



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 6SIT / pdb_00006sit
Title : Pseudo-atomic crystal structure of the desmoglein 2 - human adenovirus serotype 3 fibre knob complex
Authors : Burmeister, W.P.; Fender, P.; Vassal-Stermann, E.
Deposited on : 2019-08-11
Resolution : 4.50 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

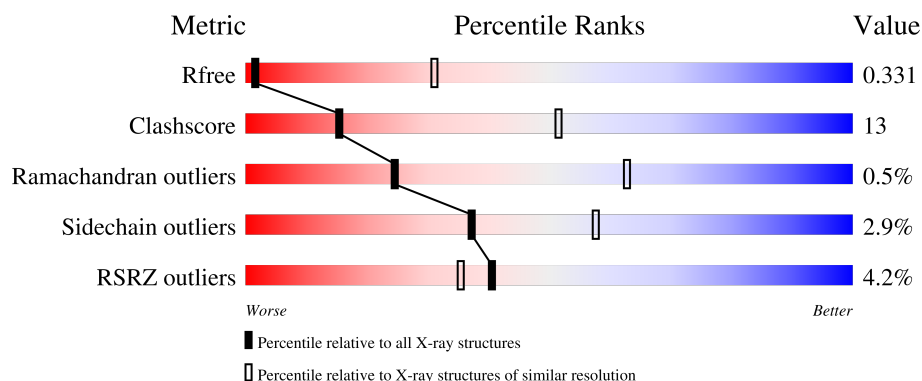
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

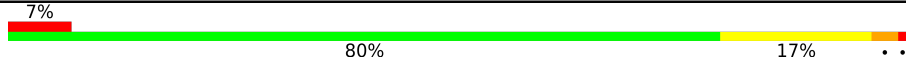
The reported resolution of this entry is 4.50 Å.

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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	191	
2	D	238	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3378 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1499	962	240	291	6			

- Molecule 2 is a protein called Desmoglein-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	238	Total	C	N	O	S	0	0	0
			1873	1182	307	381	3			

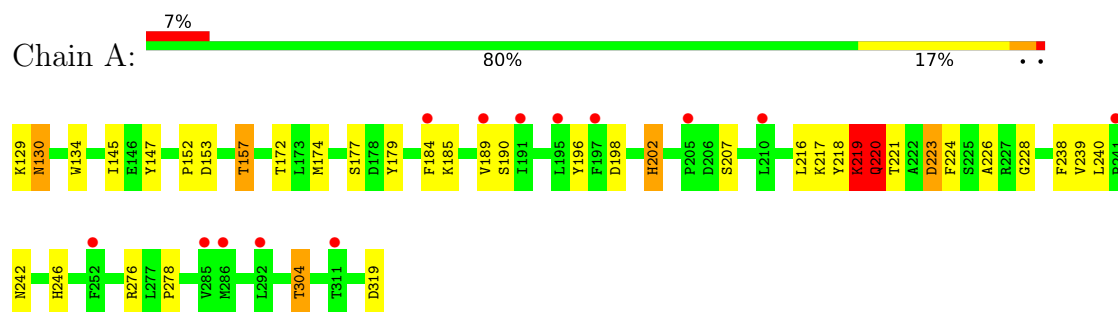
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	6	Total	Ca	0	0
			6	6		

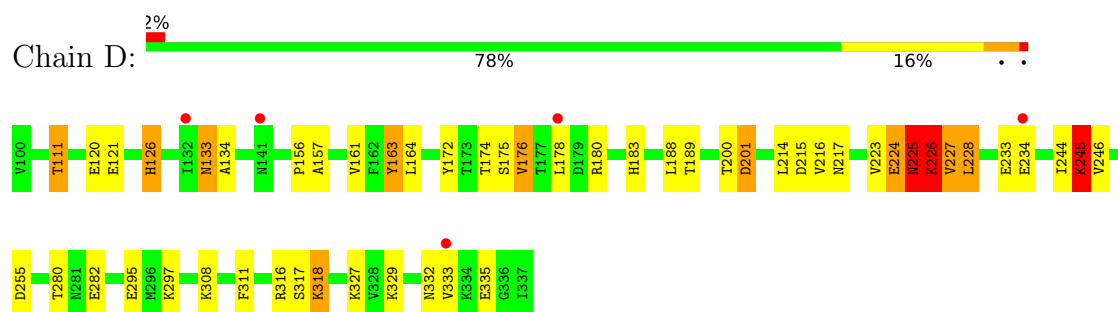
3 Residue-property plots

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: Fiber protein



• Molecule 2: Desmoglein-2



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	146.53Å 146.53Å 146.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.50 – 4.50 46.50 – 4.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.50-4.50) 97.1 (46.50-4.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 4.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.367 , 0.370 0.374 , 0.331	Depositor DCC
R_{free} test set	173 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	252.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 238.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.205 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3378	wwPDB-VP
Average B, all atoms (Å ²)	302.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

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	1.02	4/1536 (0.3%)	2.01	34/2091 (1.6%)
2	D	0.85	3/1905 (0.2%)	0.90	14/2591 (0.5%)
All	All	0.93	7/3441 (0.2%)	1.50	48/4682 (1.0%)

