



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:52 PM UTC

PDB ID : 5YPS / pdb_00005yps
Title : The structural basis of histone chaperoneVps75
Authors : Chen, Y.; Zhang, Y.; Dou, Y.; Wang, M.; Xu, S.; Jiang, H.; Limper, A.; Su, D.
Deposited on : 2017-11-03
Resolution : 2.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

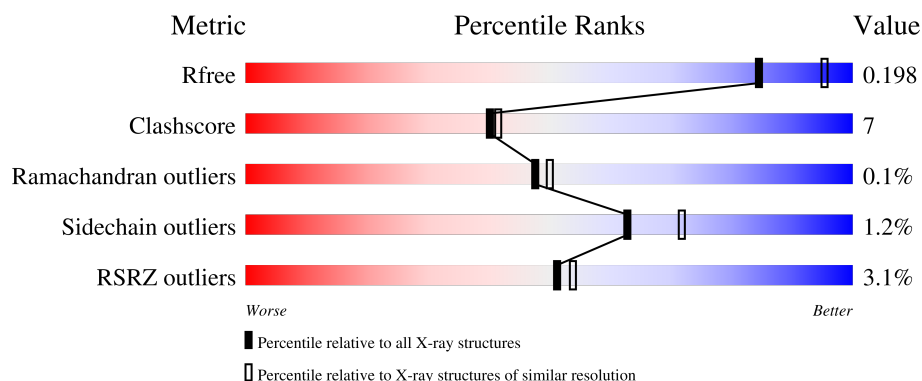
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



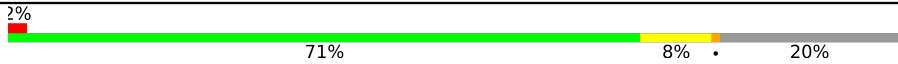
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	250	 3% 70% 10% 19%
1	B	250	 3% 72% 8% 20%
1	C	250	 3% 71% 9% 20%
1	D	250	 % 66% 13% 20%
1	E	250	 2% 72% 8% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	250	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	C	303	-	-	X	-
3	1PE	C	304	-	-	X	-
3	1PE	E	305	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10574 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 Vacuolar protein sorting-associated protein 75.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	Se	0	3	0
			1650	1061	261	324	4			
1	B	200	Total	C	N	O	Se	0	2	0
			1624	1049	256	316	3			
1	C	201	Total	C	N	O	Se	0	2	0
			1643	1060	258	322	3			
1	D	200	Total	C	N	O	Se	0	1	0
			1651	1062	259	327	3			
1	E	202	Total	C	N	O	Se	0	2	0
			1676	1077	264	331	4			
1	F	201	Total	C	N	O	Se	0	1	0
			1652	1063	260	326	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
A	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
A	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
A	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
B	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
B	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
B	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
B	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
C	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
C	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
C	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
C	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
D	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
D	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
D	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
D	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
E	1	MSE	-	initiating methionine	UNP A0A0W4ZF97

Continued on next page...

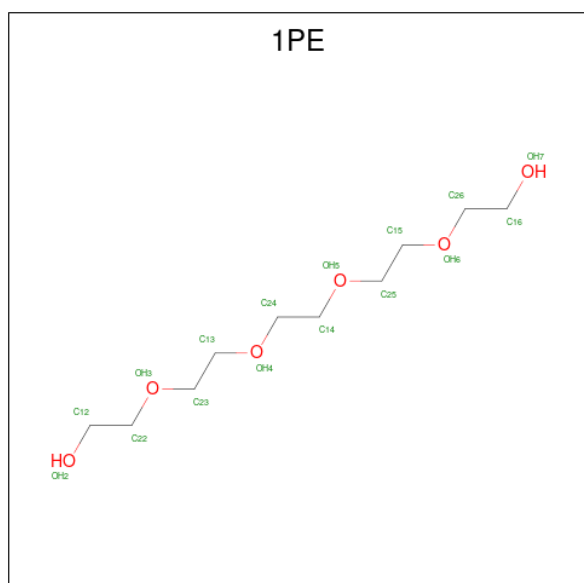
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
E	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
E	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
F	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
F	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
F	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
F	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	3	Total Ca 3 3	0	0
2	C	1	Total Ca 1 1	0	0
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		
3	F	1	Total	C	O	0	0
			16	10	6		
3	F	1	Total	C	O	0	0
			16	10	6		
3	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



