Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2020 – 07:44 PM BST

PDB ID	:	6ZLZ
Title	:	Crystal Structure of Merkel Cell Polyomavirus Virus-like Particle
Authors	:	Bayer, N.J.; Stehle, T.; Blaum, B.S.
Deposited on	:	2020-07-01
Resolution	:	3.52 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

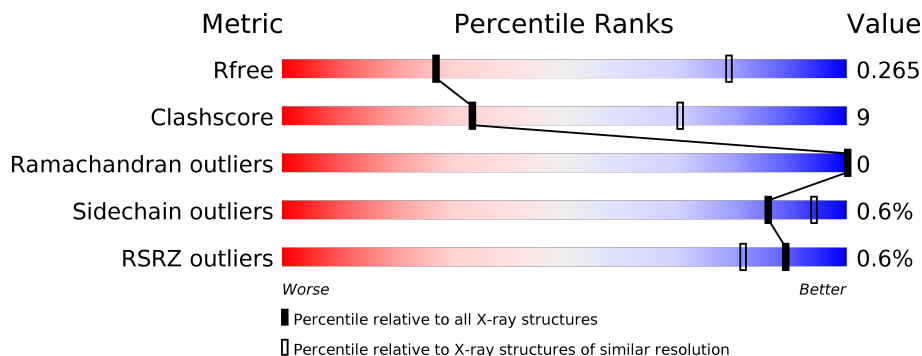|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.52 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		0.6%

Worse ← → Better

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	423	68% 17% 15%
1	B	423	% 69% 19% 12%
1	C	423	% 68% 17% 15%
1	D	423	% 66% 16% 18%
1	E	423	% 68% 17% 14%
1	F	423	69% 16% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16324 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 Capsid protein VP1.

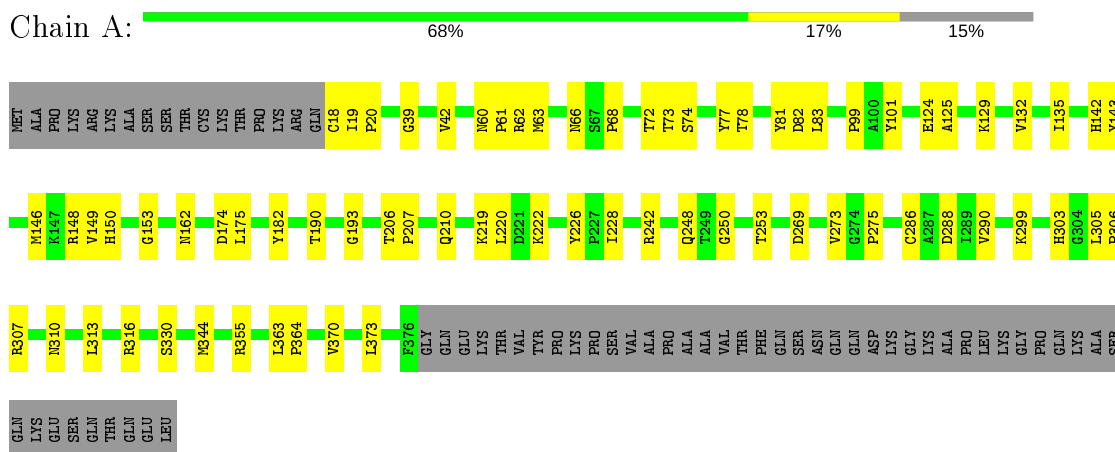| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2728	1739	446	527	16			
1	B	371	Total	C	N	O	S	0	0	0
			2800	1783	460	542	15			
1	C	360	Total	C	N	O	S	0	0	0
			2728	1742	447	523	16			
1	D	346	Total	C	N	O	S	0	0	0
			2623	1671	431	506	15			
1	E	362	Total	C	N	O	S	0	0	0
			2749	1756	449	531	13			
1	F	358	Total	C	N	O	S	0	0	0
			2690	1714	442	520	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

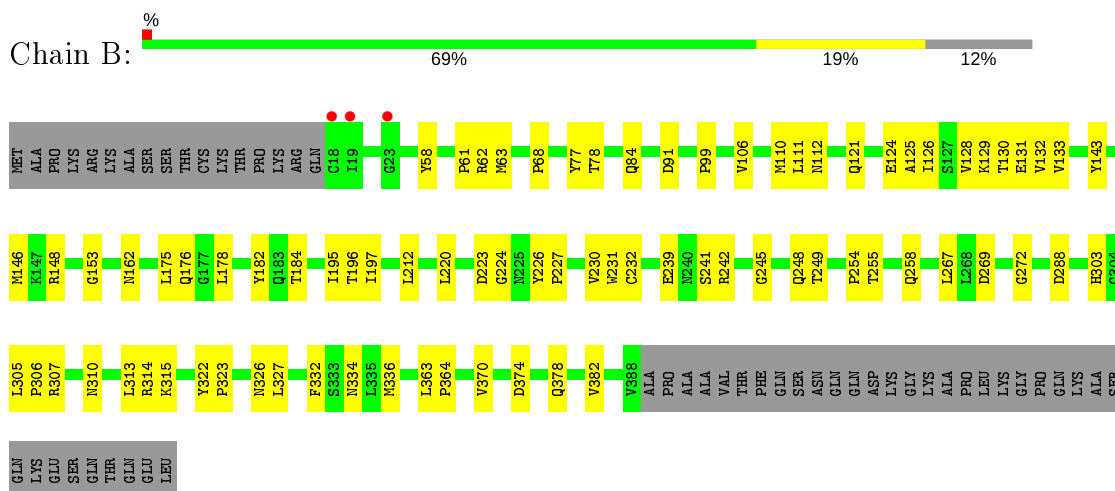| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	0
			2	2		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		

3 Residue-property plots ⓘ

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.
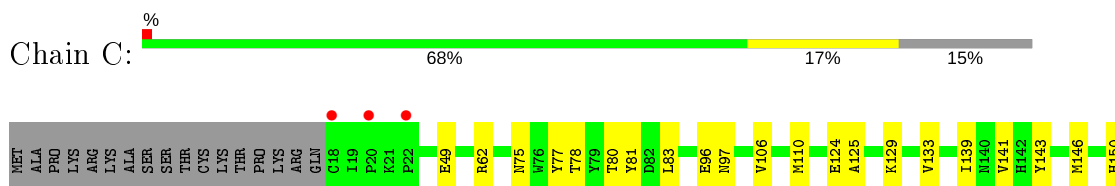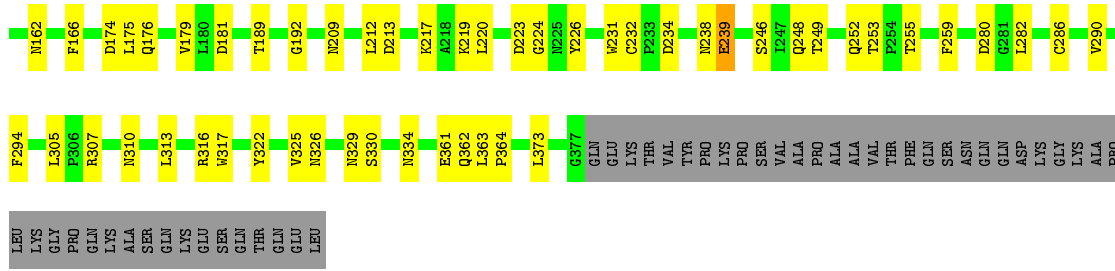
- Molecule 1: Capsid protein VP1
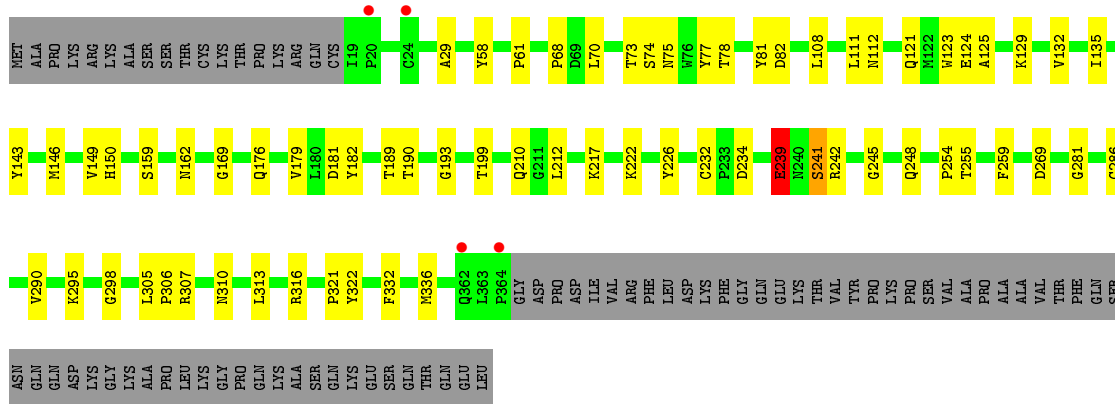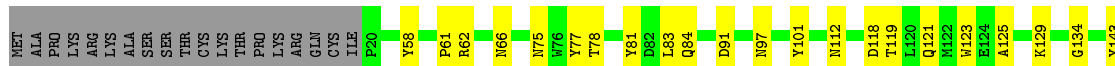
Chain A:

- Molecule 1: Capsid protein VP1

Chain B:

- Molecule 1: Capsid protein VP1

Chain C:

N162 F166 D174 L175 Q176 V179 L180 D181 T189 G192 N209 L212 D213 K217 A218 K219 L220 D223 G224 N225 Y226 W231 C232 P233 D234 N238 E239 S246 I247 Q248 T249 Q252 T253 P254 T255 F259 D280 G281 L282 C286 V290

F294 L305 P306 R307 N310 L313 R316 W317 Y322 V325 N326 N329 S330 N334 E361 Q362 L363 P364 L373 G377 GLN GLU LYS THR VAL TYR PRO LYS PRO SER VAL ALA PRO ALA ALA VAL THR PHE GLN SER ASN GLN ASP LYS GLY LYS ALA PRO

LEU LYS GLY PRO GLN LYS ALA SER GLN LYS GLU SER GLN THR GLU GLU LEU

• Molecule 1: Capsid protein VP1

Chain D:

%

66% 16% 18%

MET ALA PRO LYS ARG LYS ALA SER SER THR CYS LYS PRO LYS ARG CYS I19 P20 C24 A29 Y58 P61 P68 D69 L70 T73 S74 N75 W76 Y77 T78 Y81 D82 L108 L111 N112 Q121 M122 W123 E124 A125 K129 V132 I135

Y143 M146 V149 H150 S159 N162 G169 Q176 V179 L180 D181 Y182 T189 T190 G193 T199 Q210 G211 L212 K217 K222 Y226 C232 P233 D234 E239 N240 S241 R242 G245 Q248 P254 T255 F259 D269 G281 C286

V290 K295 G298 L305 P306 R307 N310 L313 R316 P321 Y322 F332 M336 Q362 L363 P364 GLY ASP PRO ASP ILE VAL ARG PHE LEU ASP LYS PHE GLY GLN GLU LYS THR VAL TYR PRO LYS PRO SER VAL ALA PRO ALA ALA VAL THR PHE GLN SER

ASN GLN ASP LYS GLY LYS ALA PRO LEU LYS GLY PRO GLN LYS ALA SER GLN LYS GLU SER GLN THR GLU GLU LEU

• Molecule 1: Capsid protein VP1

Chain E:

%

68% 17% 14%

MET ALA PRO ARG LYS SER ALA SER SER THR CYS LYS THR PRO LYS ARG GLN CYS ILE PRO LYS PRO LYS PRO GLY CYS CYS P26 N27 V28 A29 V42 V45 Y58 L59 N60 P61 B62 M63 Y77 T78 D91 Q92 P93 P99 P109 W123 E124 A125 V132 I135

H142 Y143 W144 D145 M146 K147 R148 V149 G153 I156 N162 Y163 P172 L173 D174 L175 Q176 Y182 T189 I195 T199 T206 P207 L212 L220 D221 K222 D223 G224 N225 Y226 C232 N238 E239 N240 S241 R242 G245 Q248 T249 G250 T253 F259

V266 L267 L268 D269 P275 L276 C277 L282 F283 D288 I289 T296 L302 H303 P306 R307 R316 F332 M336 L363 P364 D374 G377 Q378 V382 Y383 S387 VAL ALA PRO ALA ALA VAL THR PHE GLN SER ASN GLN GLN ASP LYS GLY LYS ALA

PRO LEU LYS GLY PRO GLN LYS ALA SER GLN LYS GLU SER GLN THR GLN GLU LEU

• Molecule 1: Capsid protein VP1

Chain F:

69% 16% 15%

MET ALA PRO LYS ARG LYS ALA SER SER THR CYS LYS THR PRO LYS ARG GLN CYS ILE P20 Y58 P61 R62 N66 N75 W76 Y77 T78 Y81 D82 L83 Q84 D91 N97 Y101 Y112 N112 D118 T119 L120 Q121 M122 W123 E124 A125 K129 G134 Y143

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	554.83Å 560.99Å 573.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.52 49.97 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.97-3.52) 99.9 (49.97-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.235 , (Not available) 0.266 , 0.265	Depositor DCC
R_{free} test set	1479 reflections (0.14%)	wwPDB-VP
Wilson B-factor (Å^2)	131.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.013 for l,-k,h 0.014 for -k,-h,-l 0.013 for k,-l,-h 0.013 for -l,h,-k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16324	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0/2796	0.54	0/3823
1	B	0.53	1/2871 (0.0%)	0.54	0/3932
1	C	0.52	0/2796	0.55	0/3824
1	D	0.56	1/2688 (0.0%)	0.58	1/3678 (0.0%)
1	E	0.53	0/2818	0.55	1/3857 (0.0%)
1	F	0.49	0/2759	0.55	0/3778
All	All	0.53	2/16728 (0.0%)	0.55	2/22892 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	ALA	C-N	-5.61	1.21	1.34
1	B	124	GLU	CD-OE1	-5.02	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	239	GLU	CB-CA-C	-5.18	100.04	110.40
1	E	199	THR	CA-CB-OG1	-5.10	98.30	109.00

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	2728	0	2632	49	0
1	B	2800	0	2679	60	0
1	C	2728	0	2634	50	0
1	D	2623	0	2535	47	0
1	E	2749	0	2639	58	0
1	F	2690	0	2560	43	0
2	A	2	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
All	All	16324	0	15679	273	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 9.