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	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	ASP	CG-OD1	24.50	1.72	1.25
1	A	219	LYS	C-N	-10.49	1.20	1.33
2	D	227	VAL	N-CA	7.09	1.55	1.46
1	A	219	LYS	C-O	5.97	1.31	1.24
1	A	221	THR	N-CA	-5.93	1.38	1.46
1	A	238	PHE	CA-C	5.59	1.60	1.52
2	D	327	LYS	CA-CB	-5.00	1.45	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	O-C-N	-30.59	81.90	122.59
1	A	219	LYS	CA-C-O	-19.46	92.68	120.51
1	A	220	GLN	O-C-N	-17.19	101.95	123.26
1	A	221	THR	N-CA-CB	13.24	132.22	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	CA-C-N	12.99	142.63	121.58
1	A	219	LYS	C-N-CA	12.99	142.63	121.58
1	A	219	LYS	N-CA-C	12.55	137.53	110.80
1	A	217	LYS	CA-C-N	9.83	136.63	122.77
1	A	217	LYS	C-N-CA	9.83	136.63	122.77
1	A	220	GLN	CA-C-O	-8.41	109.71	119.98
2	D	111	THR	N-CA-CB	-8.35	96.53	110.39
1	A	218	TYR	CA-C-N	7.98	136.77	121.54
1	A	218	TYR	C-N-CA	7.98	136.77	121.54
1	A	223	ASP	N-CA-C	-7.80	94.89	108.08
1	A	223	ASP	CB-CA-C	7.80	125.68	116.63
1	A	185	LYS	N-CA-C	-7.24	104.45	113.28
2	D	227	VAL	CB-CA-C	-7.22	99.45	111.29
1	A	246	HIS	CA-CB-CG	-7.03	106.77	113.80
1	A	218	TYR	O-C-N	-6.75	115.38	123.27
1	A	220	GLN	CA-C-N	6.69	131.54	122.84
1	A	220	GLN	C-N-CA	6.69	131.54	122.84
2	D	327	LYS	CG-CD-CE	-6.52	96.30	111.30
2	D	245	LYS	CA-CB-CG	-6.45	101.19	114.10
1	A	217	LYS	O-C-N	-6.31	114.04	122.43
1	A	179	TYR	O-C-N	6.09	128.34	122.07
2	D	111	THR	CB-CA-C	6.03	122.92	110.31
1	A	239	VAL	N-CA-C	5.90	115.73	108.53
1	A	134	TRP	N-CA-C	5.86	116.83	108.74
2	D	228	LEU	N-CA-C	5.86	119.24	108.58
1	A	223	ASP	CA-C-O	-5.80	109.55	119.13
2	D	224	GLU	N-CA-C	-5.68	105.46	112.90
1	A	304	THR	CA-C-N	-5.63	113.06	120.95
1	A	304	THR	C-N-CA	-5.63	113.06	120.95
2	D	318	LYS	N-CA-C	-5.58	106.42	113.18
1	A	157	THR	CA-C-O	-5.57	114.40	120.36
2	D	227	VAL	N-CA-C	5.53	120.85	109.34
1	A	207	SER	N-CA-CB	-5.49	102.45	110.53
2	D	126	HIS	N-CA-C	5.41	119.04	111.90
2	D	226	LYS	CA-C-O	-5.39	113.42	119.79
2	D	327	LYS	CA-CB-CG	-5.38	103.34	114.10
2	D	227	VAL	N-CA-CB	5.35	120.05	111.23
1	A	130	ASN	N-CA-C	-5.33	99.44	110.80
1	A	145	ILE	CB-CA-C	-5.33	105.23	111.94
1	A	202	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	276	ARG	CD-NE-CZ	5.18	131.65	124.40
2	D	226	LYS	CG-CD-CE	5.17	123.18	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	TYR	N-CA-C	5.14	116.77	108.34
1	A	198	ASP	CA-CB-CG	5.11	117.71	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LYS	Mainchain
1	A	220	GLN	Mainchain,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	1499	0	1470	42	0
2	D	1873	0	1843	56	9
3	D	6	0	0	0	0
All	All	3378	0	3313	90	9

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 13.