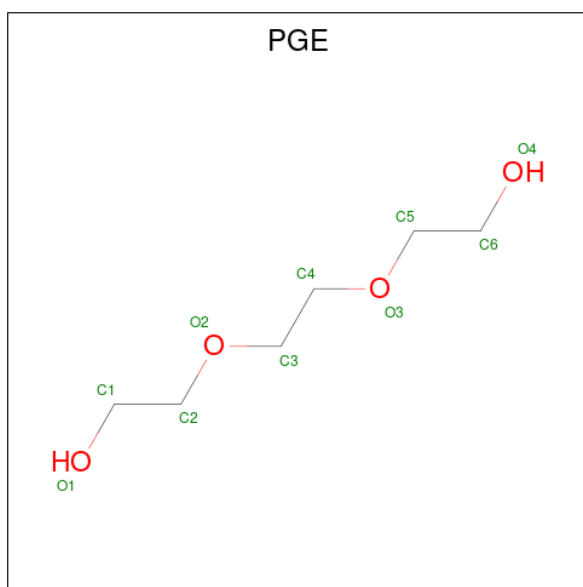
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			10	6	4		

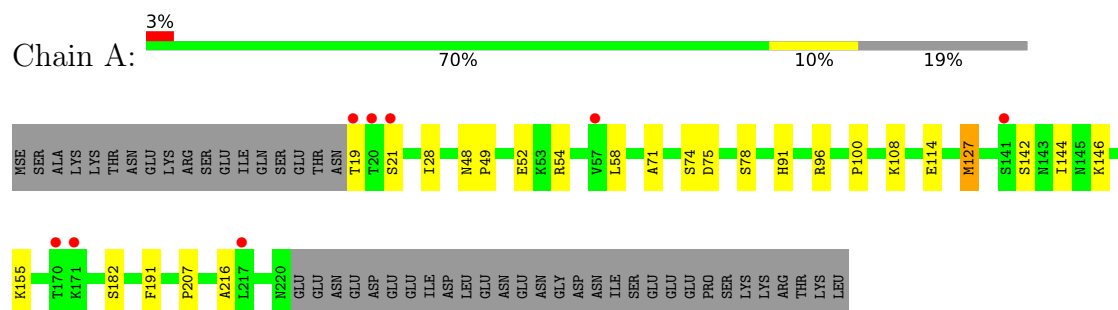
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	33	Total	O	0	0
			33	33		
7	B	37	Total	O	0	0
			37	37		
7	C	41	Total	O	0	0
			41	41		
7	D	30	Total	O	0	0
			30	30		
7	E	61	Total	O	0	0
			61	61		
7	F	30	Total	O	0	0
			30	30		

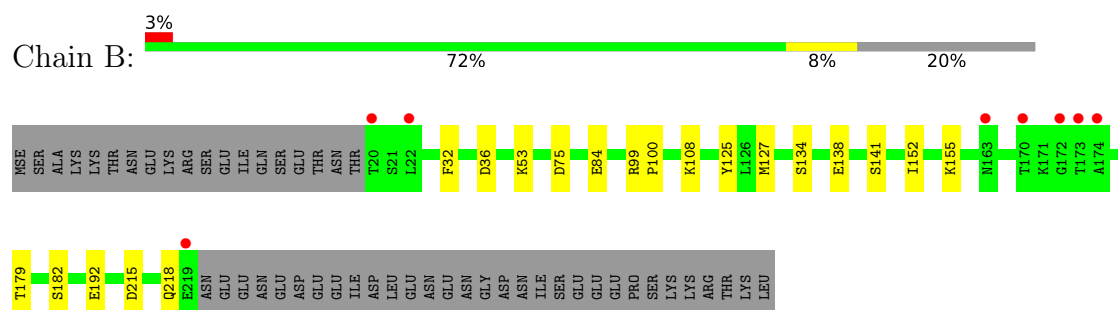
3 Residue-property plots [i](#)

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.

