Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2025 – 02:11 PM JST

PDB ID	:	8Y41
Title	:	VcFadRqm, mutant protein of Fatty Acid Responsive Transcription Factor from Vibrio cholerae, in Complex with oleoyl-CoA
Authors	:	Tsui, W.; Shi, W.
Deposited on	:	2024-01-30
Resolution	:	2.58 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:

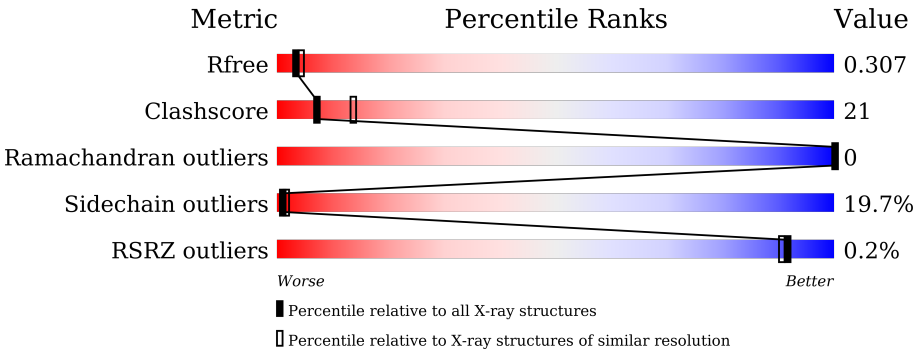
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.58 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	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	279	54% 33% 6% 6%
1	D	279	54% 29% 11% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4442 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.

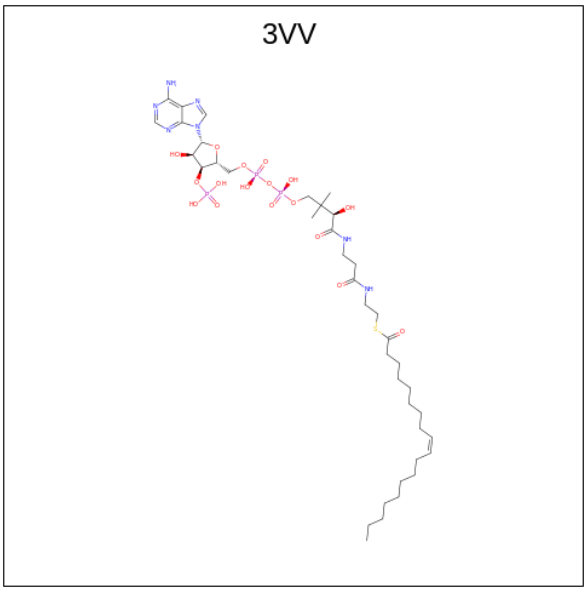
- Molecule 1 is a protein called Fatty acid metabolism regulator protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2109	1352	360	387	10			
1	D	263	Total	C	N	O	S	0	0	0
			2120	1360	362	388	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ALA	TYR	engineered mutation	UNP A0A085QQF2
A	167	GLU	LYS	engineered mutation	UNP A0A085QQF2
A	214	PHE	LEU	engineered mutation	UNP A0A085QQF2
A	219	PHE	LEU	engineered mutation	UNP A0A085QQF2
D	162	ALA	TYR	engineered mutation	UNP A0A085QQF2
D	165	GLU	LYS	engineered mutation	UNP A0A085QQF2
D	212	PHE	LEU	engineered mutation	UNP A0A085QQF2
D	217	PHE	LEU	engineered mutation	UNP A0A085QQF2

- Molecule 2 is S-{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (9Z)-octadec-9-enethioate (non-preferred name) (three-letter code: 3VV) (formula: $C_{39}H_{68}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			67	39	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			67	39	7	17	3	1		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cd	0	0
			2	2		
3	D	2	Total	Cd	0	0
			2	2		

- Molecule 4 is water.

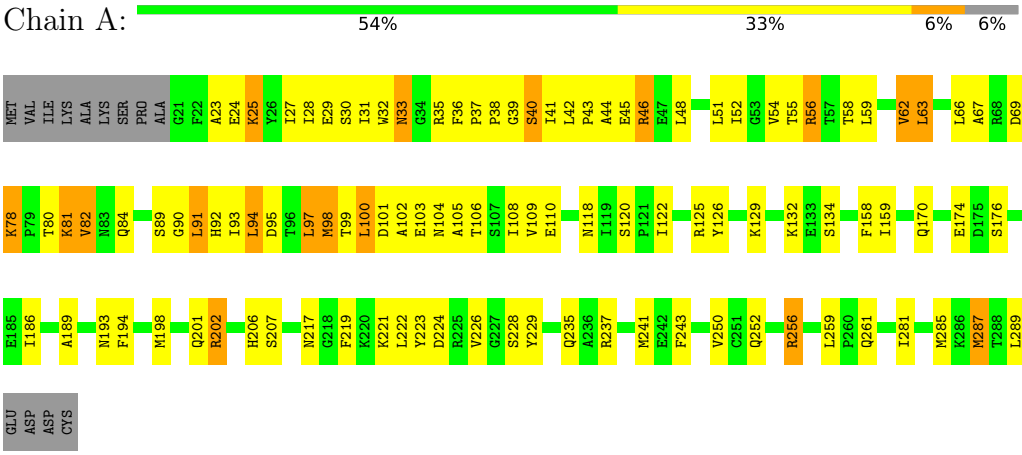
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	D	34	Total	O	0	0
			34	34		

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.

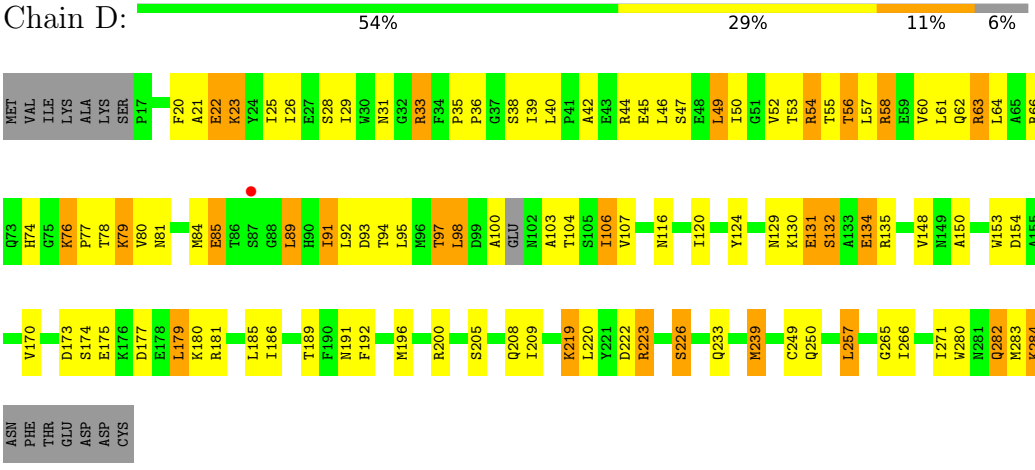
• Molecule 1: Fatty acid metabolism regulator protein

Chain A:



• Molecule 1: Fatty acid metabolism regulator protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.73Å 57.34Å 57.48Å 67.92° 63.35° 90.02°	Depositor
Resolution (Å)	19.49 – 2.58 19.49 – 2.58	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.49-2.58) 98.7 (19.49-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.248 , 0.261 0.283 , 0.307	Depositor DCC
R_{free} test set	742 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.156 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4442	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% 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: CD, 3VV

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	0.58	0/2157	0.76	0/2917
1	D	0.59	0/2168	0.76	0/2929
All	All	0.58	0/4325	0.76	0/5846

There are no bond length outliers.

