG13	2.11	0.49
1:A:82:ARG:HA	1:A:155:ILE:O	2.12	0.49
1:B:409:ILE:HG22	1:B:410:MET:HE3	1.94	0.49
1:A:227:SER:OG	1:A:322:GLU:OE2	2.27	0.49
1:A:257:LEU:HD23	1:A:258:ILE:N	2.28	0.49
1:A:312:ASP:OD1	1:A:337:LYS:NZ	2.45	0.49
1:B:192:ILE:HG22	1:B:192:ILE:O	2.12	0.49
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.78	0.49
1:A:224:VAL:HG22	1:A:313:VAL:HB	1.95	0.49
1:B:84:HIS:CD2	1:B:85:PRO:HD2	2.48	0.49
1:A:78:LYS:HE2	1:A:388:MET:HE2	1.94	0.48
1:A:358:HIS:CE1	1:A:362:ASN:OD1	2.67	0.48
1:B:9:GLU:OE1	1:B:9:GLU:N	2.42	0.48
1:A:397:TRP:CZ3	1:A:405:ARG:HD2	2.50	0.47
1:B:193[A]:ARG:NE	3:B:604:HOH:O	2.44	0.47
1:B:48:GLN:NE2	1:B:89:LEU:HD22	2.29	0.47
1:B:409:ILE:HG22	1:B:410:MET:CE	2.45	0.46
1:B:264:SER:O	1:B:295:LYS:NZ	2.37	0.46
1:A:126:ASP:CG	1:A:164:TYR:HH	2.19	0.46
1:A:74:LEU:CD1	1:A:447:VAL:HG22	2.45	0.45
1:A:202:VAL:HG21	1:A:239:LYS:HB3	1.98	0.45
1:B:198:GLY:O	1:B:201:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:HG11	1:A:132:PHE:CE1	2.52	0.45
1:B:50:ARG:NH1	3:B:606:HOH:O	2.49	0.45
1:B:277:LYS:HE3	1:B:277:LYS:HA	1.99	0.45
1:B:345:MET:HA	3:B:616:HOH:O	2.16	0.45
1:A:120:ASP:OD2	1:A:122:LYS:HG2	2.17	0.45
1:A:316:PRO:HD2	1:A:340:ALA:O	2.17	0.45
1:B:341:GLU:O	1:B:377:ASN:HB3	2.17	0.45
1:B:17:LEU:O	1:B:20:THR:OG1	2.32	0.45
1:A:70:PHE:HB3	1:A:100:ILE:HD11	1.99	0.44
1:A:257:LEU:HD21	1:A:296:PHE:HB3	1.98	0.44
1:A:199:TYR:CG	1:A:239:LYS:HE3	2.52	0.44
1:A:275:ALA:HA	1:A:278:VAL:HG12	1.98	0.44
1:B:224:VAL:HA	1:B:313:VAL:O	2.17	0.44
1:A:224:VAL:HA	1:A:313:VAL:O	2.17	0.44
1:A:259:VAL:HG13	1:A:261:ASP:N	2.27	0.44
1:A:213:THR:O	1:A:214:ASN:C	2.56	0.44
1:B:349:GLN:HA	1:B:352:ILE:HD12	1.99	0.44
1:A:197:THR:O	1:A:201:VAL:HG23	2.18	0.44
1:A:126:ASP:OD1	1:A:164:TYR:OH	2.29	0.44
1:B:78:LYS:CG	1:B:388:MET:HE1	2.47	0.44
1:B:55:ASN:C	1:B:55:ASN:OD1	2.56	0.43
1:A:203:TYR:CD2	1:A:407:LYS:HG3	2.53	0.43
1:B:273:ILE:HA	1:B:276:LEU:HD12	2.00	0.43