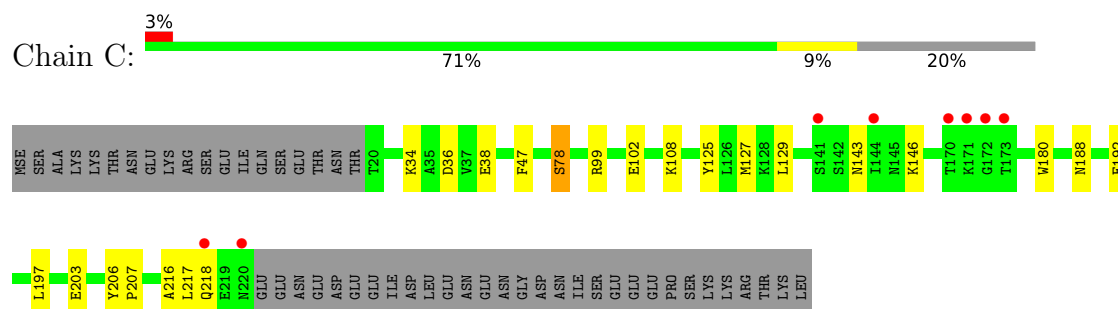
- Molecule 1: Vacuolar protein sorting-associated protein 75



- Molecule 1: Vacuolar protein sorting-associated protein 75

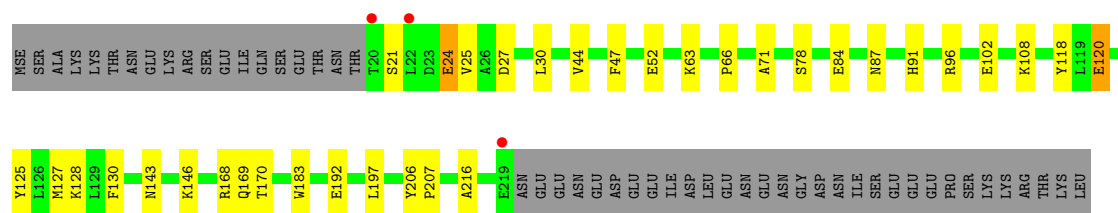


- Molecule 1: Vacuolar protein sorting-associated protein 75

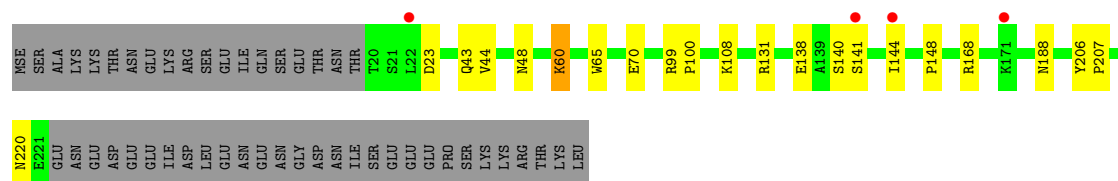
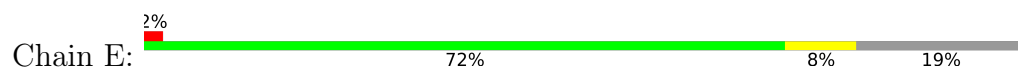