There are no bond angle outliers.

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	2109	0	2077	89	0
1	D	2120	0	2098	90	0
2	A	67	0	64	3	0
2	D	67	0	64	17	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	41	0	0	1	0
4	D	34	0	0	0	0
All	All	4442	0	4303	178	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 21.

All (178) 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:A:99:THR:HA	1:A:222:LEU:HD13	1.28	1.08
1:D:23:LYS:HE2	1:D:92:LEU:HB2	1.36	1.06
1:A:129:LYS:HB3	2:D:301:3VV:N63	1.75	1.02
1:A:42:LEU:HD22	1:A:82:VAL:HG12	1.48	0.94
1:A:129:LYS:HD3	2:D:301:3VV:H67	1.36	0.88
1:A:38:PRO:HA	1:A:82:VAL:HG22	1.62	0.81
1:A:100:LEU:HB2	1:A:105:ALA:HB3	1.61	0.80
1:D:22:GLU:HA	1:D:64:LEU:HD11	1.63	0.79
1:D:148:VAL:HG21	1:D:239:MET:HE1	1.66	0.78
1:A:99:THR:CA	1:A:222:LEU:HD13	2.14	0.76
1:A:43:PRO:HG2	1:A:48:LEU:HD13	1.67	0.75
1:A:129:LYS:CB	2:D:301:3VV:N63	2.49	0.75
1:A:129:LYS:HB3	2:D:301:3VV:H67	1.50	0.74
1:D:39:ILE:HD13	1:D:79:LYS:HB3	1.71	0.72
1:A:94:LEU:O	1:A:97:LEU:HD11	1.89	0.72
1:A:97:LEU:HD13	1:A:219:PHE:CE1	2.25	0.71
1:A:243:PHE:HA	4:A:406:HOH:O	1.91	0.70
1:D:153:TRP:HD1	1:D:186:ILE:HG22	1.57	0.69
1:D:58:ARG:O	1:D:62:GLN:HG2	1.92	0.69
1:A:23:ALA:HB2	1:A:54:VAL:HG11	1.76	0.67
1:A:129:LYS:CD	2:D:301:3VV:N63	2.58	0.67
1:A:129:LYS:HD3	2:D:301:3VV:N63	2.08	0.67
1:D:28:SER:HB2	1:D:33:ARG:HG2	1.78	0.66
1:A:129:LYS:CD	2:D:301:3VV:H67	2.06	0.66
1:A:31:ILE:HG12	1:A:36:PHE:HB2	1.78	0.66
1:A:94:LEU:HA	1:A:97:LEU:HD21	1.78	0.66
1:A:106:THR:O	1:A:110:GLU:HG2	1.95	0.65
1:D:153:TRP:CD1	1:D:186:ILE:HG22	2.32	0.64
1:A:90:GLY:HA3	1:A:92:HIS:CE1	2.33	0.63
1:A:125:ARG:HD3	2:D:301:3VV:C59	2.28	0.63
1:D:97:THR:HA	1:D:223:ARG:CZ	2.30	0.62
1:D:33:ARG:HH22	1:D:49:LEU:HD22	1.64	0.62
1:D:91:ILE:H	1:D:93:ASP:CG	2.03	0.62
1:A:129:LYS:HB3	2:D:301:3VV:H66	1.60	0.61
1:A:217:ASN:HB3	1:D:85:GLU:O	2.01	0.61
1:A:99:THR:HG22	1:A:222:LEU:HB2	1.82	0.61
1:A:180:GLU:O	1:A:184:GLN:HG2	2.01	0.61
1:D:22:GLU:HB2	1:D:64:LEU:HD21	1.83	0.61
1:D:97:THR:HB	1:D:100:ALA:HB3	1.82	0.60
1:A:122:ILE:HG21	1:D:116:ASN:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LYS:O	1:D:134:GLU:HG3	2.01	0.60
1:D:74:HIS:CE1	1:D:76:LYS:HG2	2.38	0.59
1:D:22:GLU:HG3	1:D:23:LYS:N	2.18	0.58
1:D:196:MET:HG3	1:D:200:ARG:HD2	1.85	0.58
1:A:45:GLU:HB2	1:A:56:ARG:CZ	2.34	0.58
1:D:72:ILE:HA	1:D:74:HIS:CE1	2.38	0.57
1:A:100:LEU:HD11	1:A:103:GLU:HA	1.88	0.56
1:A:44:ALA:O	1:A:48:LEU:HB2	2.06	0.55
1:A:24:GLU:HA	1:A:66:LEU:HD11	1.88	0.55
1:A:125:ARG:HD3	2:D:301:3VV:H65	1.89	0.54
1:D:42:ALA:HB3	1:D:45:GLU:OE1	2.08	0.54
1:D:20:PHE:HB2	1:D:23:LYS:HZ2	1.72	0.54
1:A:29:GLU:HB3	1:A:104:ASN:HB2	1.90	0.54
1:A:193:ASN:ND2	1:A:224:ASP:HA	2.23	0.54
1:A:27:ILE:O	1:A:31:ILE:HG13	2.07	0.54
1:A:118:ASN:HB3	1:D:120:ILE:HG21	1.89	0.53
2:D:301:3VV:H68	2:D:301:3VV:O43	2.08	0.53
1:A:193:ASN:HD21	1:A:224:ASP:HA	1.74	0.53
1:D:23:LYS:NZ	1:D:92:LEU:HD13	2.23	0.53
1:A:109:VAL:HG11	1:A:226:VAL:HG21	1.91	0.53
1:D:72:ILE:HG22	1:D:78:THR:HA	1.89	0.52
1:A:25:LYS:HZ1	1:A:98:MET:CG	2.22	0.52
1:A:30:SER:HB3	1:A:35:ARG:HB3	1.92	0.52
1:D:150:ALA:HB2	1:D:156:PHE:HB2	1.92	0.52
1:D:222:ASP:O	1:D:226:SER:HB3	2.09	0.52
1:D:23:LYS:HB3	1:D:91:ILE:C	2.31	0.51
1:D:39:ILE:HD12	1:D:77:PRO:HB2	1.91	0.51
1:A:52:ILE:HB	1:A:54:VAL:HG22	1.93	0.51
1:A:100:LEU:CD1	1:A:103:GLU:HA	2.41	0.51
1:D:40:LEU:HD22	1:D:70:LEU:HD11	1.92	0.51
1:D:107:VAL:HG22	1:D:220:LEU:HD21	1.93	0.51
1:A:91:LEU:HD21	1:D:89:LEU:HB3	1.91	0.50
1:A:35:ARG:O	1:A:37:PRO:HD3	2.11	0.50
1:A:100:LEU:CB	1:A:105:ALA:HB3	2.36	0.50
1:D:103:ALA:HB1	1:D:106:ILE:HB	1.93	0.50
1:A:102:ALA:H	1:A:104:ASN:ND2	2.10	0.50
1:D:175:GLU:OE2	1:D:180:LYS:HB3	2.12	0.50
1:A:46:ARG:HA	1:A:56:ARG:HD2	1.94	0.50
1:D:54:ARG:O	1:D:58:ARG:HB2	2.11	0.50
1:A:46:ARG:HG2	1:A:56:ARG:NH1	2.26	0.49
1:A:62:VAL:HG12	1:A:63:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:SER:HA	1:D:31:ASN:ND2	2.27	0.49
1:A:122:ILE:HD11	1:D:120:ILE:HD11	1.93	0.49
1:D:153:TRP:HB2	1:D:186:ILE:CG2	2.43	0.49
1:D:271:ILE:HA	1:D:282:GLN:NE2	2.27	0.49
1:D:52:VAL:HG23	1:D:57:LEU:HB2	1.95	0.49
1:A:75:GLN:O	1:A:78:LYS:HD2	2.13	0.48
1:D:91:ILE:HG12	1:D:93:ASP:CG	2.34	0.48
1:D:25:ILE:O	1:D:29:ILE:HG13	2.14	0.48