All (90) 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)
2:D:201:ASP:OD1	2:D:201:ASP:CG	1.71	1.32
1:A:220:GLN:HG3	1:A:223:ASP:OD1	1.44	1.18
1:A:129:LYS:O	1:A:130:ASN:HB2	1.53	1.04
1:A:240:LEU:HD13	1:A:242:ASN:OD1	1.57	1.02
1:A:220:GLN:CG	1:A:223:ASP:OD1	2.11	0.99
1:A:147:TYR:HB2	2:D:126:HIS:CE1	1.98	0.97
2:D:245:LYS:HD3	2:D:282:GLU:HG2	1.47	0.95
2:D:245:LYS:NZ	2:D:280:THR:O	2.04	0.90
1:A:147:TYR:HB2	2:D:126:HIS:HE1	1.31	0.89
2:D:245:LYS:HD3	2:D:282:GLU:CG	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:O	1:A:220:GLN:HG2	1.75	0.87
2:D:225:ASN:OD1	2:D:244:ILE:HA	1.75	0.85
2:D:174:THR:OG1	2:D:176:VAL:HG22	1.78	0.83
2:D:225:ASN:OD1	2:D:245:LYS:N	2.12	0.82
2:D:133:ASN:OD1	2:D:134:ALA:N	2.13	0.81
2:D:133:ASN:OD1	2:D:133:ASN:C	2.27	0.76
2:D:227:VAL:O	2:D:227:VAL:HG23	1.85	0.75
1:A:190:SER:O	2:D:175:SER:HB2	1.85	0.74
2:D:180:ARG:HD3	2:D:215:ASP:HB2	1.69	0.72
1:A:220:GLN:CB	1:A:223:ASP:OD1	2.38	0.72
2:D:225:ASN:CG	2:D:245:LYS:H	1.98	0.71
2:D:163:TYR:CD2	2:D:163:TYR:C	2.73	0.67
2:D:180:ARG:CD	2:D:215:ASP:HB2	2.25	0.65
1:A:219:LYS:O	1:A:219:LYS:HD3	1.96	0.65
2:D:180:ARG:HD3	2:D:215:ASP:CB	2.26	0.65
1:A:147:TYR:CB	2:D:126:HIS:CE1	2.77	0.64
2:D:245:LYS:HZ3	2:D:280:THR:HB	1.64	0.62
1:A:240:LEU:HB3	1:A:242:ASN:OD1	1.99	0.62
1:A:219:LYS:O	1:A:220:GLN:CG	2.50	0.60
2:D:225:ASN:OD1	2:D:244:ILE:CA	2.50	0.59
1:A:240:LEU:CD1	1:A:242:ASN:OD1	2.42	0.59
1:A:202:HIS:CE1	1:A:224:PHE:O	2.55	0.58
2:D:217:ASN:HD22	2:D:311:PHE:HA	1.69	0.58
1:A:147:TYR:CG	2:D:126:HIS:CE1	2.92	0.58
2:D:224:GLU:O	2:D:225:ASN:C	2.47	0.57
2:D:217:ASN:ND2	2:D:311:PHE:HA	2.20	0.57
1:A:129:LYS:O	1:A:130:ASN:CB	2.32	0.56
2:D:161:VAL:C	2:D:174:THR:HG23	2.31	0.56
2:D:295:GLU:OE2	2:D:297:LYS:NZ	2.38	0.56
2:D:245:LYS:HD3	2:D:282:GLU:HG3	1.86	0.56
2:D:223:VAL:CG1	2:D:225:ASN:HB2	2.37	0.54
1:A:220:GLN:HB3	1:A:223:ASP:OD1	2.06	0.54
1:A:224:PHE:CE2	1:A:226:ALA:HB2	2.43	0.54
2:D:332:ASN:OD1	2:D:333:VAL:N	2.41	0.53
1:A:219:LYS:O	1:A:219:LYS:CD	2.57	0.53
1:A:147:TYR:HE2	2:D:172:TYR:CG	2.27	0.53
1:A:189:VAL:HG12	1:A:190:SER:N	2.24	0.52
1:A:228:GLY:HA3	1:A:319:ASP:OD1	2.09	0.52
2:D:120:GLU:HA	2:D:214:LEU:HB2	1.90	0.52
2:D:163:TYR:CD2	2:D:163:TYR:O	2.62	0.52
2:D:126:HIS:O	2:D:172:TYR:HD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:THR:OG1	2:D:201:ASP:N	2.44	0.51
1:A:219:LYS:O	1:A:220:GLN:CB	2.58	0.51
1:A:202:HIS:HE1	1:A:224:PHE:O	1.94	0.49
2:D:121:GLU:OE1	2:D:216:VAL:HG22	2.11	0.49
2:D:224:GLU:O	2:D:226:LYS:N	2.45	0.49
2:D:156:PRO:HG3	2:D:183:HIS:NE2	2.28	0.49
1:A:224:PHE:HE2	1:A:226:ALA:HB2	1.78	0.48
2:D:161:VAL:HG21	2:D:178:LEU:HG	1.94	0.48
2:D:245:LYS:NZ	2:D:280:THR:HB	2.27	0.48
1:A:220:GLN:HB3	1:A:223:ASP:HA	1.94	0.48
2:D:161:VAL:HG23	2:D:176:VAL:CG2	2.44	0.48
2:D:161:VAL:HA	2:D:174:THR:OG1	2.13	0.48
1:A:240:LEU:C	1:A:242:ASN:H	2.22	0.47
1:A:157:THR:HB	1:A:172:THR:HG22	1.97	0.47
2:D:316:ARG:C	2:D:318:LYS:H	2.22	0.46
2:D:156:PRO:HG3	2:D:183:HIS:CE1	2.51	0.46
2:D:161:VAL:HG22	2:D:161:VAL:O	2.16	0.46
2:D:180:ARG:HD3	2:D:215:ASP:CA	2.46	0.46
1:A:174:MET:HE3	1:A:304:THR:HG21	1.98	0.44
2:D:234:GLU:OE2	2:D:335:GLU:OE2	2.34	0.44
1:A:240:LEU:CB	1:A:242:ASN:OD1	2.63	0.44
1:A:147:TYR:CE2	2:D:172:TYR:CG	3.07	0.43
1:A:153:ASP:HB2	1:A:177:SER:HB3	2.00	0.43
2:D:174:THR:HG1	2:D:176:VAL:HG22	1.78	0.43
2:D:225:ASN:HD22	2:D:225:ASN:HA	1.65	0.43
2:D:176:VAL:CG2	2:D:176:VAL:O	2.67	0.42
2:D:188:LEU:HD12	2:D:189:THR:N	2.34	0.42
1:A:220:GLN:NE2	1:A:224:PHE:CD1	2.88	0.42
1:A:130:ASN:OD1	1:A:216:LEU:HD13	2.19	0.41
1:A:184:PHE:HD1	1:A:189:VAL:HG21	1.85	0.41
2:D:163:TYR:O	2:D:163:TYR:HD2	2.03	0.41
1:A:224:PHE:CD1	1:A:224:PHE:N	2.88	0.41
1:A:220:GLN:NE2	1:A:224:PHE:CE1	2.83	0.41
1:A:147:TYR:HE2	2:D:172:TYR:CD2	2.39	0.41
1:A:174:MET:CE	1:A:304:THR:HG21	2.51	0.41
1:A:240:LEU:HB3	1:A:242:ASN:CG	2.45	0.41
2:D:156:PRO:O	2:D:157:ALA:HB3	2.20	0.40
1:A:196:TYR:CD1	1:A:278:PRO:HG3	2.56	0.40
2:D:245:LYS:CD	2:D:282:GLU:HG3	2.52	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:226:LYS:O	2:D:226:LYS:O[5_555]	1.60	0.60
2:D:111:THR:O	2:D:233:GLU:OE2[15_556]	1.66	0.54
2:D:255:ASP:OD2	2:D:308:LYS:NZ[15_556]	1.72	0.48
2:D:227:VAL:CG1	2:D:227:VAL:CG1[5_555]	1.78	0.42
2:D:111:THR:C	2:D:233:GLU:OE2[15_556]	1.90	0.30
2:D:111:THR:CB	2:D:233:GLU:OE1[15_556]	2.00	0.20
2:D:226:LYS:CB	2:D:228:LEU:N[9_555]	2.03	0.17
2:D:226:LYS:C	2:D:226:LYS:O[9_555]	2.13	0.07
2:D:111:THR:OG1	2:D:233:GLU:OE1[15_556]	2.18	0.02