- Molecule 1: Vacuolar protein sorting-associated protein 75

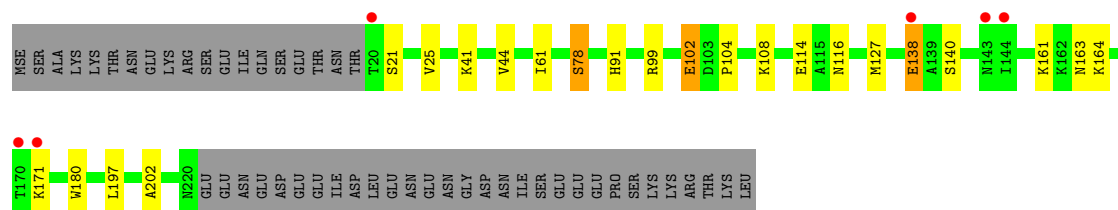




● Molecule 1: Vacuolar protein sorting-associated protein 75



● Molecule 1: Vacuolar protein sorting-associated protein 75



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.67Å 76.40Å 130.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.10 48.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.26-2.10) 99.5 (48.26-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.236 0.196 , 0.198	Depositor DCC
R_{free} test set	4187 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10574	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: PEG, 1PE, CA, PGE, GOL

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	0.49	0/1687	0.75	0/2291
1	B	0.55	0/1661	0.77	0/2255
1	C	0.55	0/1680	0.77	0/2278
1	D	0.54	0/1688	0.79	0/2288
1	E	0.60	0/1713	0.83	6/2320 (0.3%)
1	F	0.54	0/1689	0.79	1/2290 (0.0%)
All	All	0.54	0/10118	0.79	7/13722 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	ASN	CA-C-N	-6.87	111.91	119.19
1	E	48	ASN	C-N-CA	-6.87	111.91	119.19
1	E	65	TRP	CA-C-N	-5.60	113.12	119.28
1	E	65	TRP	C-N-CA	-5.60	113.12	119.28
1	E	23	ASP	N-CA-C	-5.51	107.11	113.88
1	F	61	ILE	N-CA-C	5.24	113.21	107.60
1	E	220	ASN	N-CA-C	5.16	117.47	108.76

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	1650	0	1555	21	0
1	B	1624	0	1543	21	0
1	C	1643	0	1563	28	1
1	D	1651	0	1584	25	0
1	E	1676	0	1611	19	1
1	F	1652	0	1582	16	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	48	0	66	6	0
3	B	48	0	66	9	0
3	C	48	0	66	19	0
3	D	48	0	66	6	0
3	E	64	0	88	14	0
3	F	48	0	66	7	0
4	A	7	0	10	1	0
4	B	7	0	10	0	0
4	D	7	0	10	1	0
4	E	7	0	10	1	0
4	F	14	0	20	1	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	18	0	24	2	0
5	E	18	0	24	2	0
5	F	18	0	24	1	1
6	C	10	0	14	2	0
7	A	33	0	0	0	0
7	B	37	0	0	1	0
7	C	41	0	0	1	0
7	D	30	0	0	1	0
7	E	61	0	0	2	0
7	F	30	0	0	2	0
All	All	10574	0	10034	134	2

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 7.