1:A:92:HIS:CD2	1:A:93:ILE:HG13	2.49	0.48
1:D:26:ILE:HD12	1:D:91:ILE:HD12	1.95	0.48
1:A:126:TYR:HB3	1:A:207:SER:O	2.14	0.48
1:A:182:LYS:O	1:A:186:ILE:HG12	2.14	0.48
1:D:91:ILE:HG12	1:D:93:ASP:OD2	2.14	0.48
1:D:219:LYS:HB3	1:D:219:LYS:HE2	1.51	0.47
1:A:250:VAL:HG11	1:A:259:LEU:HG	1.96	0.47
1:D:266:ILE:HG13	2:D:301:3VV:H49	1.97	0.47
1:A:37:PRO:HB2	1:A:40:SER:HB2	1.96	0.47
1:A:81:LYS:HB2	1:A:81:LYS:HE2	1.41	0.47
1:A:92:HIS:HD2	1:A:93:ILE:HG13	1.80	0.47
1:A:37:PRO:HB2	1:A:40:SER:OG	2.15	0.46
1:A:37:PRO:HB2	1:A:40:SER:CB	2.45	0.46
1:A:125:ARG:HG3	1:A:256:ARG:HB2	1.98	0.46
1:D:116:ASN:HA	2:D:301:3VV:O57	2.15	0.46
1:A:29:GLU:O	1:A:33:ASN:HB3	2.16	0.46
1:D:60:VAL:HG12	1:D:61:LEU:HD23	1.98	0.46
1:A:129:LYS:HD2	2:D:301:3VV:N64	2.31	0.46
2:A:301:3VV:O57	2:A:301:3VV:H58	2.16	0.46
1:D:130:LYS:O	1:D:134:GLU:CG	2.64	0.46
1:A:32:TRP:HE3	1:A:108:ILE:HD13	1.80	0.46
1:A:97:LEU:HD13	1:A:219:PHE:HE1	1.79	0.46
1:D:76:LYS:HE2	1:D:79:LYS:HD3	1.98	0.45
1:A:42:LEU:HD12	1:A:42:LEU:HA	1.72	0.45
1:A:94:LEU:H	1:A:94:LEU:HG	1.47	0.45
1:A:229:TYR:CE2	1:A:287:MET:O	2.69	0.45
1:A:37:PRO:HD2	1:A:41:ILE:H	1.82	0.45
1:D:170:VAL:HG12	1:D:185:LEU:HD23	1.99	0.45
1:D:76:LYS:CE	1:D:79:LYS:HD3	2.46	0.45
1:D:52:VAL:HB	1:D:56:THR:HB	1.98	0.45
1:D:157:ILE:HD11	1:D:166:ILE:HB	1.98	0.45
1:A:48:LEU:O	1:A:52:ILE:HG13	2.17	0.45
1:D:35:PRO:HD2	1:D:38:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:HG22	1:A:285:MET:CE	2.46	0.45
1:D:129:ASN:HB3	1:D:132:SER:OG	2.18	0.45
1:A:67:ALA:HB2	1:A:72:LEU:HD12	1.99	0.44
1:A:30:SER:HB2	1:A:36:PHE:CD2	2.53	0.44
1:A:39:GLY:N	1:A:82:VAL:O	2.46	0.44
1:D:103:ALA:O	1:D:104:THR:C	2.54	0.44
1:A:24:GLU:HG3	1:A:62:VAL:HG22	2.00	0.44
1:D:280:TRP:CE2	1:D:284:LYS:HB2	2.52	0.44
1:A:198:MET:O	1:A:202:ARG:HB2	2.17	0.44
1:D:179:LEU:HD12	1:D:179:LEU:HA	1.81	0.44
1:D:285:MET:HB3	1:D:285:MET:HE3	1.75	0.44
1:D:97:THR:HG22	1:D:98:LEU:H	1.83	0.44
1:A:99:THR:O	1:A:100:LEU:HB3	2.17	0.43
1:D:156:PHE:CZ	1:D:189:THR:HG21	2.54	0.43
1:A:132:LYS:NZ	1:A:252:GLN:HA	2.33	0.43
1:D:131:GLU:O	1:D:135:ARG:HG3	2.19	0.43
1:D:21:ALA:HB2	1:D:52:VAL:HG21	2.01	0.43
1:D:94:THR:HB	1:D:220:LEU:HD22	2.00	0.43
1:D:130:LYS:HE3	1:D:250:GLN:HA	2.01	0.43
1:D:130:LYS:HE3	1:D:249:CYS:O	2.18	0.43
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.43
1:D:74:HIS:HE2	1:D:79:LYS:HE3	1.82	0.43
1:D:156:PHE:CE2	1:D:189:THR:HG21	2.54	0.43
1:A:38:PRO:HA	1:A:82:VAL:CG2	2.40	0.43
1:D:131:GLU:HA	1:D:134:GLU:HG3	2.00	0.43
1:A:223:TYR:HA	2:A:301:3VV:H34	2.00	0.43
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.83	0.42
1:D:175:GLU:OE1	1:D:177:ASP:HB3	2.18	0.42
1:D:153:TRP:HB2	1:D:186:ILE:HG23	2.00	0.42
1:D:191:ASN:HD21	1:D:222:ASP:HA	1.84	0.42
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.79	0.42
1:A:129:LYS:HD2	2:D:301:3VV:C62	2.50	0.42
1:D:63:ARG:HA	1:D:66:ARG:HB2	2.01	0.42
1:D:265:GLY:HA3	2:D:301:3VV:O30	2.19	0.42
1:D:89:LEU:HD13	1:D:89:LEU:HA	1.68	0.42
1:A:42:LEU:HD23	1:A:80:THR:O	2.20	0.42
1:D:36:PRO:HB3	1:D:81:ASN:O	2.19	0.42
1:A:36:PHE:HD1	1:A:41:ILE:HG22	1.84	0.42
1:D:97:THR:CB	1:D:100:ALA:HB3	2.48	0.42
1:D:175:GLU:HB3	1:D:181:ARG:HG3	2.01	0.42
1:D:124:TYR:HB3	1:D:205:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:O	1:A:78:LYS:HB2	2.20	0.41
1:D:46:LEU:HD23	1:D:57:LEU:HD21	2.02	0.41
1:D:89:LEU:HA	1:D:93:ASP:OD2	2.21	0.41
1:D:106:ILE:HD12	1:D:106:ILE:HA	1.72	0.41
1:D:49:LEU:HD23	1:D:50:ILE:HG13	2.03	0.41
1:D:150:ALA:CB	1:D:156:PHE:HB2	2.51	0.41
1:A:46:ARG:HG2	1:A:46:ARG:H	1.54	0.41
1:A:237:ARG:O	1:A:241:MET:HG3	2.21	0.41
1:D:25:ILE:HD11	1:D:50:ILE:HD11	2.03	0.41
1:D:91:ILE:C	1:D:93:ASP:N	2.74	0.41
2:D:301:3VV:H26	2:D:301:3VV:H20	1.84	0.41
1:D:71:THR:O	1:D:79:LYS:HG3	2.22	0.40
1:A:189:ALA:HB1	1:A:228:SER:O	2.20	0.40
2:A:301:3VV:H20	2:A:301:3VV:H26	1.83	0.40
1:D:280:TRP:NE1	1:D:284:LYS:HE3	2.37	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	260/279 (93%)	230 (88%)	30 (12%)	0	100	100
1	D	259/279 (93%)	228 (88%)	31 (12%)	0	100	100
All	All	519/558 (93%)	458 (88%)	61 (12%)	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	222/241 (92%)	180 (81%)	42 (19%)	1 2
1	D	224/241 (93%)	178 (80%)	46 (20%)	1 1
All	All	446/482 (92%)	358 (80%)	88 (20%)	1 2