All (273) 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:169:GLY:HA3	1:D:241:SER:HB3	1.51	0.92
1:F:112:ASN:HD21	1:F:121:GLN:H	1.26	0.83
1:E:242:ARG:HH21	1:E:269:ASP:HB3	1.47	0.80
1:B:242:ARG:HH11	1:B:269:ASP:HB3	1.46	0.79
1:E:174:ASP:H	1:E:238:ASN:HD21	1.32	0.76
1:C:290:VAL:HG21	1:C:305:LEU:HD13	1.68	0.75
1:E:162:ASN:ND2	1:E:289:ILE:O	2.20	0.74
1:A:355:ARG:NH2	1:C:239:GLU:OE1	2.21	0.73
1:D:124:GLU:OE1	1:D:316:ARG:NE	2.23	0.71
1:A:148:ARG:NH1	1:A:153:GLY:O	2.24	0.70
1:B:112:ASN:H	1:B:121:GLN:HE21	1.39	0.70
1:A:143:TYR:HB3	1:A:146:MET:HG3	1.73	0.69
1:F:175:LEU:HA	1:F:234:ASP:H	1.57	0.69
1:B:143:TYR:HB3	1:B:146:MET:HG3	1.74	0.68
1:E:162:ASN:HB3	1:E:248:GLN:HB3	1.76	0.67
1:F:143:TYR:HB3	1:F:146:MET:HB2	1.75	0.67
1:B:128:VAL:HG12	1:B:267:LEU:HD11	1.77	0.67
1:C:133:VAL:HG21	1:D:212:LEU:HD12	1.76	0.67
1:A:162:ASN:OD1	1:A:248:GLN:NE2	2.27	0.66
1:E:143:TYR:HB3	1:E:146:MET:HB2	1.76	0.65
1:B:126:ILE:HD11	1:B:314:ARG:HD3	1.78	0.65
1:A:162:ASN:ND2	1:A:290:VAL:O	2.30	0.65
1:C:223:ASP:OD1	1:C:224:GLY:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ASP:OD1	1:F:224:GLY:N	2.30	0.64
1:B:175:LEU:HD23	1:B:231:TRP:HB3	1.78	0.64
1:C:179:VAL:HG12	1:C:181:ASP:H	1.63	0.64
1:C:175:LEU:HA	1:C:234:ASP:H	1.62	0.64
1:B:148:ARG:NH1	1:B:153:GLY:O	2.31	0.63
1:A:344:MET:HG2	1:B:106:VAL:HG22	1.80	0.63
1:F:129:LYS:HB3	1:F:310:ASN:HB3	1.82	0.62
1:D:143:TYR:HB3	1:D:146:MET:HB2	1.80	0.62
1:B:374:ASP:OD1	1:B:378:GLN:N	2.33	0.61
1:C:162:ASN:HB2	1:C:248:GLN:HB3	1.82	0.61
1:F:175:LEU:HD13	1:F:231:TRP:HB3	1.81	0.61
1:F:286:CYS:HB2	1:F:307:ARG:HD3	1.81	0.61
1:A:286:CYS:HB2	1:A:307:ARG:HD3	1.83	0.60
1:C:175:LEU:HD13	1:C:231:TRP:HB3	1.83	0.60
1:E:374:ASP:OD1	1:E:378:GLN:N	2.33	0.60
1:F:363:LEU:HD12	1:F:364:PRO:HD2	1.84	0.60
1:B:306:PRO:HG2	1:C:212:LEU:HB2	1.83	0.59
1:B:370:VAL:HG13	1:B:382:VAL:HB	1.83	0.59
1:C:325:VAL:HG12	1:C:329:ASN:HD21	1.67	0.59
1:B:322:TYR:HB3	1:B:327:LEU:HD11	1.83	0.59
1:D:179:VAL:HG12	1:D:181:ASP:H	1.66	0.59
1:C:363:LEU:HD12	1:C:364:PRO:HD2	1.83	0.59
1:A:129:LYS:HB3	1:A:310:ASN:HB3	1.83	0.59
1:E:220:LEU:HA	1:E:226:TYR:HE2	1.68	0.59
1:C:143:TYR:HB3	1:C:146:MET:HG3	1.85	0.58
1:F:361:GLU:OE2	1:F:371:ARG:NH2	2.34	0.58
1:B:242:ARG:NH1	1:B:269:ASP:HB3	2.15	0.58
1:D:290:VAL:HG21	1:D:305:LEU:HG	1.86	0.58
1:B:220:LEU:HA	1:B:226:TYR:HE2	1.69	0.58
1:F:125:ALA:HB3	1:F:275:PRO:HG2	1.85	0.58
1:B:182:TYR:OH	1:F:75:ASN:OD1	2.21	0.58
1:C:209:ASN:ND2	1:C:213:ASP:OD2	2.37	0.57
1:D:242:ARG:NH2	1:D:269:ASP:HB3	2.19	0.57
1:A:373:LEU:HD21	1:C:330:SER:HB3	1.86	0.57
1:B:254:PRO:HB3	1:C:253:THR:HG21	1.87	0.57
1:B:220:LEU:HA	1:B:226:TYR:CE2	2.40	0.56
1:E:174:ASP:N	1:E:238:ASN:HD21	2.01	0.56
1:E:363:LEU:HD12	1:E:364:PRO:HD2	1.88	0.56
1:A:18:CYS:SG	1:A:19:ILE:N	2.79	0.56
1:C:49:GLU:OE2	1:C:317:TRP:NE1	2.36	0.56
1:A:190:THR:HG23	1:A:193:GLY:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:SER:O	1:F:261:ASN:ND2	2.36	0.55
1:A:63:MET:HG3	1:A:99:PRO:HB3	1.88	0.55
1:B:363:LEU:HD12	1:B:364:PRO:HD2	1.89	0.55
1:C:174:ASP:OD1	1:C:219:LYS:HG2	2.07	0.55
1:A:288:ASP:OD2	1:A:307:ARG:NH1	2.34	0.54
1:D:254:PRO:HB3	1:E:253:THR:HG21	1.90	0.54
1:E:240:ASN:O	1:E:240:ASN:ND2	2.41	0.54
1:C:124:GLU:OE1	1:C:316:ARG:NE	2.37	0.54
1:E:125:ALA:HB3	1:E:275:PRO:HG2	1.90	0.54
1:D:73:THR:HG1	1:D:81:TYR:HH	1.53	0.53
1:E:266:VAL:HG12	1:E:268:LEU:H	1.74	0.53
1:C:220:LEU:HA	1:C:226:TYR:HE2	1.73	0.53
1:D:111:LEU:HD11	1:D:123:TRP:NE1	2.24	0.53
1:E:148:ARG:NH1	1:E:153:GLY:O	2.42	0.52
1:C:62:ARG:HG3	1:C:223:ASP:OD1	2.07	0.52
1:D:129:LYS:HB3	1:D:310:ASN:HB3	1.92	0.52
1:B:223:ASP:OD1	1:B:224:GLY:N	2.42	0.52
1:B:269:ASP:OD1	1:B:272:GLY:N	2.43	0.52
1:C:217:LYS:NZ	1:C:234:ASP:OD2	2.33	0.52
1:D:182:TYR:H	1:D:210:GLN:HE21	1.57	0.52
1:B:143:TYR:HE1	1:C:181:ASP:OD2	1.92	0.51
1:B:162:ASN:ND2	1:B:248:GLN:HE21	2.08	0.51
1:D:162:ASN:HD22	1:D:248:GLN:HE21	1.57	0.51
1:F:81:TYR:O	1:F:83:LEU:HD12	2.11	0.51
1:E:132:VAL:HB	1:E:135:ILE:HD11	1.92	0.51
1:E:223:ASP:OD1	1:E:224:GLY:N	2.43	0.51
1:A:125:ALA:HB3	1:A:275:PRO:HG2	1.93	0.51
1:A:174:ASP:OD1	1:A:219:LYS:NZ	2.36	0.51
1:D:162:ASN:ND2	1:D:248:GLN:HE21	2.09	0.51
1:A:330:SER:HB2	1:C:373:LEU:HD23	1.92	0.51
1:A:363:LEU:HD12	1:A:364:PRO:HD2	1.93	0.51
1:C:220:LEU:HA	1:C:226:TYR:CE2	2.45	0.51
1:E:58:TYR:CD2	1:F:212:LEU:HD23	2.46	0.51
1:B:227:PRO:HG2	1:B:230:VAL:HG22	1.92	0.50