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:192:GLU:OE2	7:B:401:HOH:O	1.95	0.85
1:C:192:GLU:OE2	7:C:401:HOH:O	1.96	0.83
1:C:99:ARG:HE	3:C:303:1PE:H142	1.41	0.83
1:B:99:ARG:HE	3:B:305:1PE:H232	1.46	0.80
1:C:108:LYS:HE2	3:C:304:1PE:H251	1.68	0.76
1:F:127:MSE:HE2	3:F:304:1PE:H131	1.68	0.76
1:D:169:GLN:H	1:D:169:GLN:CD	1.93	0.75
1:D:192:GLU:OE2	7:D:401:HOH:O	2.07	0.72
1:C:99:ARG:HH21	3:C:303:1PE:H252	1.55	0.71
1:A:146:LYS:NZ	1:B:75:ASP:OD1	2.24	0.70
1:D:127:MSE:HG3	3:D:304:1PE:H222	1.74	0.70
3:C:302:1PE:H231	1:D:207:PRO:HB3	1.73	0.69
1:B:127[B]:MSE:HE1	3:B:304:1PE:H222	1.73	0.69
1:F:138:GLU:OE2	7:F:401:HOH:O	2.09	0.68
1:A:155:LYS:HE3	1:A:182:SER:HB2	1.76	0.66
1:B:99:ARG:HH21	3:B:305:1PE:H242	1.61	0.66
1:D:168:ARG:HH11	1:D:170:THR:HG21	1.61	0.65
1:A:28:ILE:HD11	1:B:53:LYS:HE2	1.79	0.65
1:A:142:SER:OG	1:B:215:ASP:OD2	2.12	0.63
1:F:102:GLU:H	1:F:102:GLU:CD	2.05	0.63
1:B:108:LYS:NZ	3:B:304:1PE:H142	2.13	0.63
1:E:141:SER:O	4:F:307:PEG:H12	2.00	0.62
1:E:99:ARG:HH21	3:E:305:1PE:H242	1.65	0.61
1:E:99:ARG:HE	3:E:305:1PE:H242	1.66	0.61
1:E:168:ARG:NH2	3:E:306:1PE:OH7	2.33	0.61
3:C:304:1PE:H242	3:C:304:1PE:H262	1.83	0.61
1:C:78:SER:HB2	6:C:306:PGE:H32	1.84	0.60
1:E:108:LYS:HD2	3:E:303:1PE:H162	1.83	0.60
1:E:100:PRO:HB3	3:E:303:1PE:H252	1.84	0.59
1:C:108:LYS:HZ3	3:C:304:1PE:H132	1.66	0.59
1:B:155[B]:LYS:HG3	1:B:182:SER:HA	1.84	0.59
1:C:125:TYR:CE2	1:C:127[A]:MSE:HE3	2.38	0.59
1:E:44:VAL:HA	3:E:305:1PE:H121	1.85	0.59
1:B:134:SER:O	1:B:138:GLU:HG2	2.02	0.58
1:D:120:GLU:OE2	5:D:307:GOL:O1	2.19	0.58
1:E:100:PRO:HA	4:E:307:PEG:H42	1.85	0.58
1:B:108:LYS:HZ2	3:B:304:1PE:H142	1.69	0.57
1:C:143:ASN:HB3	1:C:146:LYS:HB2	1.86	0.57
1:C:207:PRO:HB3	3:D:303:1PE:H141	1.85	0.57
1:A:108:LYS:HE3	1:A:127[A]:MSE:SE	2.55	0.56
1:F:44:VAL:HA	3:F:305:1PE:H222	1.86	0.56
3:A:303:1PE:H231	1:B:32:PHE:HD2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:NE	3:C:303:1PE:H142	2.18	0.56
1:C:99:ARG:NH2	3:C:303:1PE:H252	2.21	0.56
1:E:140:SER:HB2	7:E:430:HOH:O	2.06	0.56
1:A:91:HIS:HB3	1:A:114:GLU:HG2	1.89	0.55
1:B:100:PRO:HB3	3:B:304:1PE:H141	1.89	0.54
1:A:74:SER:HA	1:A:78:SER:HB3	1.90	0.54
1:F:21:SER:O	1:F:25:VAL:HG23	2.08	0.53
1:C:125:TYR:HE2	1:C:127[A]:MSE:HE3	1.74	0.53
1:A:127[A]:MSE:SE	3:A:304:1PE:H261	2.59	0.53
1:E:43:GLN:HE22	3:E:305:1PE:H252	1.74	0.52
1:A:52:GLU:CD	1:A:96:ARG:HH22	2.18	0.52
1:D:108:LYS:HE3	1:D:127:MSE:HE2	1.91	0.52
3:E:303:1PE:OH2	3:E:303:1PE:OH7	2.23	0.52
1:E:43:GLN:HE22	3:E:305:1PE:H141	1.74	0.51
1:A:207:PRO:HB3	3:A:303:1PE:H131	1.92	0.51
3:E:304:1PE:OH7	3:E:304:1PE:OH2	2.26	0.51
1:A:75:ASP:HB3	1:D:146:LYS:HE3	1.93	0.51
1:D:143:ASN:HB3	1:D:146:LYS:HB2	1.93	0.51
1:F:78:SER:O	5:F:308:GOL:H32	2.10	0.50
1:C:108:LYS:HD2	3:C:304:1PE:H221	1.93	0.50
1:F:116:ASN:O	1:F:161:LYS:NZ	2.31	0.50
1:F:163:ASN:C	1:F:164:LYS:HD2	2.37	0.50
1:D:27:ASP:HA	1:D:30:LEU:HD12	1.94	0.50
1:C:108:LYS:HZ2	3:C:304:1PE:H122	1.78	0.49
1:C:108:LYS:HE3	1:C:127[A]:MSE:HE2	1.94	0.49