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	ILE
1	A	33	ASN
1	A	40	SER
1	A	46	ARG
1	A	51	LEU
1	A	55	THR
1	A	56	ARG
1	A	58	THR
1	A	62	VAL
1	A	63	LEU
1	A	69	ASP
1	A	78	LYS
1	A	81	LYS
1	A	82	VAL
1	A	84	GLN
1	A	89	SER
1	A	91	LEU
1	A	94	LEU
1	A	95	ASP
1	A	97	LEU
1	A	98	MET
1	A	100	LEU
1	A	101	ASP
1	A	120	SER
1	A	134	SER
1	A	158	PHE
1	A	170	GLN
1	A	174	GLU
1	A	176	SER
1	A	181	LEU

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Mol	Chain	Res	Type
1	A	183	ARG
1	A	194	PHE
1	A	201	GLN
1	A	202	ARG
1	A	206	HIS
1	A	221	LYS
1	A	235	GLN
1	A	256	ARG
1	A	261	GLN
1	A	287	MET
1	A	289	LEU
1	D	22	GLU
1	D	23	LYS
1	D	33	ARG
1	D	44	ARG
1	D	47	SER
1	D	49	LEU
1	D	53	THR
1	D	54	ARG
1	D	55	THR
1	D	56	THR
1	D	58	ARG
1	D	63	ARG
1	D	70	LEU
1	D	72	ILE
1	D	76	LYS
1	D	79	LYS
1	D	80	VAL
1	D	84	MET
1	D	85	GLU
1	D	89	LEU
1	D	91	ILE
1	D	95	LEU
1	D	97	THR
1	D	98	LEU
1	D	106	ILE
1	D	131	GLU
1	D	132	SER
1	D	134	GLU
1	D	154	ASP
1	D	156	PHE
1	D	157	ILE

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Mol	Chain	Res	Type
1	D	173	ASP
1	D	174	SER
1	D	179	LEU
1	D	192	PHE
1	D	208	GLN
1	D	209	ILE
1	D	219	LYS
1	D	223	ARG
1	D	226	SER
1	D	233	GLN
1	D	239	MET
1	D	257	LEU
1	D	282	GLN
1	D	283	MET
1	D	284	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	92	HIS
1	A	118	ASN
1	A	193	ASN
1	A	217	ASN
1	D	116	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	3VV	A	301	-	61,69,69	0.57	1 (1%)	72,95,95	0.78	2 (2%)
2	3VV	D	301	-	61,69,69	0.59	2 (3%)	72,95,95	0.70	1 (1%)

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
2	3VV	A	301	-	-	26/64/84/84	0/3/3/3
2	3VV	D	301	-	-	26/64/84/84	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	3VV	P54-O53	2.27	1.63	1.59
2	D	301	3VV	C59-N60	-2.06	1.31	1.34
2	A	301	3VV	P54-O53	2.04	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	3VV	P42-O41-P38	-2.85	123.04	132.83
2	D	301	3VV	C61-C62-N63	2.31	123.86	120.35
2	A	301	3VV	C61-C62-N63	2.22	123.73	120.35

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	3VV	S20-C21-C22-N23
2	A	301	3VV	C36-O37-P38-O39
2	A	301	3VV	C36-O37-P38-O41
2	A	301	3VV	C46-O45-P42-O41
2	A	301	3VV	C29-C31-C33-C34
2	A	301	3VV	C29-C31-C33-C36
2	A	301	3VV	O32-C31-C33-C34
2	A	301	3VV	O32-C31-C33-C35
2	A	301	3VV	O32-C31-C33-C36
2	A	301	3VV	C31-C33-C36-O37
2	A	301	3VV	C34-C33-C36-O37
2	A	301	3VV	C35-C33-C36-O37
2	A	301	3VV	C47-C52-O53-P54
2	D	301	3VV	S20-C21-C22-N23
2	D	301	3VV	C26-C24-N23-C22
2	D	301	3VV	O25-C24-N23-C22
2	D	301	3VV	C24-C26-C27-N28
2	D	301	3VV	C36-O37-P38-O39
2	D	301	3VV	C46-O45-P42-O41
2	D	301	3VV	C46-O45-P42-O43
2	D	301	3VV	C46-O45-P42-O44
2	D	301	3VV	C29-C31-C33-C34
2	D	301	3VV	C29-C31-C33-C36
2	D	301	3VV	O32-C31-C33-C34
2	D	301	3VV	O32-C31-C33-C36
2	A	301	3VV	C03-C04-C05-C06
2	D	301	3VV	C03-C04-C05-C06
2	A	301	3VV	O45-C46-C47-O48
2	A	301	3VV	C10-C11-C12-C13
2	A	301	3VV	C14-C15-C16-C17
2	A	301	3VV	C01-C02-C03-C04
2	D	301	3VV	C01-C02-C03-C04
2	A	301	3VV	C11-C12-C13-C14
2	A	301	3VV	C06-C07-C08-C09
2	D	301	3VV	C06-C07-C08-C09
2	A	301	3VV	C05-C06-C07-C08
2	D	301	3VV	O32-C31-C33-C35
2	A	301	3VV	C08-C09-C10-C11
2	D	301	3VV	C05-C06-C07-C08
2	A	301	3VV	C29-C31-C33-C35
2	D	301	3VV	C36-O37-P38-O41
2	D	301	3VV	P38-O41-P42-O44
2	A	301	3VV	C46-O45-P42-O43

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Mol	Chain	Res	Type	Atoms
2	D	301	3VV	C36-O37-P38-O40
2	D	301	3VV	C14-C15-C16-C17
2	D	301	3VV	P38-O41-P42-O43
2	A	301	3VV	C22-C21-S20-C18
2	D	301	3VV	C22-C21-S20-C18
2	A	301	3VV	C13-C14-C15-C16
2	D	301	3VV	C07-C08-C09-C10
2	D	301	3VV	C29-C31-C33-C35
2	D	301	3VV	O45-C46-C47-C52