1:A:78:LYS:HG2	1:A:110:MET:SD	2.59	0.43
1:B:272:ALA:O	1:B:276:LEU:HG	2.19	0.43
1:A:122:LYS:HE3	3:A:623:HOH:O	2.18	0.42
1:A:74:LEU:HD11	1:A:447:VAL:HG22	2.00	0.42
1:B:88:ASN:OD1	1:B:91:ILE:HG13	2.19	0.42
1:B:229:SER:OG	1:B:251:SER:O	2.37	0.42
1:A:254:GLN:O	1:A:298:TYR:OH	2.37	0.42
1:A:349:GLN:HA	1:A:352:ILE:HD12	2.01	0.42
1:A:229:SER:N	3:A:601:HOH:O	2.38	0.42
1:B:220:ALA:HA	1:B:244:GLY:O	2.18	0.42
1:B:266:THR:CG2	1:B:267:PRO:HD2	2.50	0.42
1:A:37:LEU:HA	1:A:40:VAL:HG12	2.01	0.41
1:B:94:PHE:CZ	1:B:345:MET:SD	3.13	0.41
1:A:337:LYS:HA	1:A:368:ILE:HA	2.02	0.41
1:B:224:VAL:O	1:B:224:VAL:HG13	2.20	0.41
1:A:224:VAL:O	1:A:248:VAL:HG12	2.20	0.41
1:B:322:GLU:N	1:B:346:GLY:O	2.53	0.41
1:A:246:ARG:HA	1:A:264:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TRP:HA	1:A:305:TRP:CE3	2.56	0.41
1:B:224:VAL:HG23	1:B:313:VAL:HB	2.02	0.41
1:B:287:VAL:O	1:B:288:THR:CG2	2.66	0.41
1:A:81:LEU:HA	1:A:115:GLY:O	2.21	0.41
1:B:68:VAL:N	1:B:114:LYS:O	2.47	0.41
1:B:193[A]:ARG:HD3	3:B:604:HOH:O	2.21	0.41
1:B:316:PRO:HD2	1:B:340:ALA:O	2.21	0.41
1:B:385:GLY:O	1:B:388:MET:HB2	2.21	0.41
1:A:127:SER:OG	1:A:130:ARG:NH2	2.54	0.41
1:A:140:LEU:O	1:A:141:CYS:C	2.59	0.41
1:A:269:GLU:HG2	1:A:292:PHE:CE1	2.56	0.41
1:B:126:ASP:HB2	3:B:613:HOH:O	2.20	0.41
1:B:305:TRP:HA	1:B:305:TRP:CE3	2.56	0.41
1:A:130:ARG:O	1:A:134:VAL:HG23	2.21	0.41
1:B:172:LEU:HA	1:B:172:LEU:HD12	1.86	0.40
1:B:35:LYS:O	1:B:39:VAL:HG23	2.22	0.40
1:B:169:TYR:CD2	1:B:179:VAL:HG11	2.57	0.40
1:B:287:VAL:O	1:B:288:THR:CB	2.70	0.40
1:B:220:ALA:HA	1:B:244:GLY:C	2.42	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	462/458 (101%)	432 (94%)	26 (6%)	4 (1%)	14	29
1	B	456/458 (100%)	434 (95%)	20 (4%)	2 (0%)	30	49
All	All	918/916 (100%)	866 (94%)	46 (5%)	6 (1%)	19	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	192	ILE
1	A	154	ASP
1	B	23	ASN
1	A	214	ASN
1	A	28	GLN