1:B:179:THR:HG21	1:C:188:ASN:O	2.12	0.49
1:D:91:HIS:NE2	3:D:305:1PE:H162	2.28	0.49
1:E:99:ARG:HH21	3:E:305:1PE:C24	2.26	0.48
1:D:71:ALA:HB2	1:D:216:ALA:HB2	1.95	0.48
1:C:108:LYS:HZ3	3:C:304:1PE:C13	2.25	0.48
1:A:108:LYS:NZ	3:A:304:1PE:OH4	2.47	0.48
1:B:108:LYS:HZ3	3:B:304:1PE:H232	1.78	0.47
3:B:306:1PE:H151	3:B:306:1PE:H142	1.50	0.47
1:E:43:GLN:NE2	3:E:305:1PE:H141	2.29	0.47
1:C:216:ALA:O	1:C:218:GLN:N	2.46	0.47
1:A:19:THR:HG22	1:A:21:SER:H	1.80	0.47
1:A:54:ARG:O	1:A:58:LEU:HG	2.14	0.47
1:D:206:TYR:HB3	1:D:207:PRO:HD3	1.97	0.47
1:A:71:ALA:HB2	1:A:216:ALA:HB2	1.96	0.46
1:B:125:TYR:CE2	1:B:127[B]:MSE:HE3	2.50	0.46
1:D:125:TYR:HE2	3:D:304:1PE:H122	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:1PE:H222	1:B:36:ASP:OD2	2.15	0.46
1:F:99:ARG:HG3	3:F:305:1PE:H132	1.97	0.46
1:E:188:ASN:HA	5:E:310:GOL:H2	1.97	0.45
1:F:180:TRP:CD1	1:F:197:LEU:HD23	2.50	0.45
1:C:203:GLU:HA	3:C:303:1PE:H251	1.98	0.45
1:E:206:TYR:HB3	1:E:207:PRO:HD3	1.99	0.45
1:E:60:LYS:HA	1:E:60:LYS:HD2	1.52	0.45
1:C:108:LYS:NZ	3:C:304:1PE:H132	2.32	0.44
1:F:91:HIS:HB3	1:F:114:GLU:HG2	1.99	0.44
3:D:304:1PE:H221	3:D:304:1PE:H132	1.63	0.44
1:F:202:ALA:O	3:F:305:1PE:H142	2.17	0.44
1:A:100:PRO:HB2	3:A:304:1PE:H231	1.98	0.44
1:D:128:LYS:HE3	1:D:130:PHE:CZ	2.52	0.44
3:C:302:1PE:H131	1:D:47:PHE:CE1	2.53	0.44
1:C:36:ASP:OD2	3:C:302:1PE:OH7	2.28	0.44
5:D:307:GOL:H11	5:D:308:GOL:O3	2.18	0.44
1:D:63:LYS:C	1:D:66:PRO:HD2	2.43	0.43
3:C:302:1PE:H251	3:C:302:1PE:H261	1.81	0.43
1:D:52:GLU:OE1	1:D:96:ARG:NH2	2.39	0.43
1:C:129:LEU:HD22	3:C:304:1PE:H222	2.00	0.42
1:D:84:GLU:O	1:D:87:ASN:HB2	2.20	0.42
1:C:206:TYR:HB3	1:C:207:PRO:HD3	2.00	0.42
1:A:146:LYS:HA	1:A:146:LYS:HD3	1.72	0.42
1:C:99:ARG:NH2	3:C:303:1PE:H261	2.34	0.42
1:D:87:ASN:HB3	1:D:118:TYR:CE2	2.55	0.42
1:C:180:TRP:CD1	1:C:197:LEU:HD23	2.55	0.42
1:B:141:SER:O	6:C:306:PGE:H62	2.20	0.42
1:A:142:SER:O	1:A:144:ILE:HD12	2.20	0.41
1:F:140:SER:HB2	7:F:409:HOH:O	2.20	0.41
1:D:24:GLU:HA	1:D:24:GLU:OE1	2.21	0.41
1:E:44:VAL:HA	3:E:305:1PE:C12	2.50	0.41
1:F:108:LYS:NZ	3:F:304:1PE:H241	2.36	0.41
1:C:47:PHE:CE1	3:D:303:1PE:H242	2.55	0.41
1:F:41:LYS:HG3	1:F:104:PRO:HG3	2.03	0.41
1:D:183:TRP:HE1	1:D:192:GLU:CD	2.28	0.41
1:E:131:ARG:HG2	7:E:419:HOH:O	2.20	0.41
1:A:48:ASN:HB3	1:A:49:PRO:HD3	2.02	0.41
1:B:152:ILE:HD11	5:E:309:GOL:H2	2.03	0.41
1:D:21:SER:O	1:D:25:VAL:HG23	2.20	0.41
1:A:191:PHE:CE1	1:D:197:LEU:HD22	2.55	0.41
1:B:192:GLU:HA	1:C:192:GLU:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:304:1PE:H122	3:E:304:1PE:H231	1.75	0.41
1:A:127[A]:MSE:HE3	1:A:127[A]:MSE:HB3	1.93	0.41
1:C:34:LYS:O	1:C:38:GLU:HG2	2.21	0.41
1:E:144:ILE:HD12	1:E:148:PRO:HB3	2.01	0.41
1:B:108:LYS:HZ3	3:B:304:1PE:H142	1.86	0.40
3:C:303:1PE:OH5	3:C:303:1PE:OH2	2.29	0.40
4:A:306:PEG:H41	4:A:306:PEG:H21	1.93	0.40
1:D:44:VAL:HA	4:D:306:PEG:H12	2.03	0.40
1:F:108:LYS:HE3	3:F:304:1PE:H132	2.03	0.40
3:F:303:1PE:H142	3:F:303:1PE:H132	1.71	0.40