1:D:112:ASN:HB2	1:D:121:GLN:NE2	2.26	0.50
1:D:61:PRO:HG2	1:D:78:THR:HG22	1.93	0.50
1:B:178:LEU:HD13	1:F:134:GLY:HA3	1.94	0.50
1:B:212:LEU:HD23	1:F:58:TYR:CG	2.46	0.50
1:D:77:TYR:O	1:D:78:THR:OG1	2.26	0.50
1:F:176:GLN:HB2	1:F:234:ASP:HB2	1.94	0.50
1:B:230:VAL:HG23	1:B:231:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:GLU:OE1	1:E:316:ARG:NE	2.41	0.49
1:A:39:GLY:O	1:A:42:VAL:HG22	2.12	0.49
1:B:63:MET:HA	1:B:99:PRO:HA	1.93	0.49
1:D:162:ASN:HD21	1:D:255:THR:HG22	1.76	0.49
1:A:61:PRO:HG2	1:A:78:THR:HG22	1.93	0.49
1:A:242:ARG:NH2	1:A:269:ASP:HB3	2.27	0.49
1:D:132:VAL:HB	1:D:135:ILE:HD11	1.94	0.49
1:D:217:LYS:NZ	1:D:234:ASP:OD2	2.34	0.49
1:E:220:LEU:HA	1:E:226:TYR:CE2	2.45	0.49
1:B:61:PRO:HG2	1:B:78:THR:HG22	1.94	0.49
1:D:286:CYS:HB2	1:D:307:ARG:HD3	1.95	0.49
1:A:124:GLU:OE1	1:A:316:ARG:NE	2.43	0.49
1:B:196:THR:HG22	1:B:197:ILE:H	1.78	0.49
1:B:162:ASN:HD22	1:B:248:GLN:HE21	1.61	0.49
1:F:149:VAL:HG23	1:F:150:HIS:ND1	2.28	0.49
1:F:149:VAL:HG12	1:F:156:ILE:HG12	1.93	0.49
1:D:82:ASP:OD1	1:D:295:LYS:NZ	2.36	0.48
1:D:259:PHE:CZ	1:E:245:GLY:HA3	2.48	0.48
1:E:42:VAL:O	1:E:45:VAL:HG12	2.12	0.48
1:A:78:THR:O	1:A:303:HIS:ND1	2.46	0.48
1:B:125:ALA:HA	1:B:313:LEU:HD23	1.95	0.48
1:B:196:THR:HG22	1:B:197:ILE:N	2.28	0.48
1:E:78:THR:O	1:E:303:HIS:ND1	2.43	0.48
1:B:245:GLY:HA3	1:F:259:PHE:CZ	2.49	0.48
1:C:174:ASP:O	1:C:238:ASN:ND2	2.29	0.48
1:C:81:TYR:O	1:C:97:ASN:ND2	2.47	0.48
1:A:19:ILE:N	1:A:20:PRO:HD3	2.29	0.47
1:E:77:TYR:O	1:E:78:THR:OG1	2.29	0.47
1:B:212:LEU:HD23	1:F:58:TYR:CD2	2.49	0.47
1:B:130:THR:O	1:B:130:THR:HG23	2.14	0.47
1:B:176:GLN:N	1:B:232:CYS:O	2.44	0.47
1:E:145:ASP:O	1:E:296:THR:N	2.48	0.47
1:B:129:LYS:HB3	1:B:310:ASN:HB3	1.96	0.47
1:A:72:THR:HG23	1:A:73:THR:HG22	1.95	0.47
1:C:75:ASN:OD1	1:D:182:TYR:OH	2.21	0.47
1:B:323:PRO:HG2	1:B:326:ASN:ND2	2.30	0.47
1:D:68:PRO:HA	1:D:74:SER:HB3	1.97	0.47
1:A:222:LYS:H	1:A:226:TYR:HE2	1.63	0.47
1:A:101:TYR:CE1	1:A:228:ILE:HG12	2.50	0.47
1:F:62:ARG:HG3	1:F:223:ASP:OD1	2.14	0.47
1:C:143:TYR:HE1	1:D:181:ASP:OD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:PHE:O	1:B:336:MET:N	2.31	0.46
1:C:166:PHE:HA	1:C:286:CYS:HA	1.97	0.46
1:D:75:ASN:OD1	1:E:182:TYR:OH	2.24	0.46
1:E:125:ALA:O	1:E:275:PRO:HD2	2.14	0.46
1:A:206:THR:HB	1:A:207:PRO:HD2	1.96	0.46
1:E:288:ASP:OD2	1:E:307:ARG:HD2	2.16	0.46
1:A:250:GLY:HA3	1:A:253:THR:OG1	2.16	0.46
1:B:143:TYR:HB3	1:B:146:MET:CG	2.45	0.46
1:E:143:TYR:HE1	1:F:181:ASP:OD2	1.97	0.46
1:C:150:HIS:NE2	1:D:298:GLY:O	2.49	0.46
1:B:112:ASN:N	1:B:121:GLN:HE21	2.12	0.46
1:C:80:THR:HG23	1:C:96:GLU:O	2.16	0.46
1:E:162:ASN:HD22	1:E:163:TYR:N	2.12	0.46
1:B:323:PRO:HG2	1:B:326:ASN:HD22	1.81	0.46
1:B:58:TYR:CE2	1:C:212:LEU:HD22	2.51	0.46
1:C:176:GLN:N	1:C:232:CYS:O	2.35	0.46
1:A:273:VAL:HG12	1:A:316:ARG:CZ	2.46	0.45
1:F:101:TYR:CE1	1:F:228:ILE:HG12	2.51	0.45
1:A:132:VAL:HB	1:A:135:ILE:HD11	1.98	0.45
1:E:172:PRO:HD3	1:E:283:PHE:HE2	1.81	0.45
1:B:62:ARG:HG3	1:B:223:ASP:OD1	2.16	0.45
1:D:176:GLN:N	1:D:232:CYS:O	2.44	0.45
1:E:61:PRO:HG2	1:E:78:THR:HG22	1.99	0.45
1:E:259:PHE:CZ	1:F:245:GLY:HA3	2.52	0.45
1:D:108:LEU:HD13	1:D:281:GLY:HA2	1.99	0.45
1:D:159:SER:HA	1:D:255:THR:HG23	1.98	0.45
1:D:332:PHE:O	1:D:336:MET:HG2	2.16	0.45
1:C:259:PHE:CZ	1:D:245:GLY:HA3	2.52	0.45
1:D:321:PRO:HG2	1:D:322:TYR:CD2	2.52	0.45
1:F:159:SER:OG	1:F:253:THR:O	2.32	0.45
1:A:182:TYR:H	1:A:210:GLN:HE21	1.65	0.45
1:E:221:ASP:H	1:E:226:TYR:HE2	1.64	0.45
1:A:143:TYR:HB3	1:A:146:MET:CG	2.44	0.44
1:F:62:ARG:HD2	1:F:66:ASN:HB3	1.99	0.44
1:B:110:MET:C	1:B:111:LEU:HD12	2.38	0.44
1:F:209:ASN:ND2	1:F:213:ASP:OD2	2.50	0.44
1:A:370:VAL:HG12	1:C:322:TYR:OH	2.17	0.44
1:D:70:LEU:O	1:D:74:SER:OG	2.22	0.44
1:B:77:TYR:O	1:B:78:THR:OG1	2.29	0.44
1:D:77:TYR:CD2	1:D:78:THR:HG23	2.53	0.44
1:E:242:ARG:NH2	1:E:269:ASP:HB3	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ASN:HA	1:C:329:ASN:HD22	1.82	0.44
1:F:91:ASP:HB3	1:F:184:THR:HG22	2.00	0.44
1:C:129:LYS:HB3	1:C:310:ASN:HB3	1.99	0.44
1:F:118:ASP:OD1	1:F:119:THR:N	2.50	0.44
1:F:162:ASN:HB2	1:F:248:GLN:HG2	1.99	0.44
1:B:91:ASP:HB3	1:B:184:THR:HG22	1.99	0.44
1:C:106:VAL:HB	1:C:282:LEU:HB3	1.99	0.44
1:F:77:TYR:CD2	1:F:78:THR:HG23	2.53	0.44
1:A:162:ASN:HB2	1:A:248:GLN:HG2	1.99	0.44
1:C:255:THR:HG21	1:C:290:VAL:HG13	2.00	0.44
1:E:109:PRO:HG2	1:E:123:TRP:HZ2	1.83	0.43