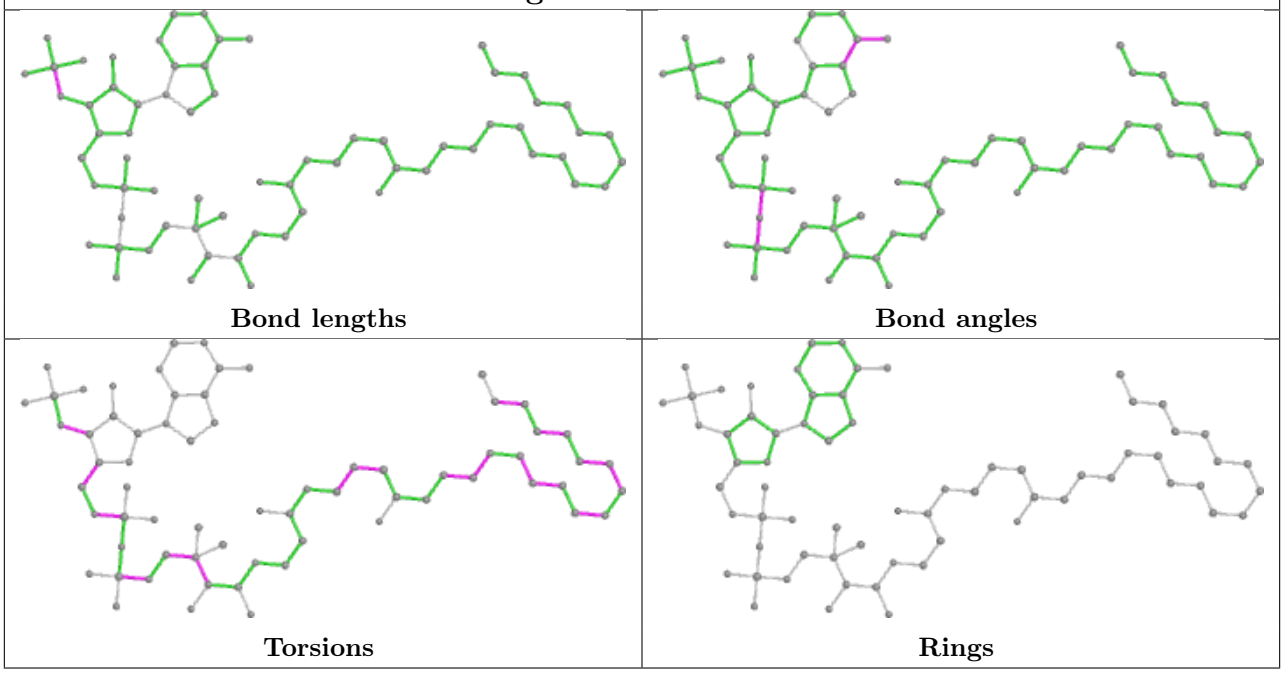
There are no ring outliers.

2 monomers are involved in 20 short contacts:

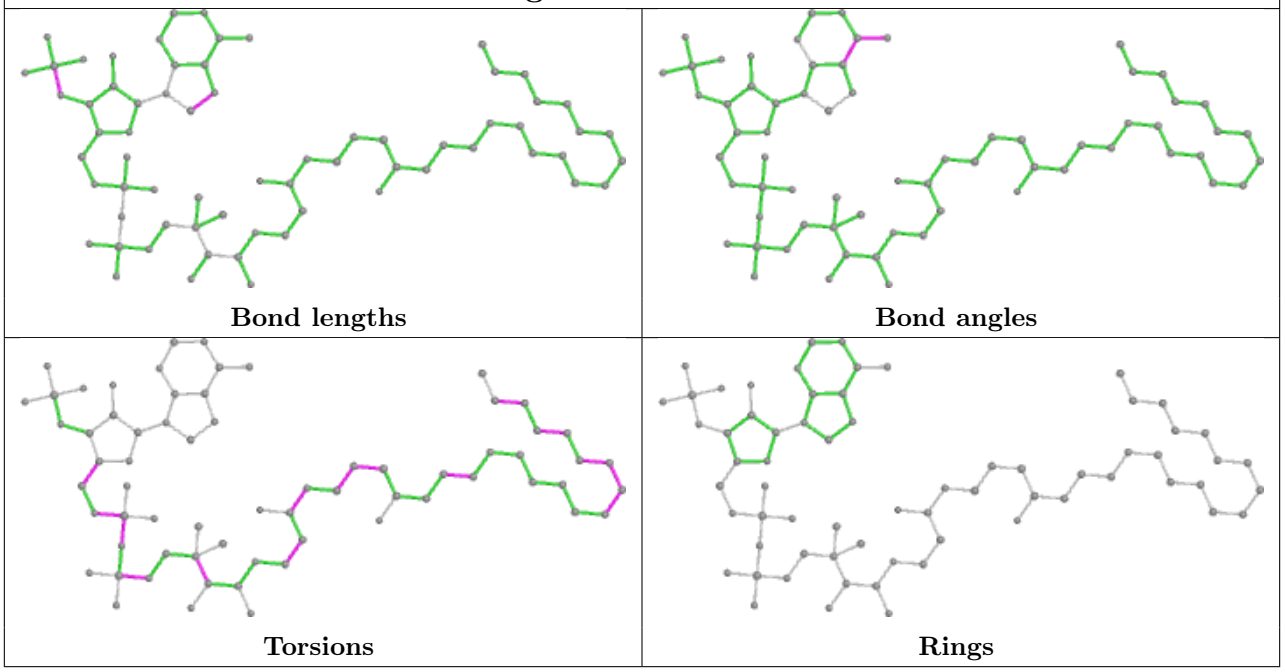
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	3VV	3	0
2	D	301	3VV	17	0

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 then 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.

Ligand 3VV A 301



Ligand 3VV D 301



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, 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	262/279 (93%)	-1.08	0 100 100	25, 43, 126, 208	0
1	D	263/279 (94%)	-1.04	1 (0%) 89 87	24, 44, 120, 202	0
All	All	525/558 (94%)	-1.06	1 (0%) 92 90	24, 43, 126, 208	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	SER	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

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	3VV	A	301	67/67	0.97	0.06	23,44,119,122	0
2	3VV	D	301	67/67	0.98	0.05	22,38,70,81	0
3	CD	A	302	1/1	0.99	0.02	44,44,44,44	0
3	CD	D	302	1/1	0.99	0.03	53,53,53,53	0