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	189/191 (99%)	179 (95%)	9 (5%)	1 (0%)	24	63
2	D	236/238 (99%)	224 (95%)	11 (5%)	1 (0%)	30	67
All	All	425/429 (99%)	403 (95%)	20 (5%)	2 (0%)	24	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	LYS
2	D	225	ASN

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	167/167 (100%)	166 (99%)	1 (1%)	78	80
2	D	213/213 (100%)	203 (95%)	10 (5%)	23	45
All	All	380/380 (100%)	369 (97%)	11 (3%)	37	58

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

Mol	Chain	Res	Type
1	A	152	PRO
2	D	133	ASN
2	D	163	TYR
2	D	164	LEU
2	D	176	VAL
2	D	225	ASN
2	D	226	LYS
2	D	245	LYS
2	D	246	VAL
2	D	317	SER
2	D	329	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	163	ASN
1	A	202	HIS
1	A	293	ASN
2	D	126	HIS
2	D	219	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 [i](#)

There are no oligosaccharides 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	191/191 (100%)	0.23	13 (6%)	23	25	290, 300, 322, 345	0
2	D	238/238 (100%)	0.21	5 (2%)	63	50	271, 302, 334, 361	0
All	All	429/429 (100%)	0.22	18 (4%)	40	35	271, 301, 330, 361	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PHE	4.7
2	D	132	ILE	4.3
1	A	191	ILE	3.8
1	A	241	PRO	3.4
2	D	178	LEU	3.3
1	A	210	LEU	3.1
1	A	286	MET	3.1
1	A	195	LEU	3.1
1	A	189	VAL	2.7
1	A	252	PHE	2.7
1	A	197	PHE	2.6
2	D	234	GLU	2.4
1	A	311	THR	2.4
1	A	205	PRO	2.3
1	A	292	LEU	2.3
1	A	285	VAL	2.2
2	D	141	ASN	2.2
2	D	333	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