1:A:175:LEU:HD11	1:A:220:LEU:HD12	1.99	0.43
1:A:62:ARG:HD2	1:A:66:ASN:HB3	2.00	0.43
1:A:68:PRO:HA	1:A:74:SER:HB3	2.00	0.43
1:C:110:MET:HG3	1:C:280:ASP:OD2	2.17	0.43
1:D:125:ALA:HA	1:D:313:LEU:HD23	2.00	0.43
1:E:77:TYR:CD2	1:E:78:THR:HG23	2.53	0.43
1:E:91:ASP:OD2	1:E:93:PRO:HD3	2.18	0.43
1:B:258:GLN:HA	1:C:246:SER:HA	2.00	0.43
1:E:162:ASN:HD22	1:E:163:TYR:H	1.64	0.43
1:A:290:VAL:HG21	1:A:305:LEU:HG	2.00	0.43
1:A:82:ASP:OD2	1:A:299:LYS:HD3	2.17	0.43
1:D:70:LEU:HD23	1:D:70:LEU:H	1.83	0.43
1:E:332:PHE:O	1:E:336:MET:HG2	2.19	0.43
1:C:77:TYR:O	1:C:78:THR:OG1	2.29	0.43
1:D:190:THR:O	1:D:193:GLY:N	2.51	0.43
1:D:306:PRO:HG2	1:E:212:LEU:HB2	2.01	0.43
1:F:123:TRP:HB2	1:F:277:CYS:HB2	2.01	0.43
1:D:189:THR:OG1	1:D:199:THR:OG1	2.22	0.43
1:D:222:LYS:H	1:D:226:TYR:HE2	1.66	0.43
1:F:242:ARG:HH21	1:F:269:ASP:HB3	1.82	0.43
1:F:164:HIS:HB2	1:F:246:SER:HB3	2.01	0.43
1:A:99:PRO:HB2	1:A:228:ILE:HD12	1.99	0.43
1:E:277:CYS:SG	1:E:282:LEU:HB3	2.58	0.43
1:E:148:ARG:HH12	1:F:84:GLN:HG2	1.84	0.43
1:B:195:ILE:HB	1:B:226:TYR:CE1	2.54	0.43
1:E:374:ASP:OD1	1:E:377:GLY:N	2.52	0.43
1:B:111:LEU:HD21	1:B:315:LYS:HG2	2.00	0.42
1:B:77:TYR:CD2	1:B:78:THR:HG23	2.54	0.42
1:E:149:VAL:HG22	1:E:156:ILE:HG12	2.00	0.42
1:B:78:THR:O	1:B:303:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:THR:HG22	1:C:249:THR:OG1	2.19	0.42
1:E:63:MET:HA	1:E:99:PRO:HA	2.01	0.42
1:F:180:LEU:O	1:F:210:GLN:NE2	2.50	0.42
1:F:61:PRO:HG2	1:F:78:THR:HG22	2.00	0.42
1:D:149:VAL:HG13	1:D:150:HIS:ND1	2.34	0.42
1:A:149:VAL:HG13	1:A:150:HIS:ND1	2.34	0.42
1:A:18:CYS:HB3	1:A:20:PRO:HD3	2.01	0.42
1:A:68:PRO:HD3	1:A:77:TYR:CE1	2.54	0.42
1:E:124:GLU:CD	1:E:316:ARG:HE	2.22	0.42
1:C:189:THR:O	1:C:192:GLY:N	2.51	0.42
1:D:58:TYR:CD2	1:E:212:LEU:HD23	2.55	0.42
1:D:73:THR:OG1	1:D:81:TYR:OH	2.23	0.42
1:A:60:ASN:HA	1:A:306:PRO:HB3	2.02	0.42
1:E:142:HIS:NE2	1:F:229:GLU:OE2	2.53	0.41
1:A:81:TYR:O	1:A:83:LEU:HD12	2.20	0.41
1:E:195:ILE:HB	1:E:226:TYR:CE1	2.55	0.41
1:B:84:GLN:HG2	1:F:148:ARG:HH22	1.84	0.41
1:F:174:ASP:OD1	1:F:219:LYS:NZ	2.40	0.41
1:F:81:TYR:O	1:F:97:ASN:ND2	2.53	0.41
1:B:288:ASP:OD2	1:B:307:ARG:HD3	2.20	0.41
1:E:288:ASP:OD2	1:E:307:ARG:NH1	2.33	0.41
1:B:249:THR:OG1	1:F:255:THR:HG22	2.20	0.41
1:E:60:ASN:HA	1:E:306:PRO:HB3	2.02	0.41
1:D:135:ILE:H	1:D:135:ILE:HD12	1.85	0.41
1:C:125:ALA:HA	1:C:313:LEU:HD23	2.02	0.41
1:E:206:THR:HB	1:E:207:PRO:HD2	2.02	0.41
1:A:125:ALA:HA	1:A:313:LEU:HD23	2.02	0.41
1:C:252:GLN:HG2	1:C:294:PHE:CE2	2.56	0.41
1:B:133:VAL:O	1:B:305:LEU:HD13	2.21	0.41
1:B:132:VAL:HG12	1:B:305:LEU:CD1	2.51	0.41
1:E:189:THR:O	1:E:189:THR:HG22	2.21	0.41
1:E:382:VAL:HG22	1:E:383:TYR:H	1.86	0.41
1:E:289:ILE:HG21	1:E:302:LEU:HD22	2.02	0.41
1:A:142:HIS:O	1:A:142:HIS:ND1	2.54	0.40
1:A:101:TYR:CD1	1:A:228:ILE:HG12	2.56	0.40
1:A:124:GLU:OE2	1:A:273:VAL:HA	2.20	0.40
1:C:139:ILE:O	1:C:141:VAL:HG23	2.21	0.40
1:C:361:GLU:HG3	1:C:362:GLN:O	2.21	0.40
1:E:240:ASN:HD22	1:E:240:ASN:C	2.23	0.40
1:E:176:GLN:N	1:E:232:CYS:O	2.48	0.40
1:D:239:GLU:H	1:D:239:GLU:HG2	1.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLY:HA3	1:E:253:THR:HG23	2.04	0.40
1:C:286:CYS:HB2	1:C:307:ARG:HD3	2.04	0.40
1:C:81:TYR:O	1:C:83:LEU:HD12	2.22	0.40
1:B:68:PRO:HD3	1:B:77:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/423 (84%)	347 (97%)	10 (3%)	0	100	100
1	B	369/423 (87%)	361 (98%)	8 (2%)	0	100	100
1	C	358/423 (85%)	351 (98%)	7 (2%)	0	100	100
1	D	344/423 (81%)	333 (97%)	11 (3%)	0	100	100
1	E	360/423 (85%)	348 (97%)	12 (3%)	0	100	100
1	F	354/423 (84%)	337 (95%)	17 (5%)	0	100	100
All	All	2142/2538 (84%)	2077 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	299/372 (80%)	299 (100%)	0	100	100
1	B	305/372 (82%)	302 (99%)	3 (1%)	76	88
1	C	297/372 (80%)	295 (99%)	2 (1%)	84	93
1	D	288/372 (77%)	286 (99%)	2 (1%)	84	93
1	E	298/372 (80%)	295 (99%)	3 (1%)	76	88
1	F	289/372 (78%)	288 (100%)	1 (0%)	92	97
All	All	1776/2232 (80%)	1765 (99%)	11 (1%)	86	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	GLU
1	B	239	GLU
1	B	334	ASN
1	C	239	GLU
1	C	334	ASN
1	D	239	GLU
1	D	241	SER
1	E	162	ASN
1	E	239	GLU
1	E	240	ASN
1	F	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	210	GLN
1	A	329	ASN
1	B	75	ASN
1	B	121	GLN
1	B	162	ASN
1	B	183	GLN
1	B	210	GLN
1	B	326	ASN
1	B	334	ASN
1	B	350	GLN
1	C	329	ASN
1	C	334	ASN
1	C	350	GLN