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	356/350 (102%)	330 (93%)	26 (7%)	11	24
1	B	350/350 (100%)	323 (92%)	27 (8%)	10	22
All	All	706/700 (101%)	653 (92%)	53 (8%)	11	24

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	15	LYS
1	A	32	GLU
1	A	39	VAL
1	A	48	GLN
1	A	60	VAL
1	A	70	PHE
1	A	125	SER
1	A	129	ILE
1	A	191	LEU
1	A	219	PHE
1	A	223	ARG
1	A	247	VAL
1	A	259	VAL
1	A	261	ASP
1	A	264	SER
1	A	278	VAL
1	A	280	ARG

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Mol	Chain	Res	Type
1	A	286	LEU
1	A	289	ASP
1	A	308[A]	VAL
1	A	308[B]	VAL
1	A	319	THR
1	A	320	GLN
1	A	326	GLU
1	A	436	VAL
1	B	3	ASN
1	B	9	GLU
1	B	16	GLU
1	B	19	SER
1	B	21	LEU
1	B	24	SER
1	B	42	VAL
1	B	64	ARG
1	B	70	PHE
1	B	78	LYS
1	B	92	LEU
1	B	141	CYS
1	B	157	VAL
1	B	172	LEU
1	B	229	SER
1	B	239	LYS
1	B	248	VAL
1	B	260	LYS
1	B	263	ASP
1	B	264	SER
1	B	277	LYS
1	B	280	ARG
1	B	288	THR
1	B	299	LEU
1	B	308	VAL
1	B	418	LEU
1	B	446	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	214	ASN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	329	GLN
1	B	23	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	457/458 (99%)	-0.28	4 (0%)	81	79	12, 33, 61, 91	7 (1%)
1	B	456/458 (99%)	-0.24	10 (2%)	62	59	15, 32, 64, 117	2 (0%)
All	All	913/916 (99%)	-0.26	14 (1%)	71	68	12, 32, 63, 117	9 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	THR	4.3
1	A	345[A]	MET	3.5
1	B	290	ALA	3.5
1	B	310	ALA	3.0
1	B	286	LEU	2.8
1	B	291	ALA	2.8
1	B	262	LYS	2.6
1	A	262	LYS	2.6
1	B	260	LYS	2.4
1	B	277	LYS	2.3
1	A	256	SER	2.3
1	B	292	PHE	2.2
1	B	279	ASP	2.2
1	A	285	GLU	2.1

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

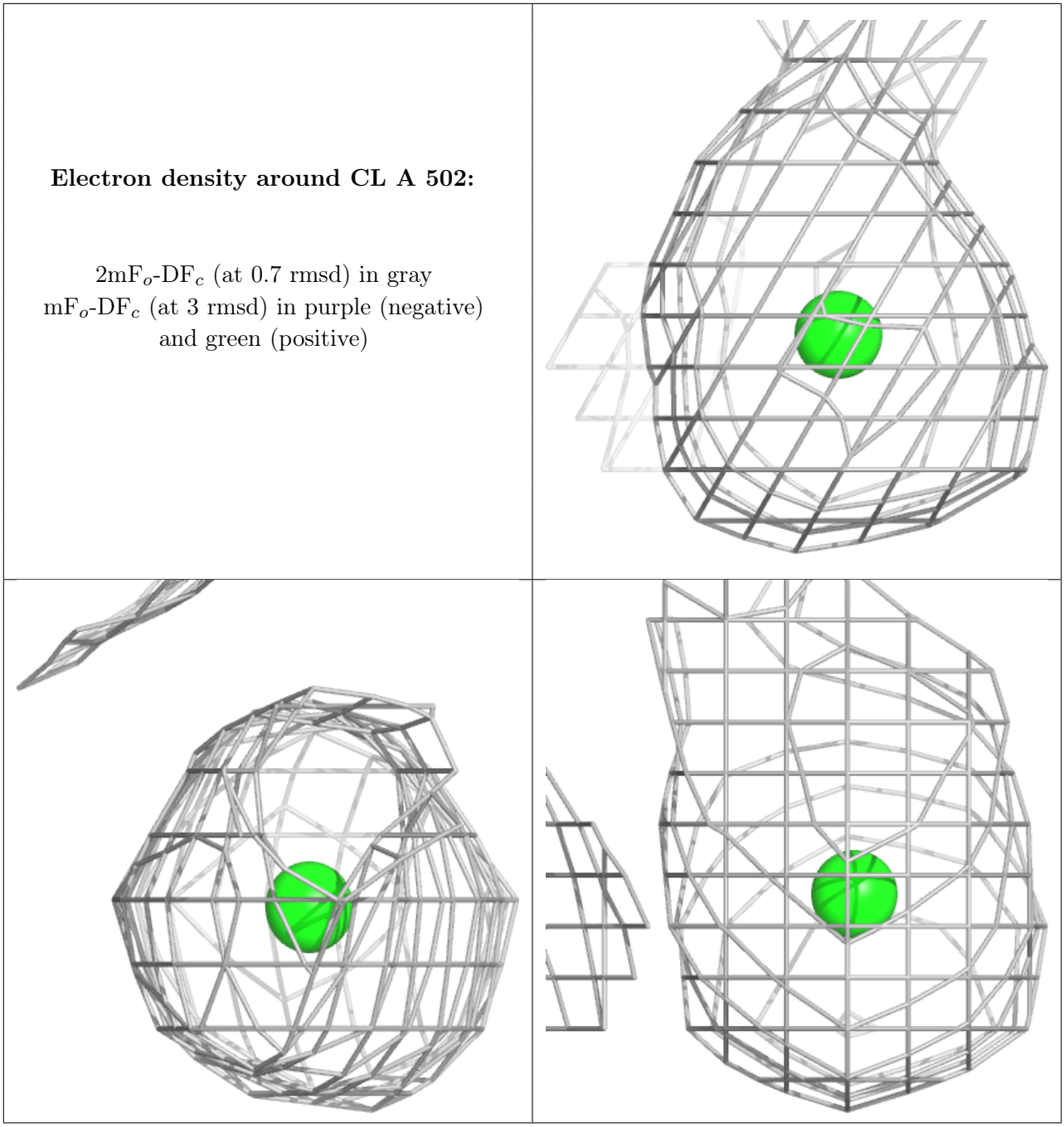
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	CL	A	502	1/1	0.96	0.06	38,38,38,38	0
2	CL	B	501	1/1	0.96	0.06	52,52,52,52	0
2	CL	B	503	1/1	0.96	0.08	46,46,46,46	0
2	CL	B	502	1/1	0.97	0.08	48,48,48,48	0
2	CL	A	501	1/1	0.98	0.10	50,50,50,50	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.