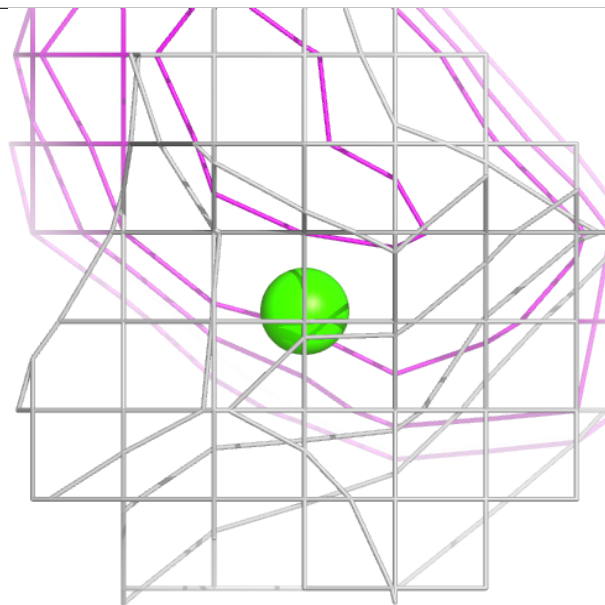
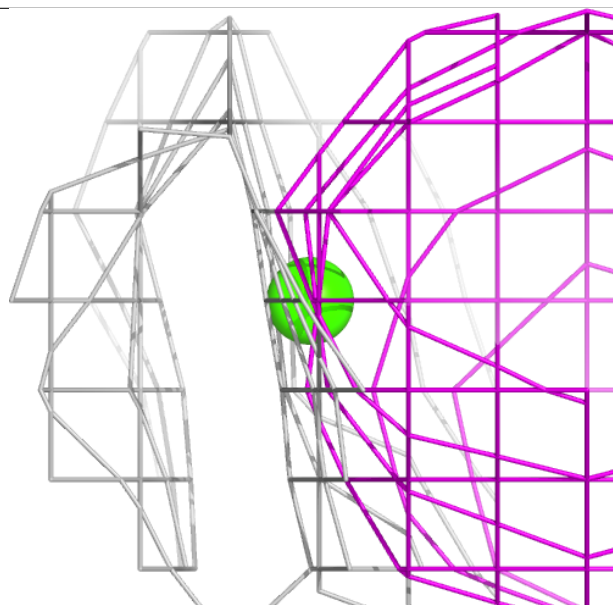
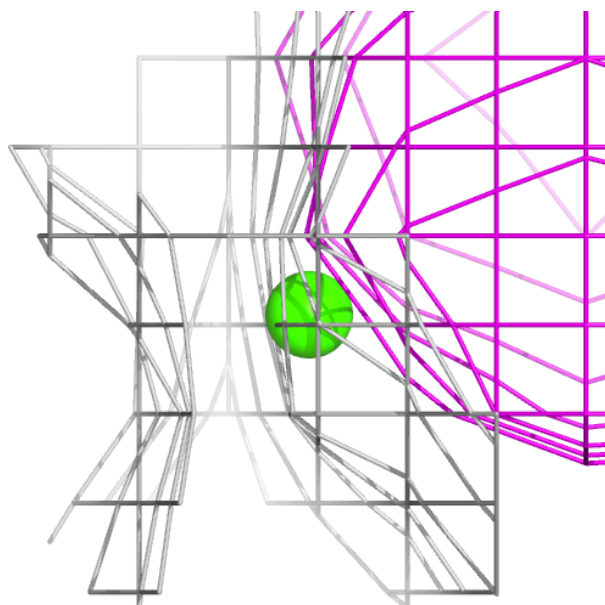
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	D	406	1/1	0.01	0.18	297,297,297,297	0
3	CA	D	405	1/1	0.67	0.14	297,297,297,297	0
3	CA	D	403	1/1	0.78	0.12	297,297,297,297	0
3	CA	D	402	1/1	0.89	0.07	297,297,297,297	0
3	CA	D	404	1/1	0.90	0.12	297,297,297,297	0
3	CA	D	401	1/1	0.93	0.14	297,297,297,297	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.

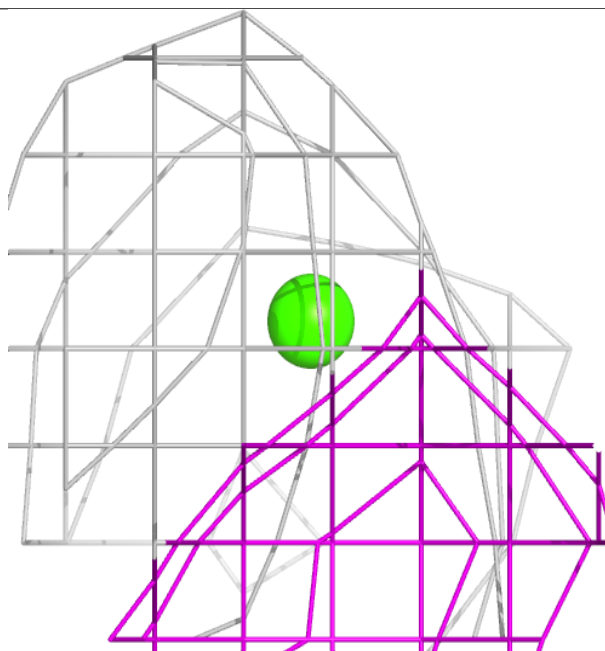
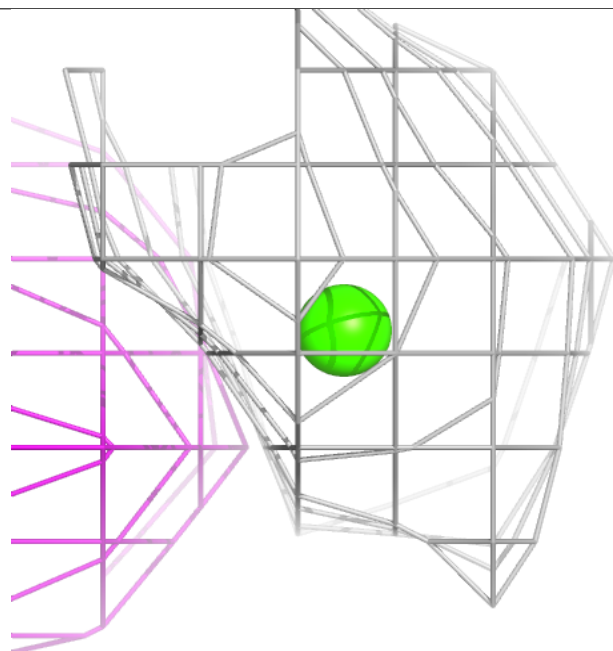
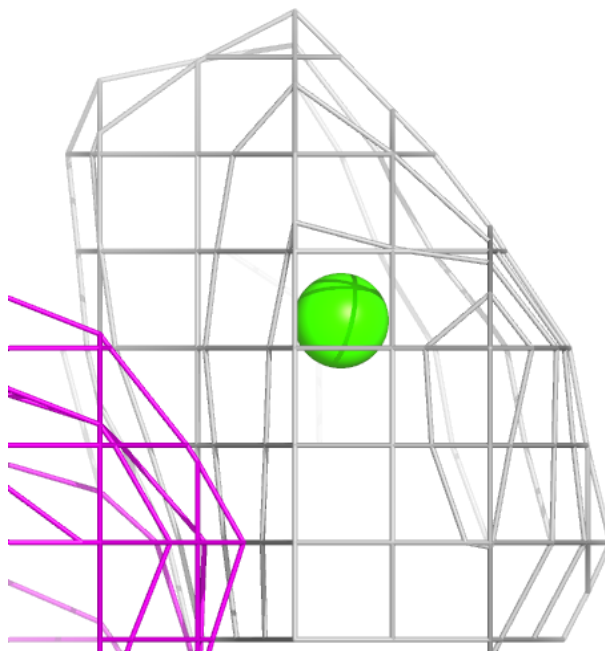
Electron density around CA D 406:

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



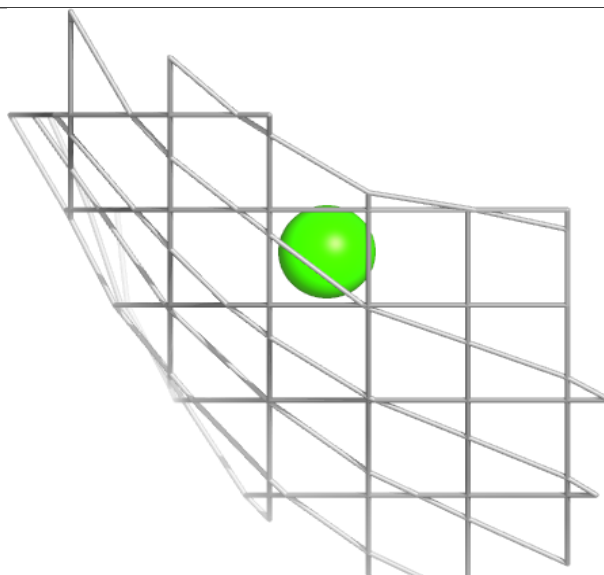
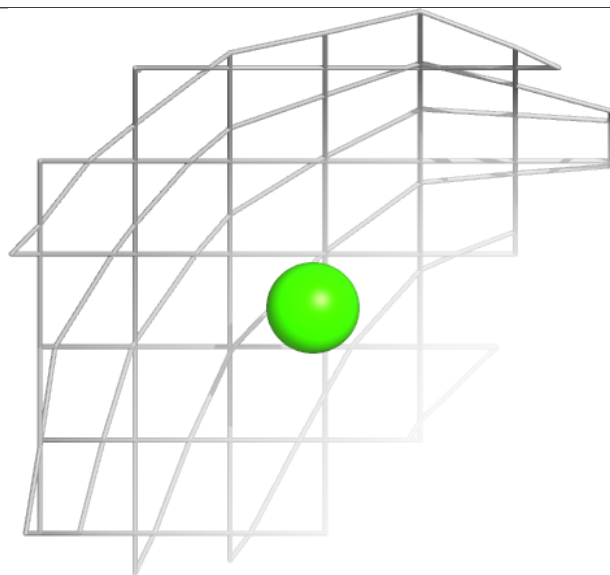
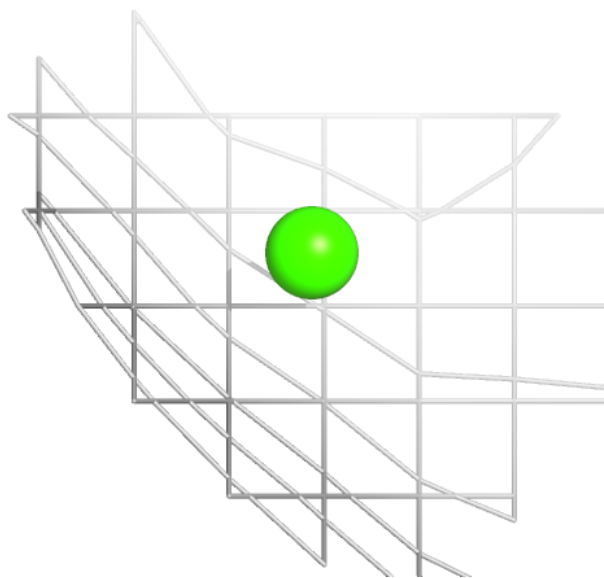
Electron density around CA D 405:

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and green (positive)



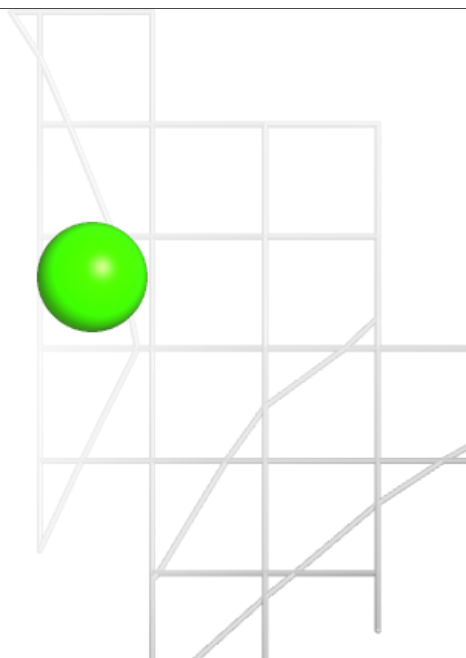
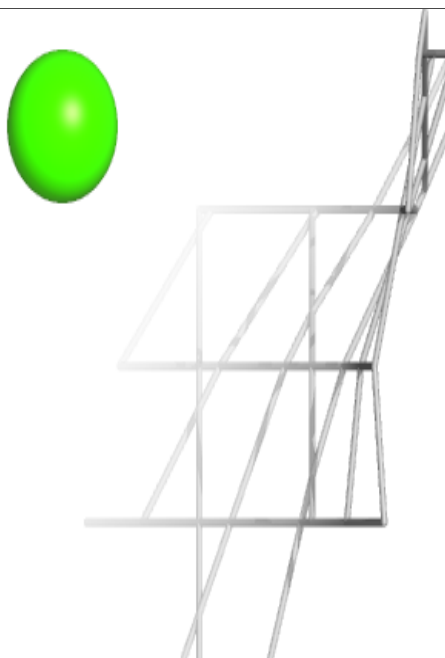
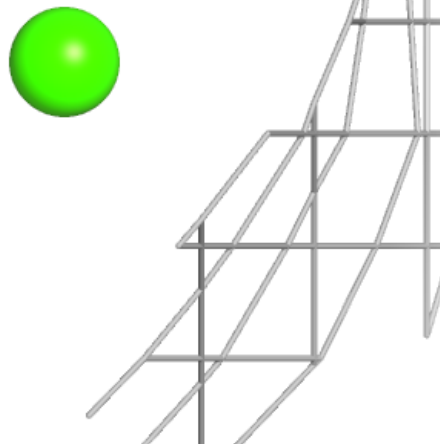
Electron density around CA D 403:

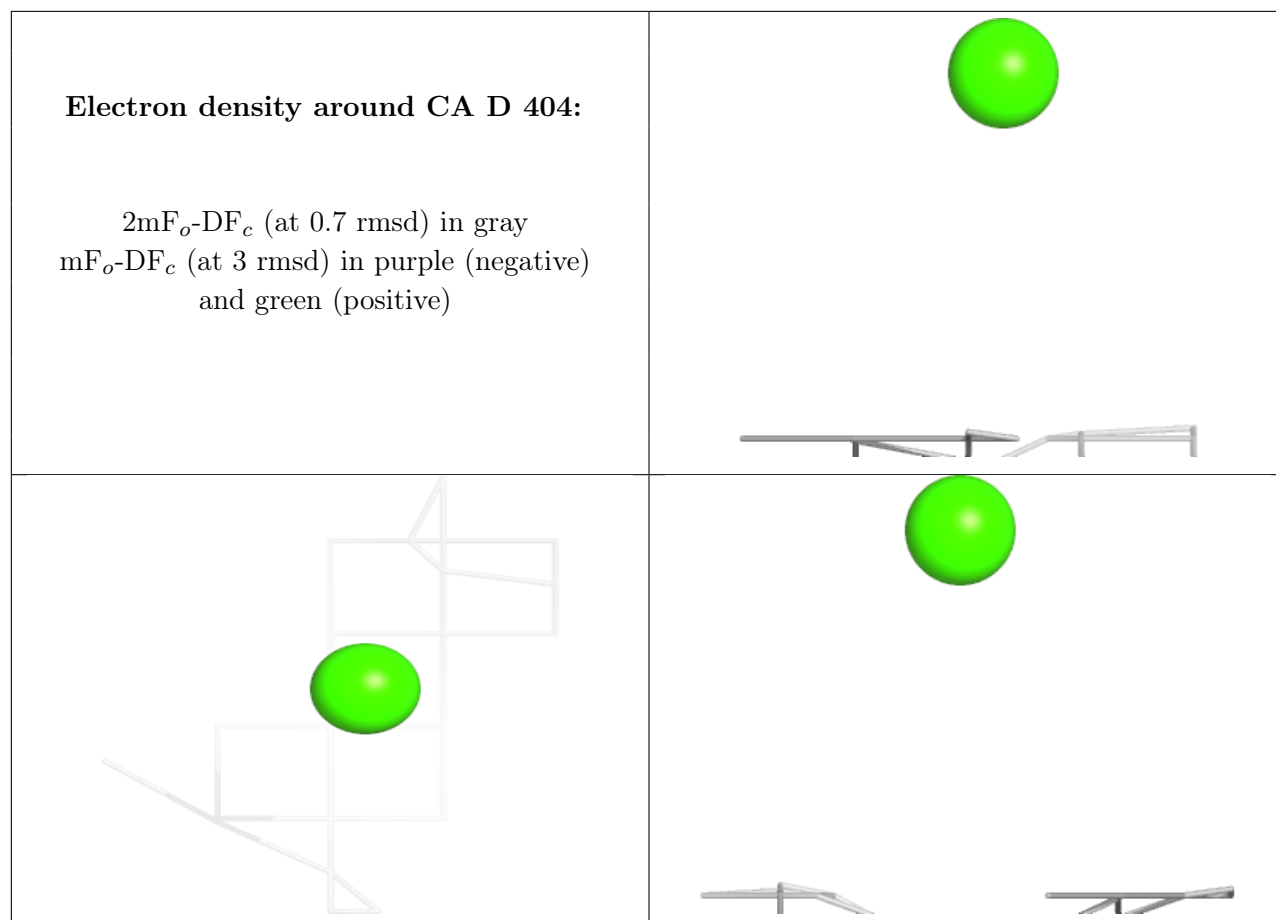
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