All (2) 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)
1:E:70:GLU:OE2	5:F:309:GOL:O2[2_565]	2.14	0.06
1:C:102:GLU:OE2	1:F:171:LYS:NZ[4_455]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	203/250 (81%)	197 (97%)	6 (3%)	0	100	100
1	B	200/250 (80%)	191 (96%)	9 (4%)	0	100	100
1	C	201/250 (80%)	195 (97%)	5 (2%)	1 (0%)	24	22
1	D	199/250 (80%)	192 (96%)	7 (4%)	0	100	100
1	E	202/250 (81%)	197 (98%)	5 (2%)	0	100	100
1	F	200/250 (80%)	192 (96%)	8 (4%)	0	100	100
All	All	1205/1500 (80%)	1164 (97%)	40 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	217	LEU

5.3.2 Protein sidechains ⓘ

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	176/228 (77%)	174 (99%)	2 (1%)	65	74
1	B	173/228 (76%)	171 (99%)	2 (1%)	63	72
1	C	176/228 (77%)	175 (99%)	1 (1%)	78	86
1	D	181/228 (79%)	177 (98%)	4 (2%)	45	53
1	E	184/228 (81%)	182 (99%)	2 (1%)	65	74
1	F	180/228 (79%)	177 (98%)	3 (2%)	53	62
All	All	1070/1368 (78%)	1056 (99%)	14 (1%)	63	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127[A]	MSE
1	A	127[B]	MSE
1	B	84	GLU
1	B	218	GLN
1	C	78	SER
1	D	24	GLU
1	D	78	SER
1	D	102	GLU
1	D	120	GLU
1	E	60	LYS
1	E	138	GLU
1	F	78	SER
1	F	102	GLU
1	F	138	GLU