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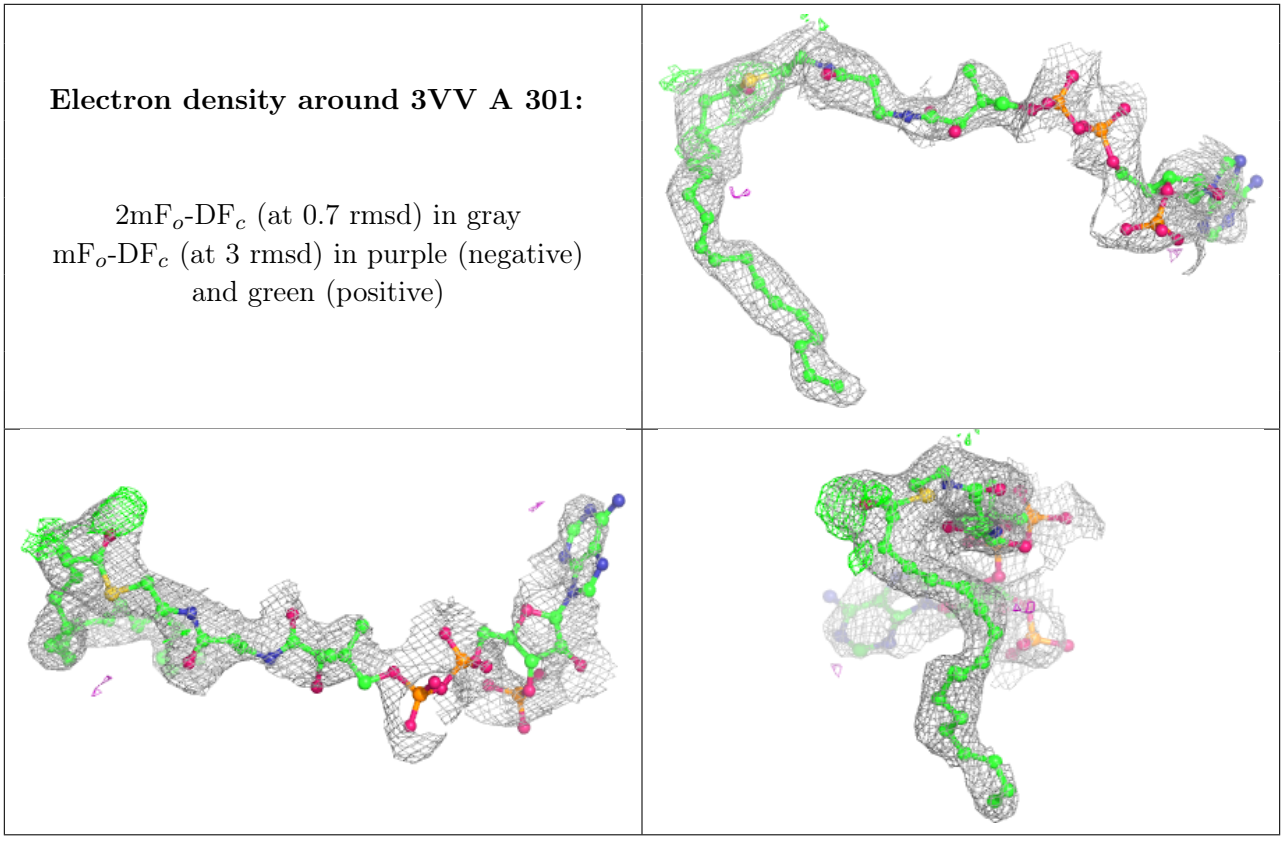
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CD	A	303	1/1	1.00	0.01	62,62,62,62	0
3	CD	D	303	1/1	1.00	0.02	67,67,67,67	0

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.

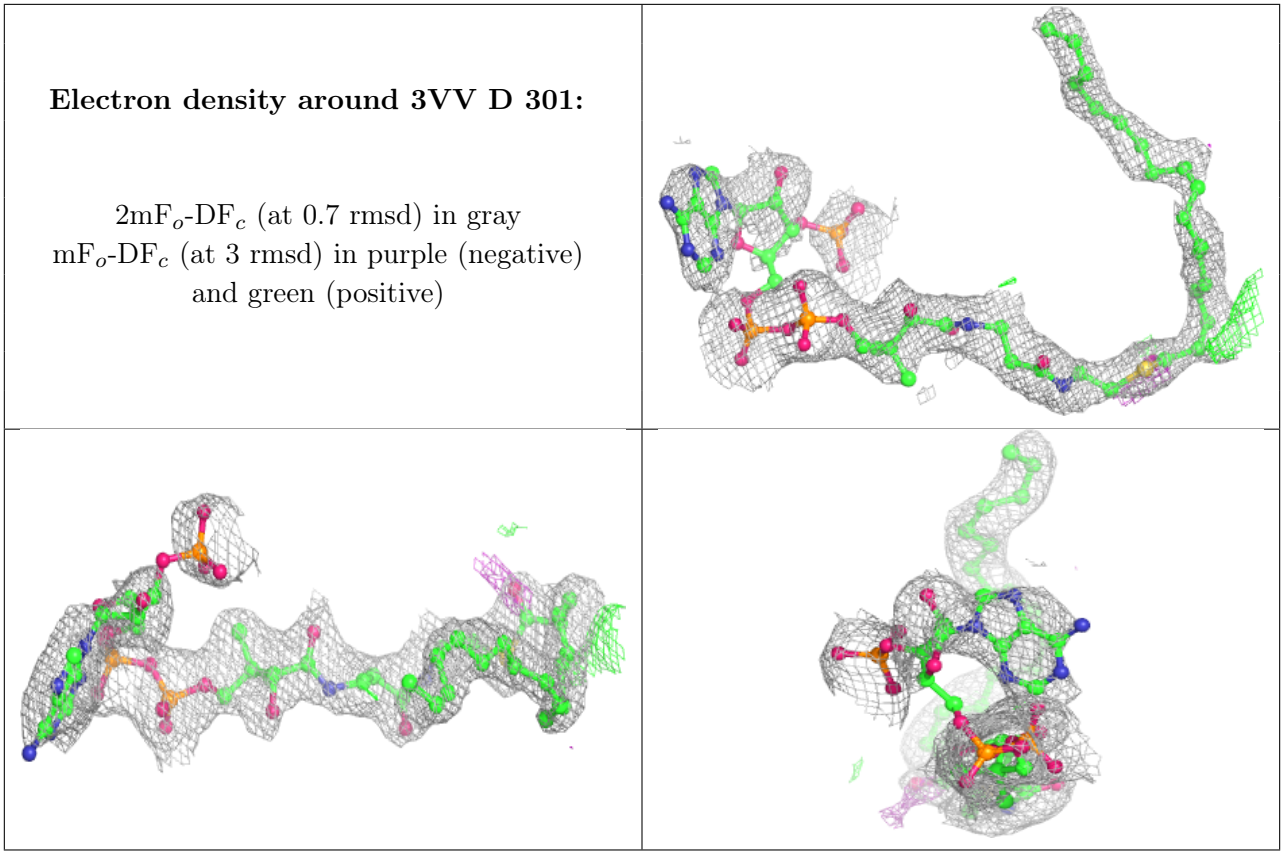
Electron density around 3VV A 301:

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



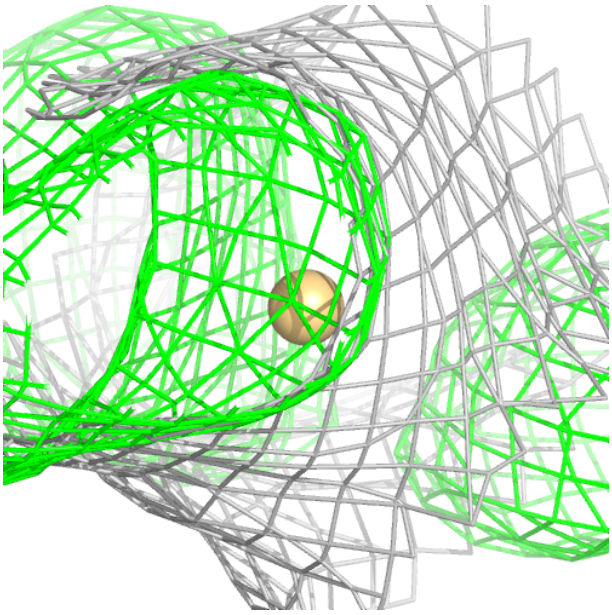
Electron density around 3VV D 301:

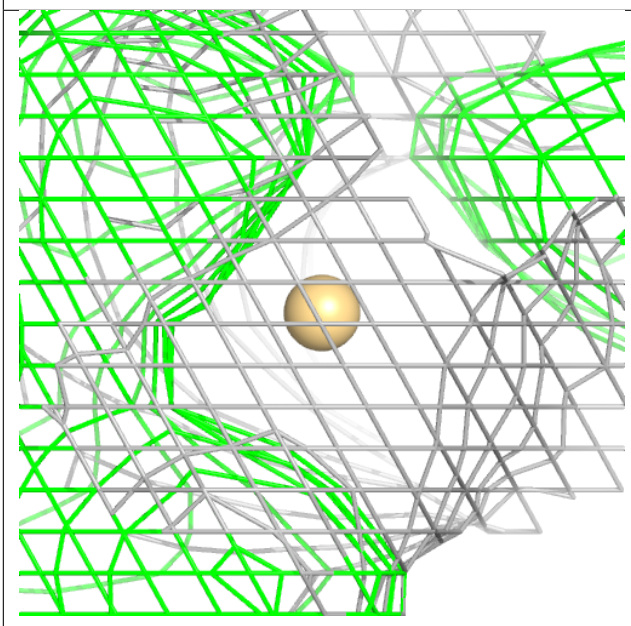
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

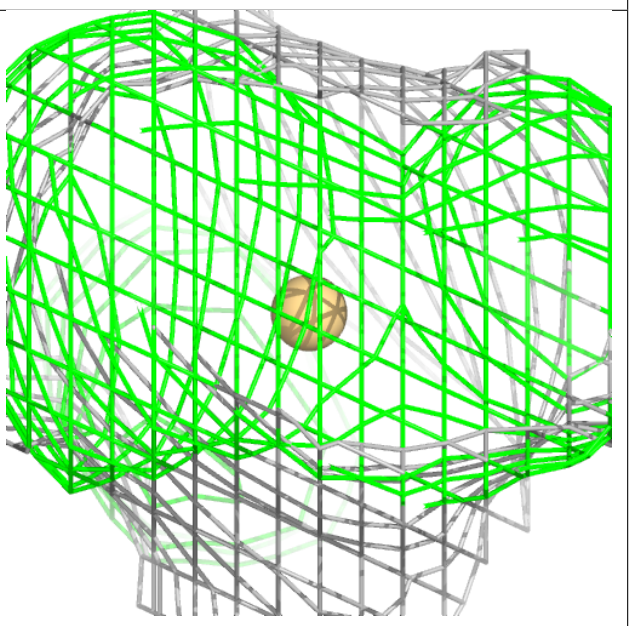


Electron density around CD A 302:

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

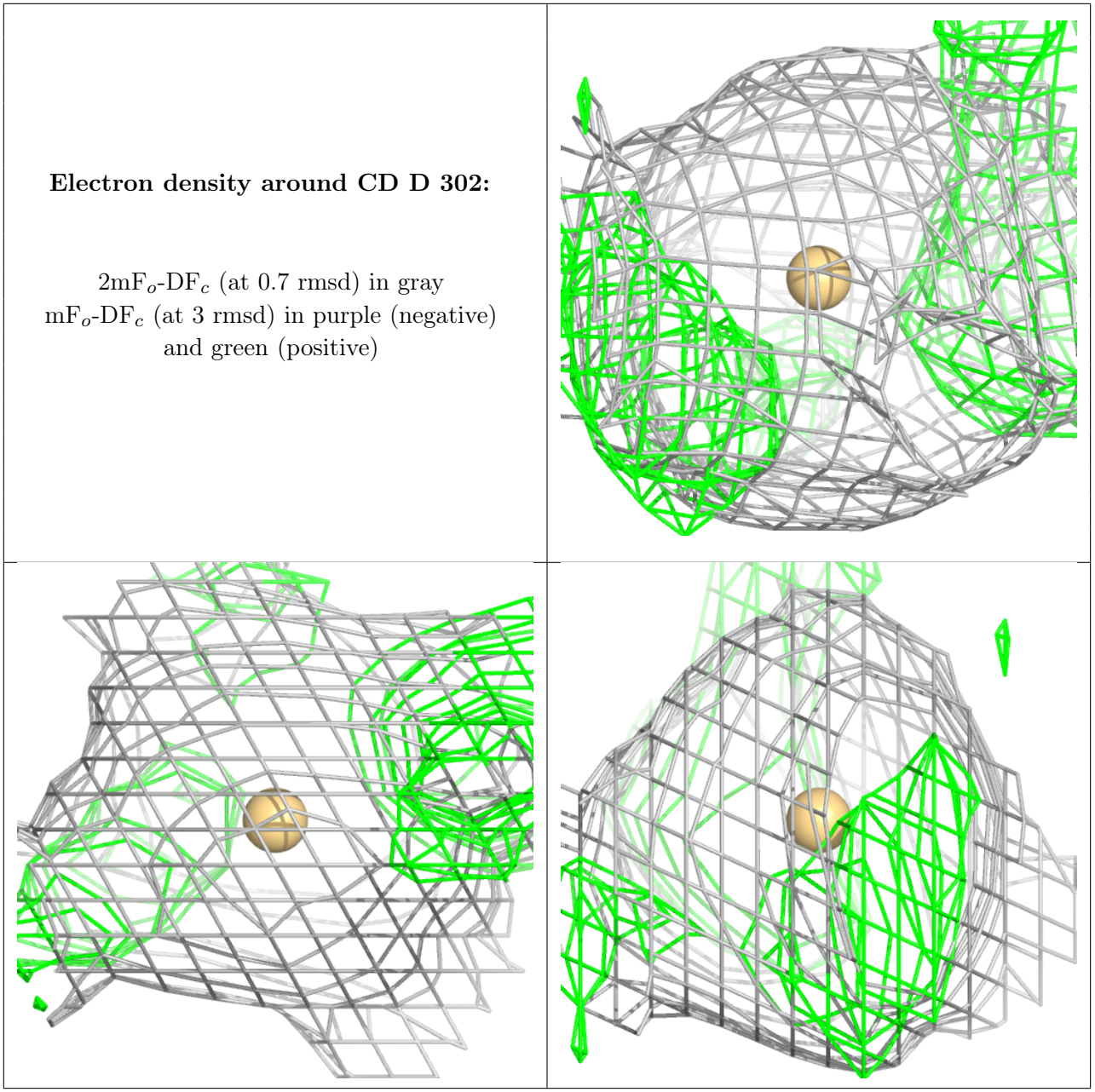






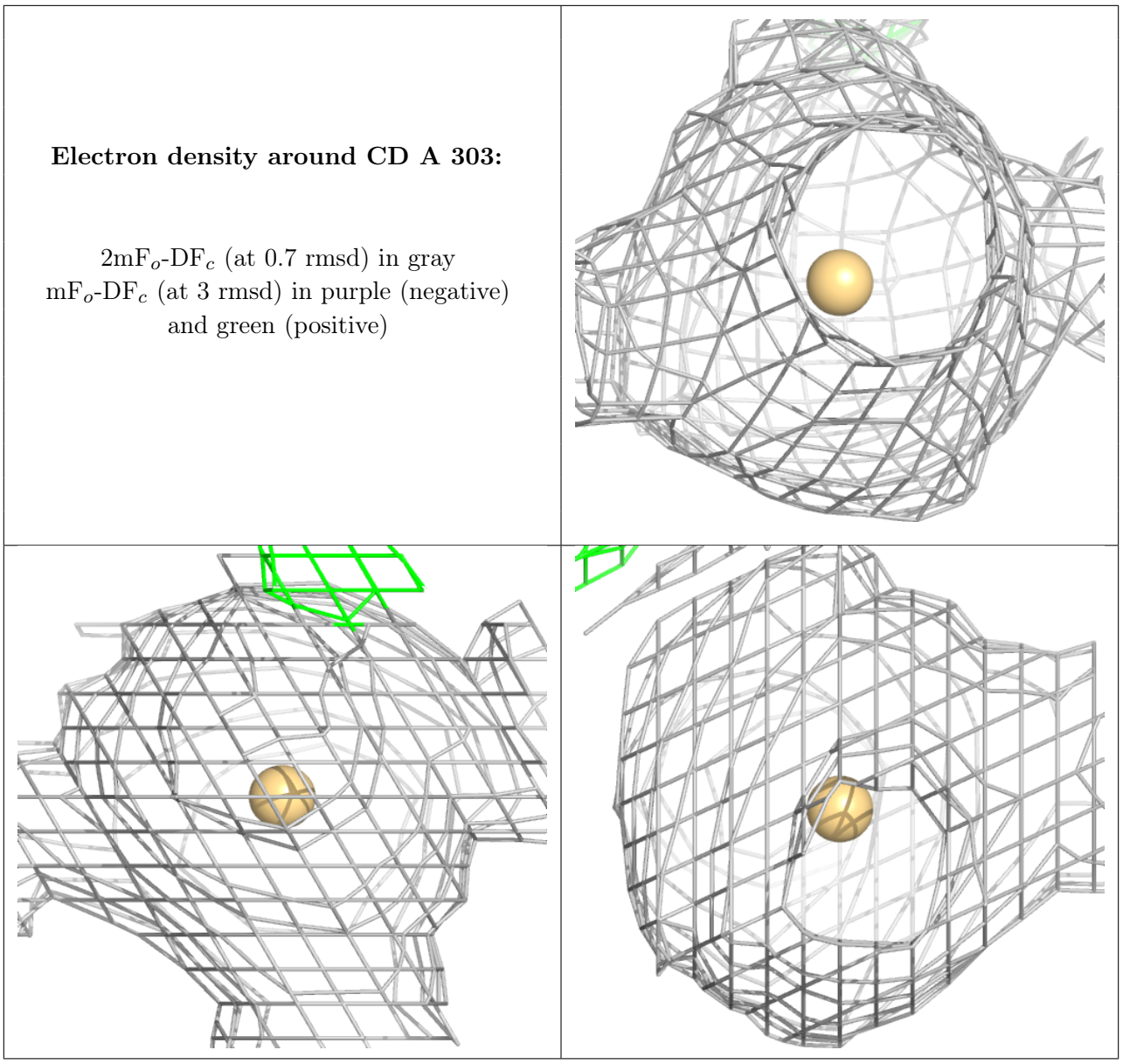
Electron density around CD D 302:

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



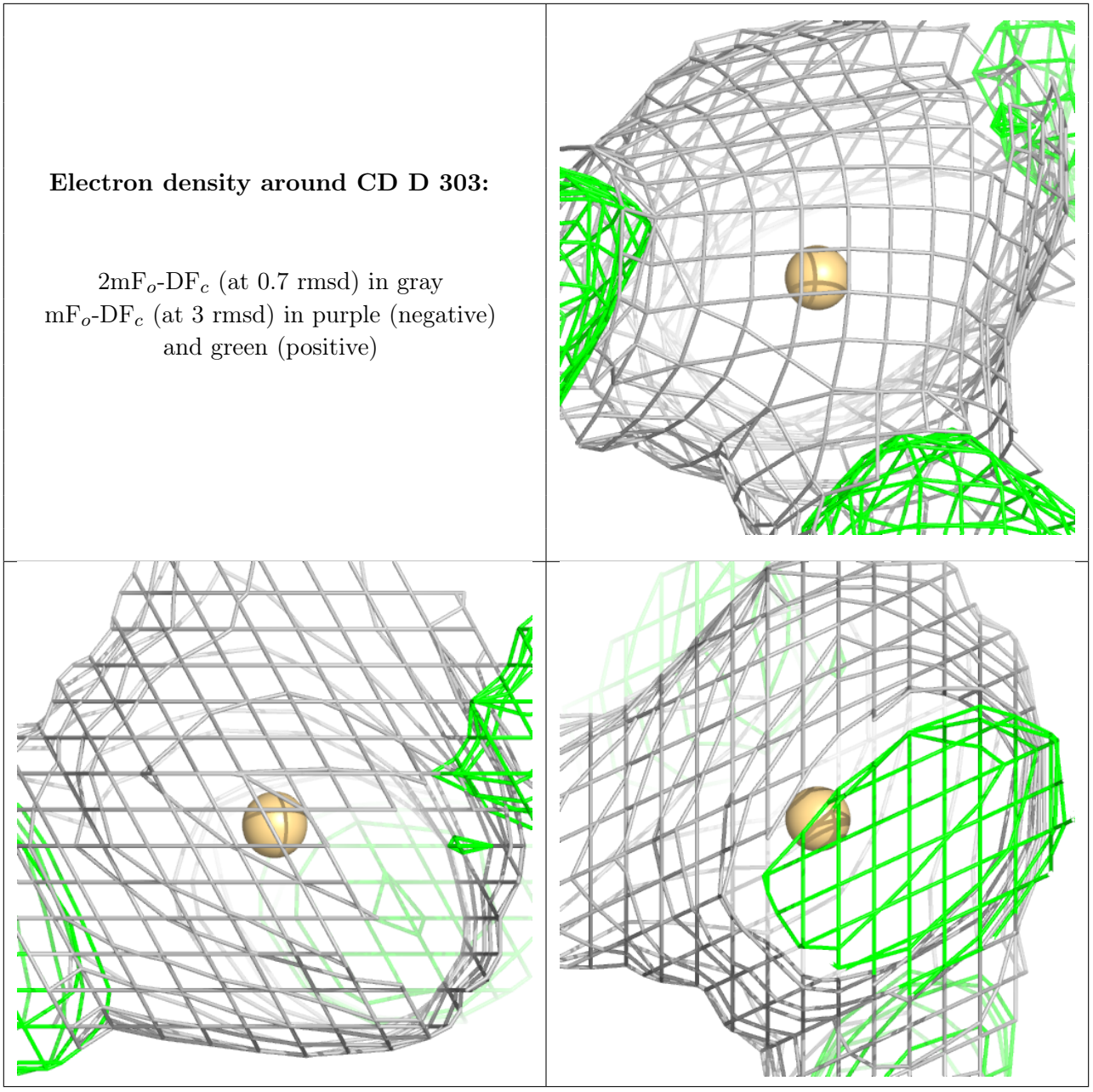
Electron density around CD A 303:

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



Electron density around CD D 303:

$2mF_o$-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.