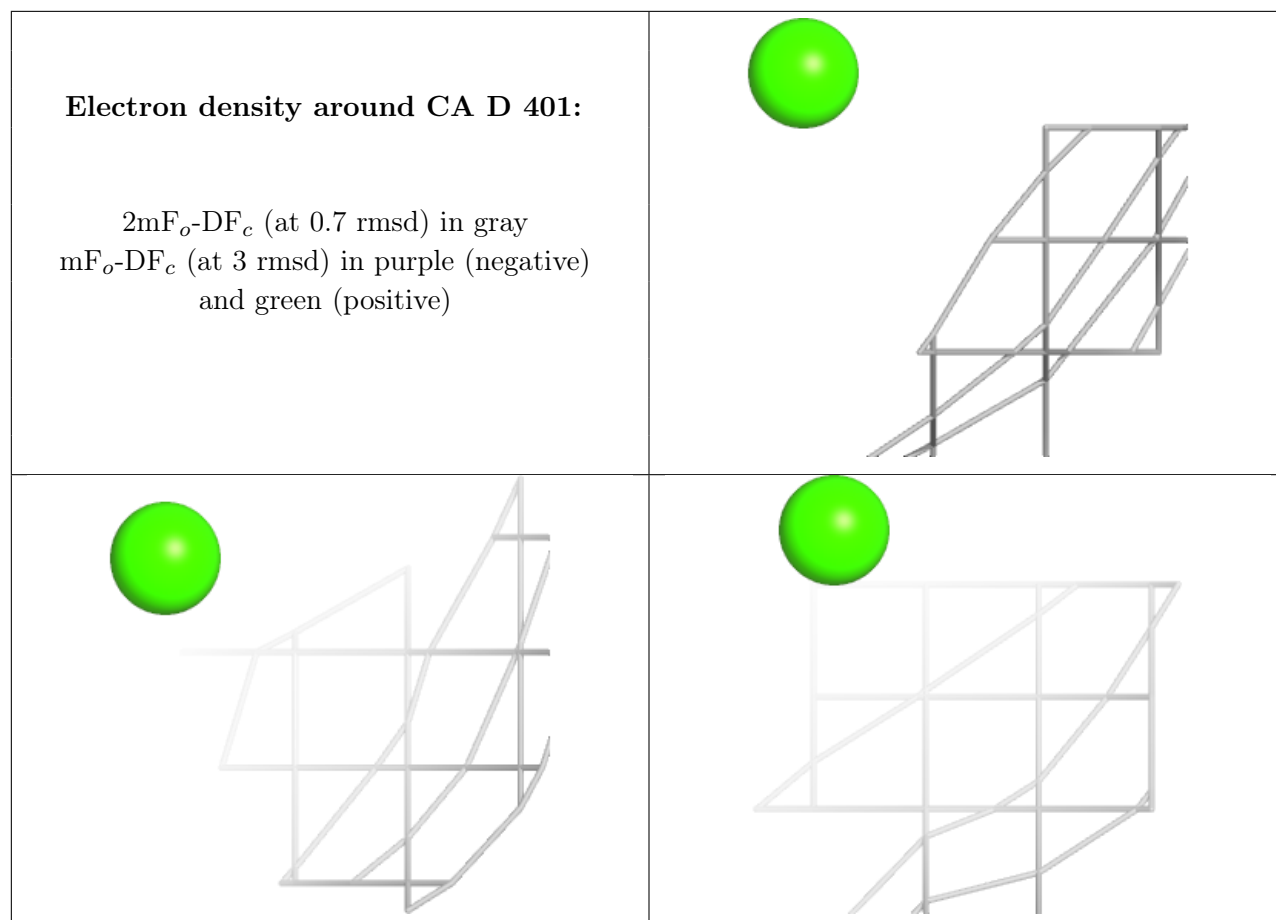


Electron density around CA D 402:

$2mF_o-DF_c$ (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.