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Mol	Chain	Res	Type
1	D	66	ASN
1	D	121	GLN
1	D	150	HIS
1	D	162	ASN
1	D	183	GLN
1	D	209	ASN
1	D	210	GLN
1	D	350	GLN
1	E	121	GLN
1	E	162	ASN
1	E	225	ASN
1	E	238	ASN
1	E	240	ASN
1	E	350	GLN
1	F	97	ASN
1	F	112	ASN
1	F	162	ASN

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 (i)

Of 6 ligands modelled in this entry, 6 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	359/423 (84%)	-0.32	0	100	100	97, 113, 137, 188	2 (0%)
1	B	371/423 (87%)	-0.31	3 (0%)	86	75	96, 114, 147, 184	2 (0%)
1	C	360/423 (85%)	-0.31	3 (0%)	86	75	92, 106, 134, 175	4 (1%)
1	D	346/423 (81%)	-0.29	4 (1%)	79	67	90, 104, 134, 178	3 (0%)
1	E	362/423 (85%)	-0.28	3 (0%)	86	75	93, 108, 138, 165	0
1	F	358/423 (84%)	-0.28	0	100	100	100, 118, 155, 171	2 (0%)
All	All	2156/2538 (84%)	-0.30	13 (0%)	89	81	90, 110, 143, 188	13 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	PRO	3.5
1	E	387	SER	3.4
1	D	362	GLN	3.1
1	B	19	ILE	2.9
1	E	29	ALA	2.8
1	D	20	PRO	2.7
1	D	24	CYS	2.4
1	B	23	GLY	2.3
1	C	22	PRO	2.3
1	B	18	CYS	2.3
1	D	364	PRO	2.3
1	E	27	ASN	2.3
1	C	18	CYS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.
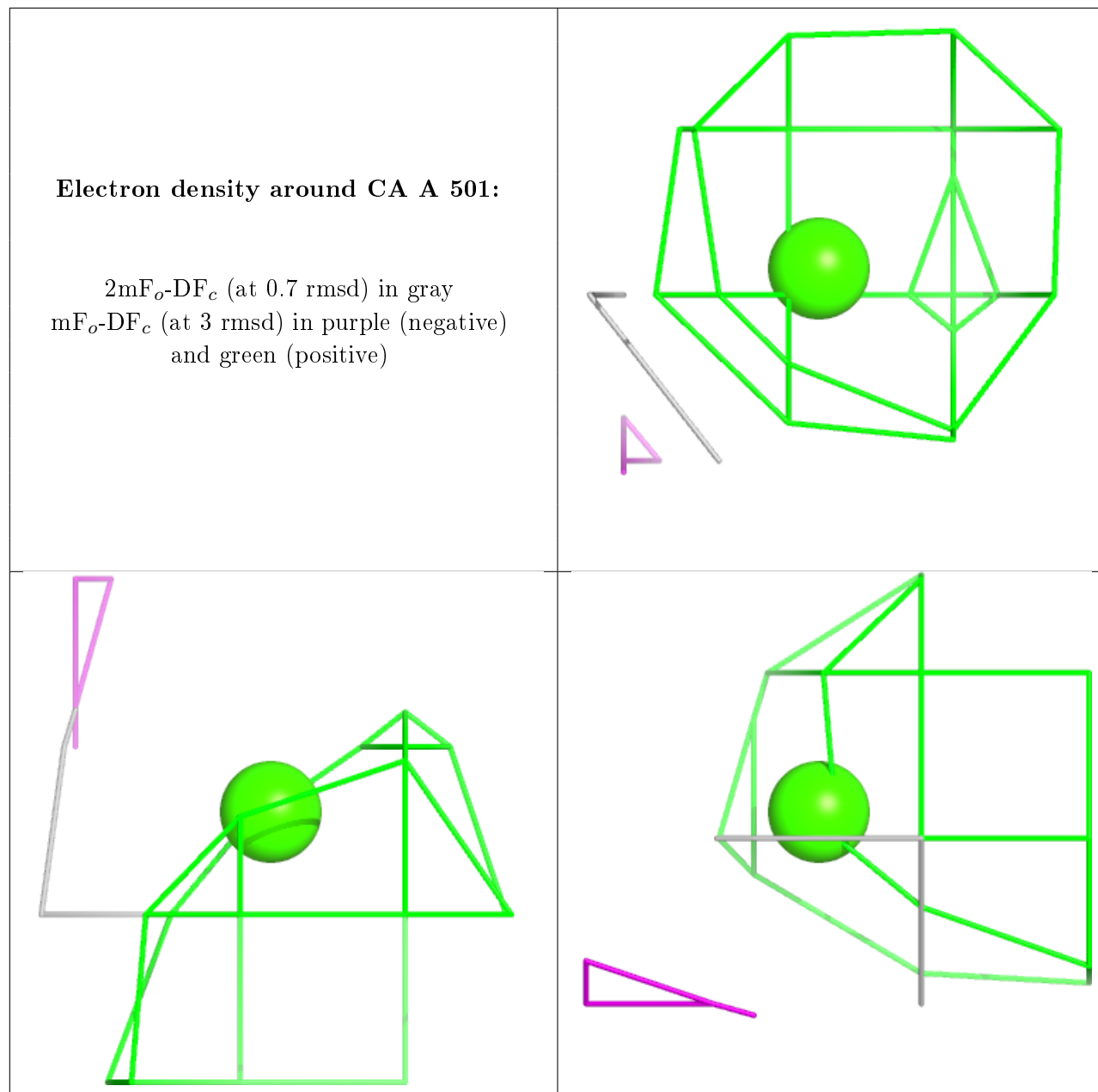
6.3 Carbohydrates (i)
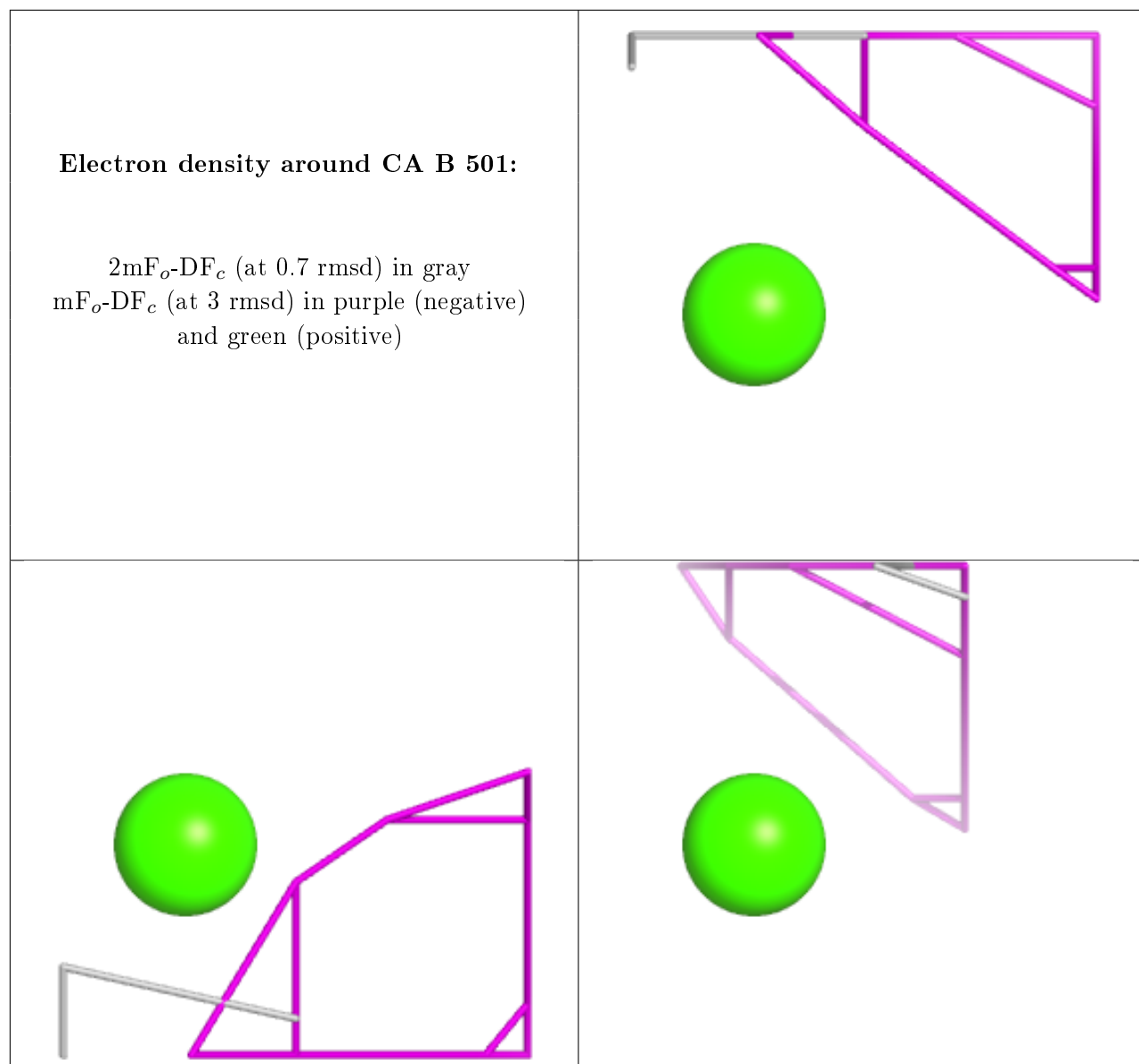
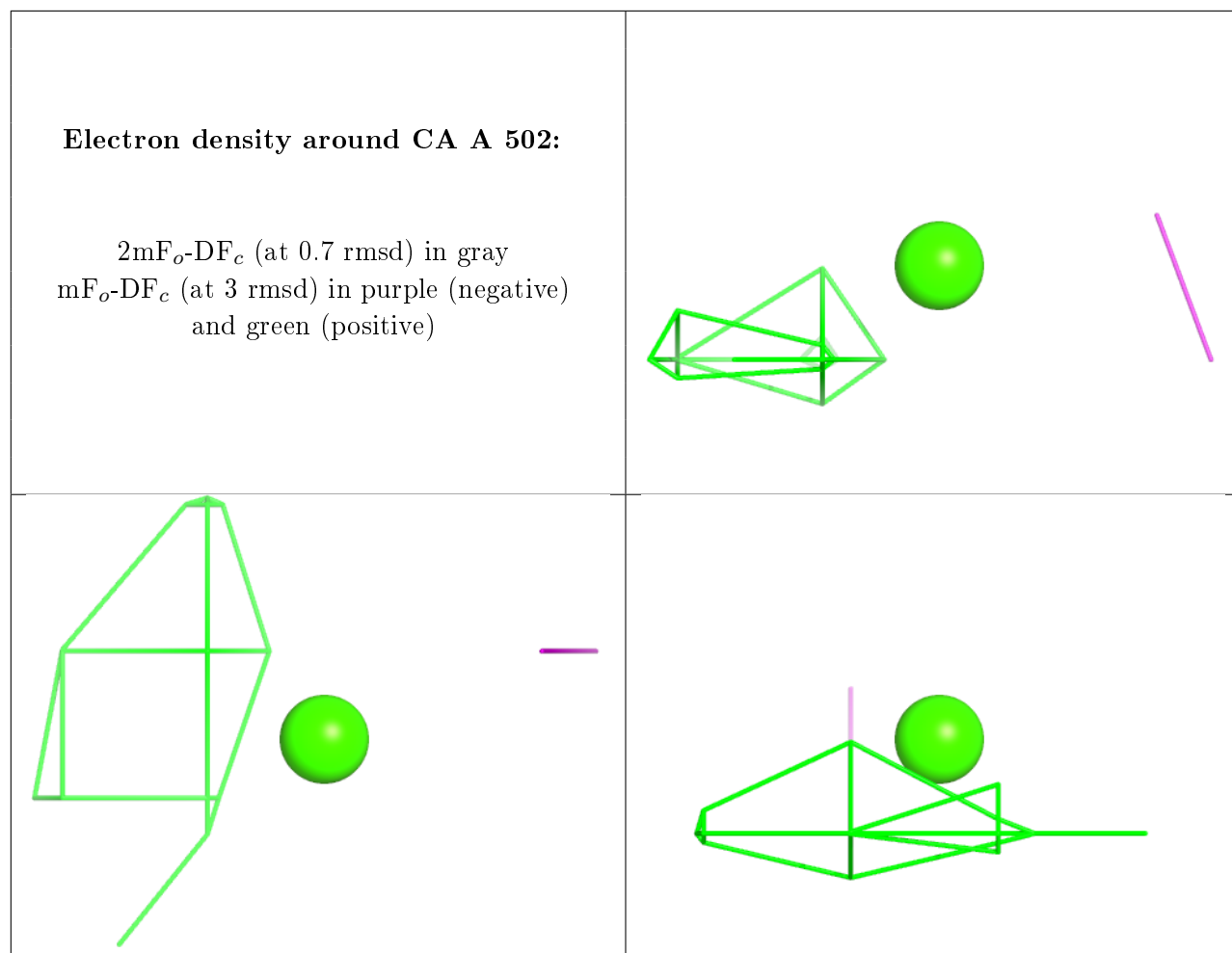There are no monosaccharides in this entry.