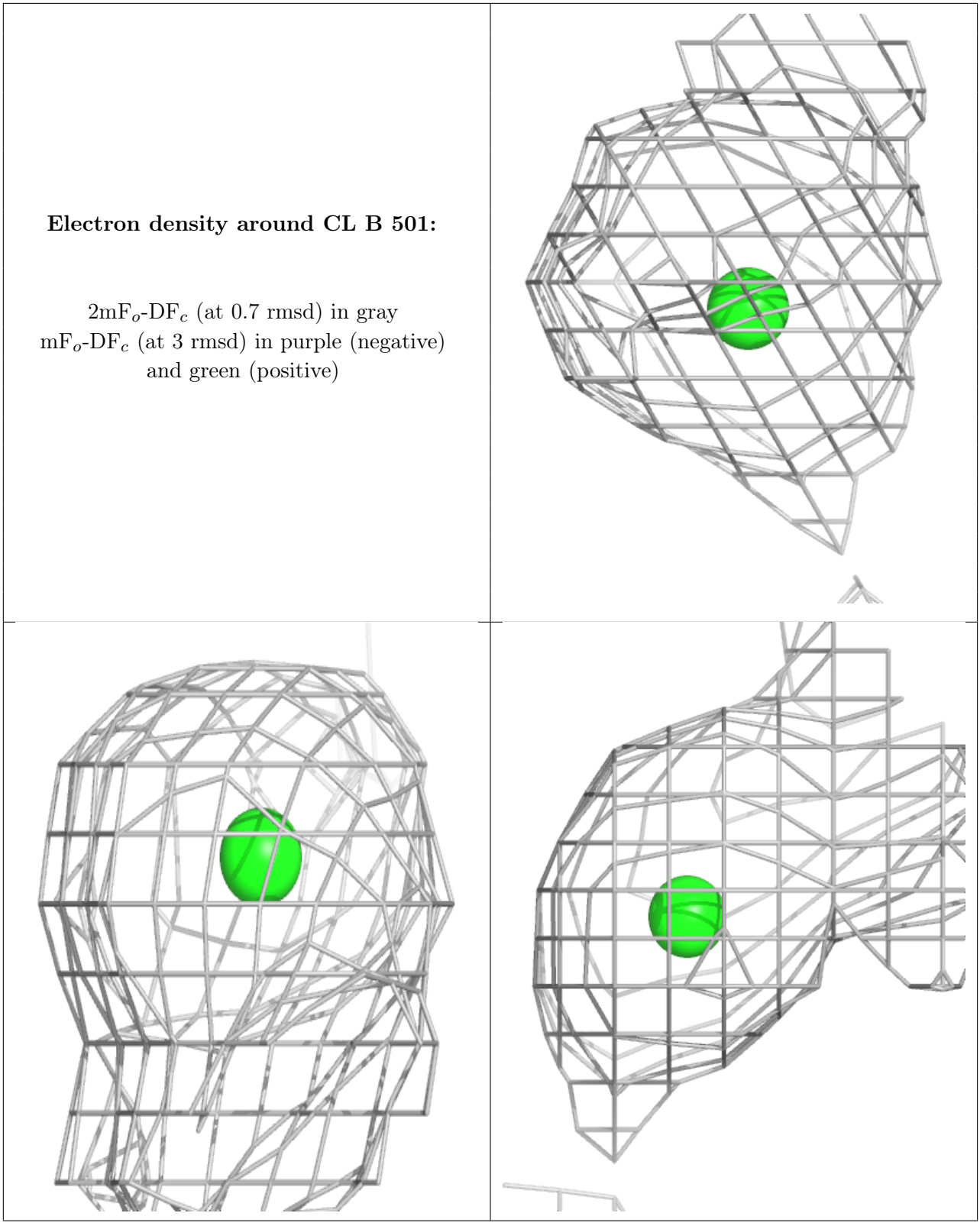
Electron density around CL A 502:

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



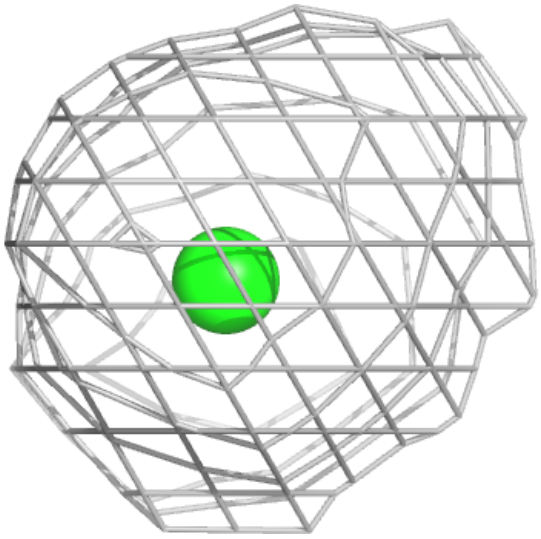
Electron density around CL B 501:

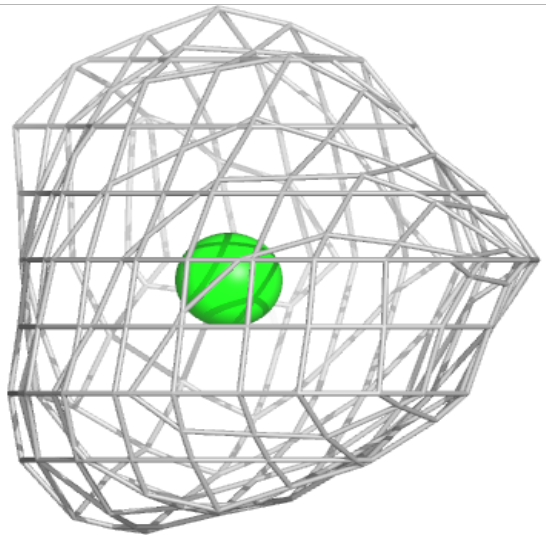
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

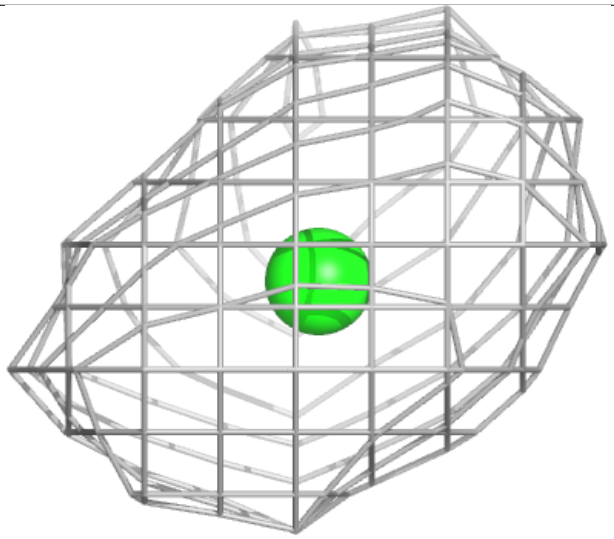


Electron density around CL B 503:

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

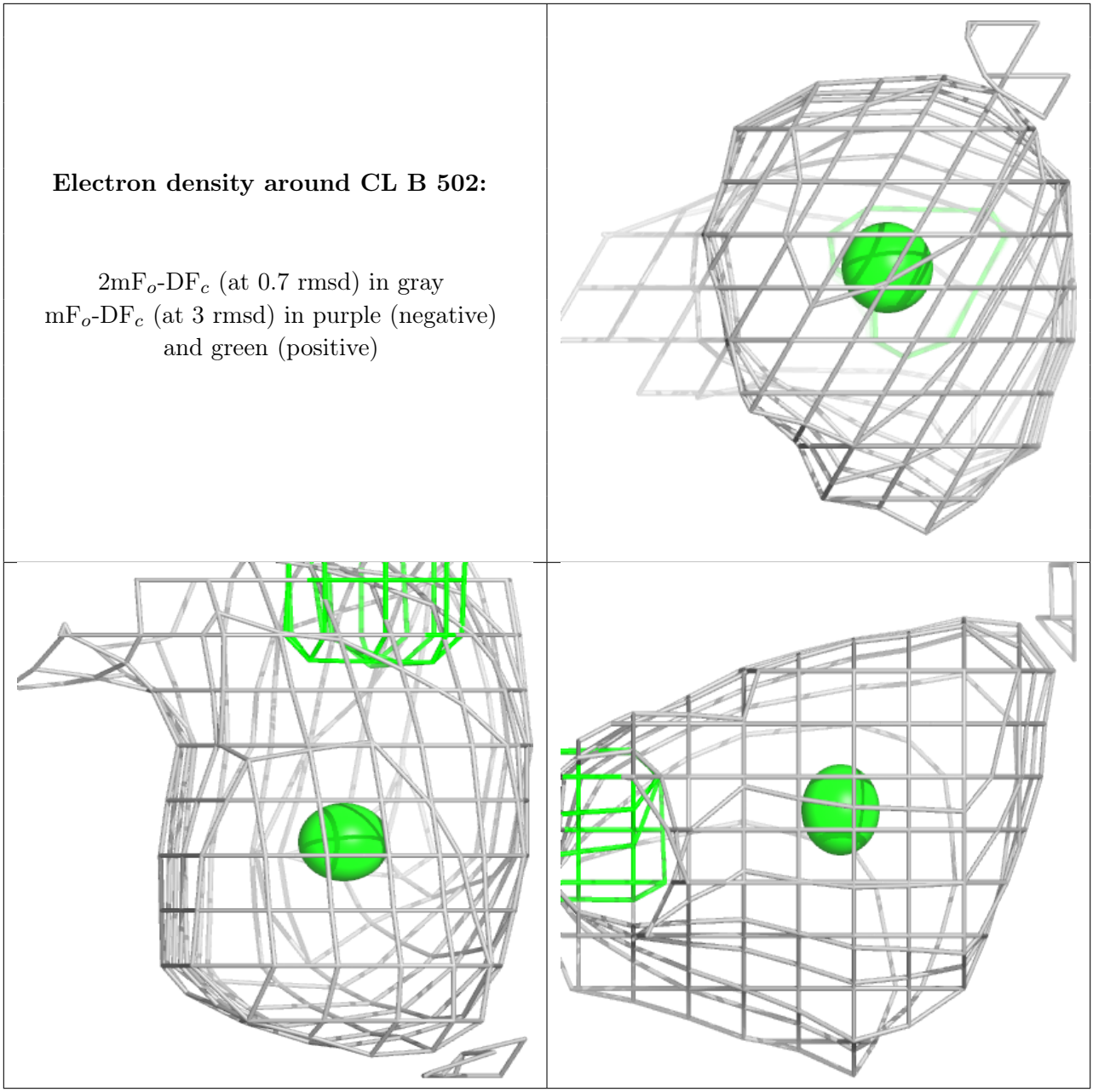






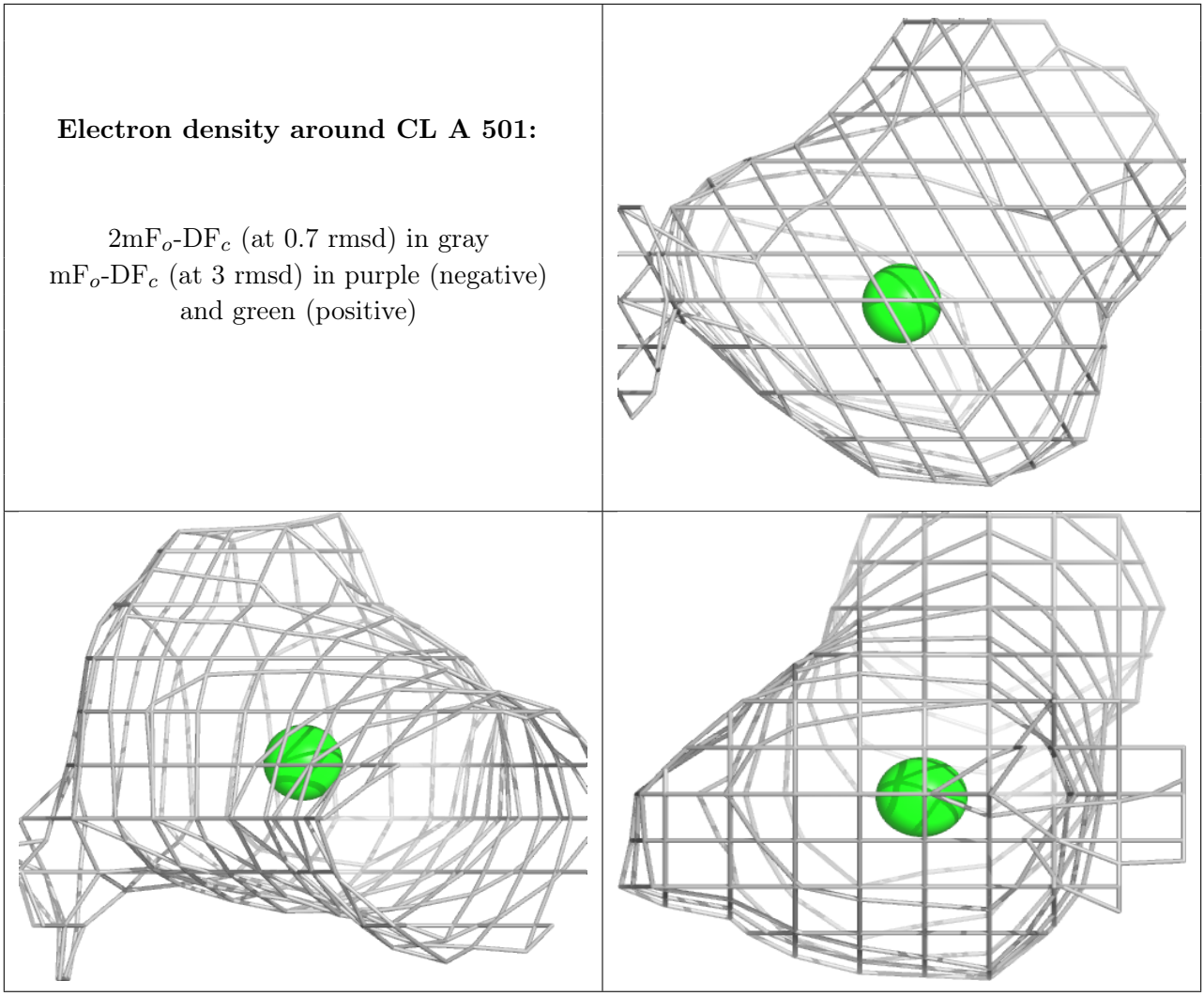
Electron density around CL B 502:

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



Electron density around CL 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)



6.5 Other polymers

There are no such residues in this entry.