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(Å^2)	Q<0.9
2	CA	A	501	1/1	0.41	0.22	116,116,116,116	1
2	CA	B	501	1/1	0.54	0.17	116,116,116,116	1
2	CA	A	502	1/1	0.58	0.18	116,116,116,116	1
2	CA	D	501	1/1	0.67	0.18	116,116,116,116	0
2	CA	E	501	1/1	0.74	0.17	116,116,116,116	1
2	CA	C	501	1/1	0.85	0.10	116,116,116,116	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.
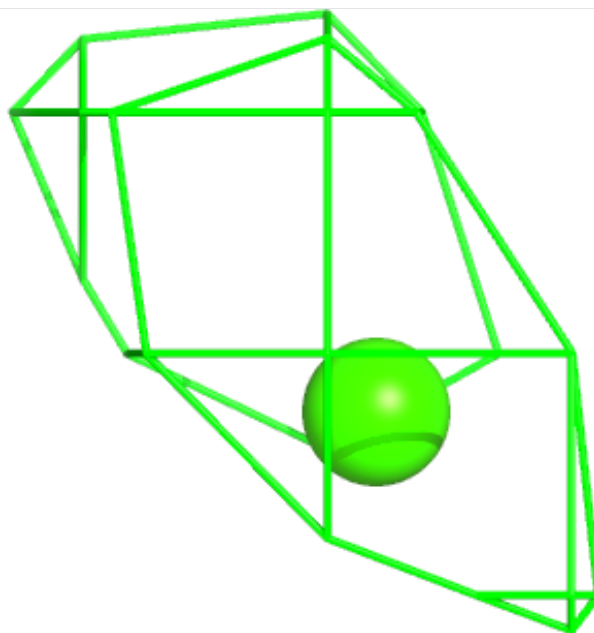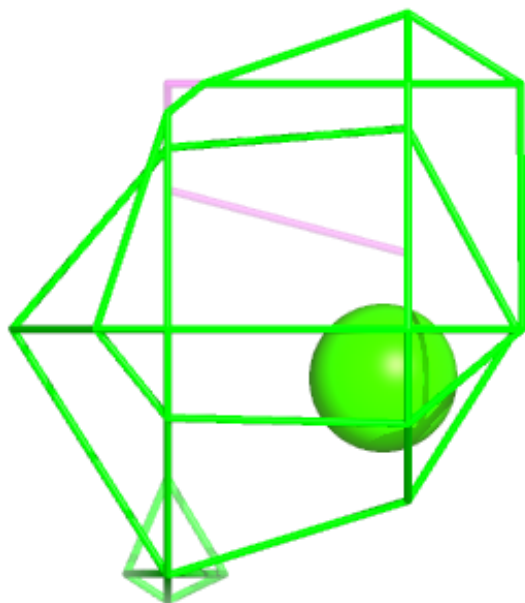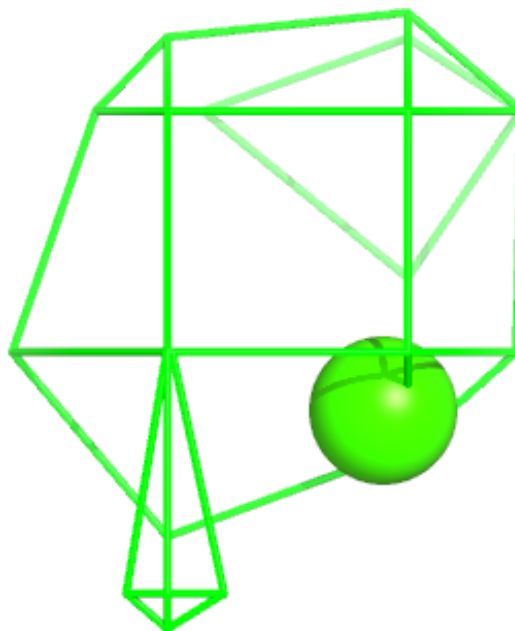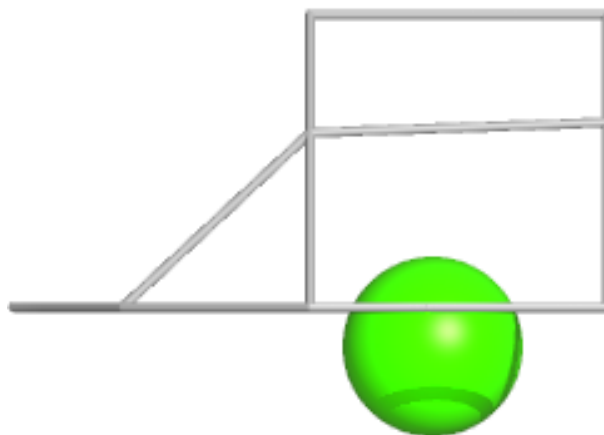
Electron density around CA A 501:

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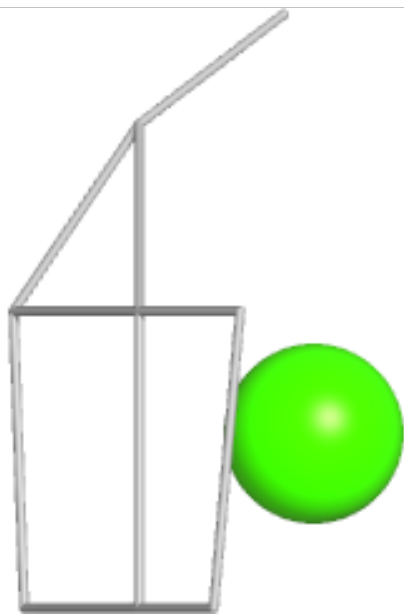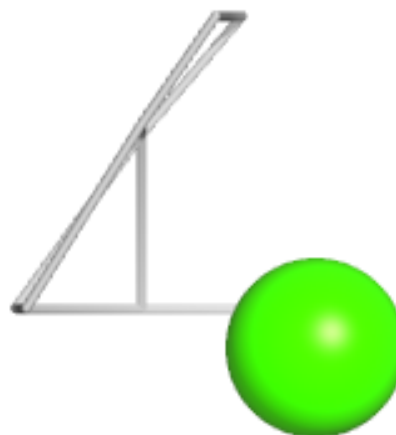and green (positive)

Electron density around CA 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 CA 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)
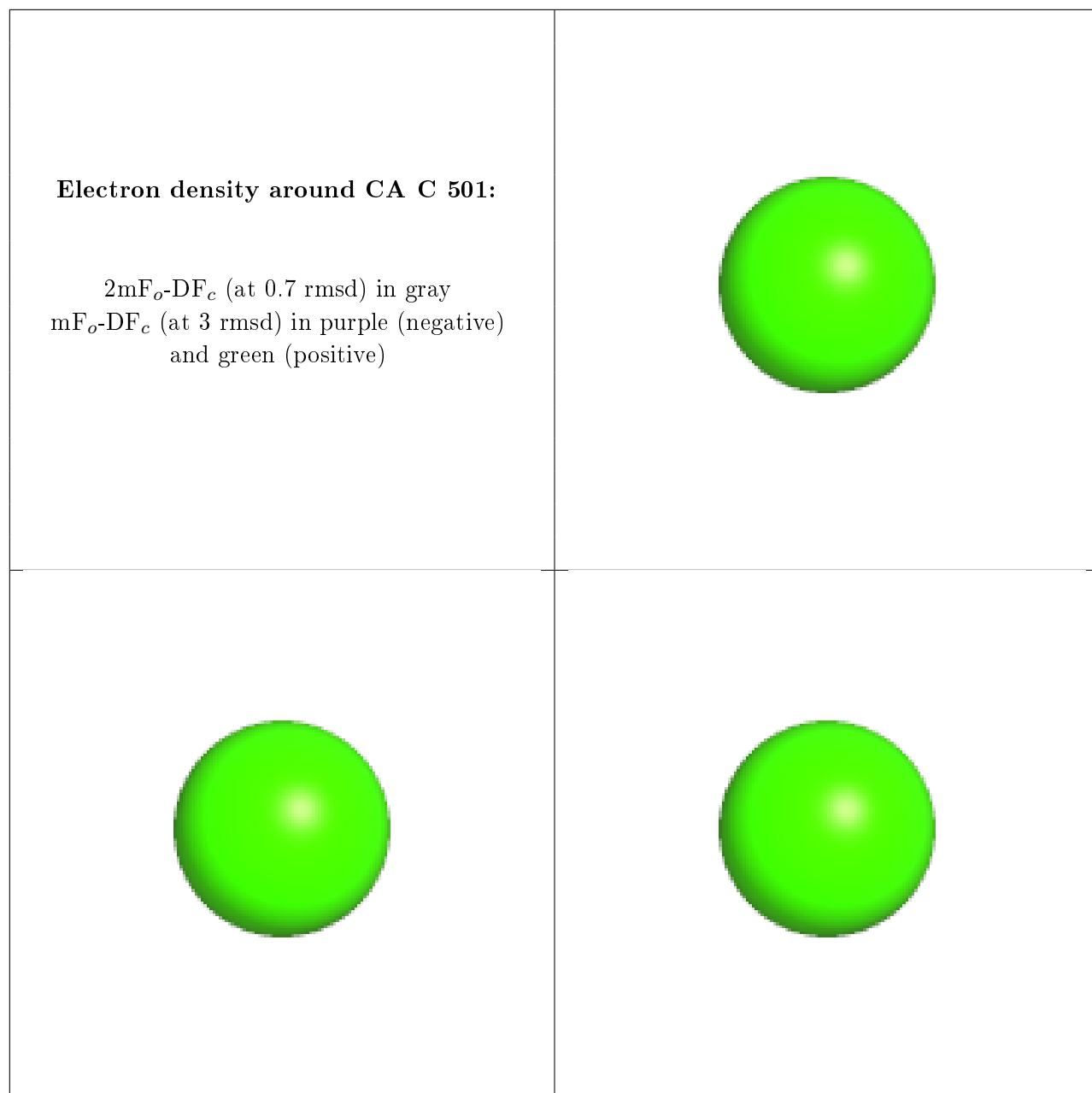
Electron density around CA D 501:

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

Electron density around CA 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 CA 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)

6.5 Other polymers (i)

There are no such residues in this entry.