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	43	GLN
1	A	48	ASN
1	B	208	ASN
1	C	150	GLN
1	E	43	GLN
1	E	48	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 51 ligands modelled in this entry, 12 are monoatomic - leaving 39 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	$\# Z > 2$
5	GOL	E	309	-	5,5,5	0.34	0	5,5,5	0.33	0
3	1PE	B	304	-	15,15,15	0.74	0	14,14,14	0.40	0
4	PEG	B	307	-	6,6,6	0.55	0	5,5,5	0.30	0
5	GOL	F	308	-	5,5,5	0.31	0	5,5,5	1.04	0
3	1PE	E	303	-	15,15,15	0.75	0	14,14,14	0.37	0
5	GOL	A	307	-	5,5,5	0.39	0	5,5,5	0.25	0
5	GOL	E	310	-	5,5,5	0.37	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGE	C	306	-	9,9,9	0.32	0	8,8,8	0.43	0
3	1PE	E	304	-	15,15,15	0.73	0	14,14,14	0.37	0
5	GOL	C	305	-	5,5,5	0.46	0	5,5,5	0.22	0
3	1PE	F	303	-	15,15,15	0.78	0	14,14,14	0.25	0
5	GOL	D	309	-	5,5,5	0.35	0	5,5,5	0.39	0
3	1PE	E	305	-	15,15,15	0.76	0	14,14,14	0.27	0
3	1PE	A	303	-	15,15,15	0.74	0	14,14,14	0.36	0
5	GOL	B	308	-	5,5,5	0.35	0	5,5,5	0.29	0
4	PEG	F	306	-	6,6,6	0.53	0	5,5,5	0.30	0
5	GOL	F	310	-	5,5,5	0.40	0	5,5,5	0.30	0
5	GOL	E	308	-	5,5,5	0.35	0	5,5,5	0.35	0
5	GOL	A	308	-	5,5,5	0.35	0	5,5,5	0.43	0
3	1PE	B	305	-	15,15,15	0.81	0	14,14,14	0.25	0
4	PEG	A	306	-	6,6,6	0.58	0	5,5,5	0.29	0
5	GOL	F	309	-	5,5,5	0.46	0	5,5,5	0.26	0
3	1PE	D	304	-	15,15,15	0.74	0	14,14,14	0.37	0
5	GOL	D	307	-	5,5,5	0.35	0	5,5,5	0.45	0
3	1PE	A	305	-	15,15,15	0.77	0	14,14,14	0.28	0
4	PEG	E	307	-	6,6,6	0.56	0	5,5,5	0.23	0
3	1PE	F	305	-	15,15,15	0.75	0	14,14,14	0.38	0
3	1PE	C	302	-	15,15,15	0.79	0	14,14,14	0.29	0
3	1PE	E	306	-	15,15,15	0.74	0	14,14,14	0.31	0
3	1PE	A	304	-	15,15,15	0.79	0	14,14,14	0.32	0
3	1PE	C	303	-	15,15,15	0.79	0	14,14,14	0.31	0
3	1PE	B	306	-	15,15,15	0.75	0	14,14,14	0.27	0
3	1PE	F	304	-	15,15,15	0.76	0	14,14,14	0.30	0
3	1PE	D	303	-	15,15,15	0.70	0	14,14,14	0.38	0
4	PEG	F	307	-	6,6,6	0.52	0	5,5,5	0.50	0
5	GOL	D	308	-	5,5,5	0.37	0	5,5,5	0.27	0
3	1PE	C	304	-	15,15,15	0.77	0	14,14,14	0.27	0
4	PEG	D	306	-	6,6,6	0.54	0	5,5,5	0.29	0
3	1PE	D	305	-	15,15,15	0.76	0	14,14,14	0.40	0

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
5	GOL	E	309	-	-	0/4/4/4	-
3	1PE	B	304	-	-	10/13/13/13	-
4	PEG	B	307	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	308	-	-	4/4/4/4	-
3	1PE	E	303	-	-	5/13/13/13	-
5	GOL	A	307	-	-	1/4/4/4	-
5	GOL	E	310	-	-	2/4/4/4	-
6	PGE	C	306	-	-	2/7/7/7	-
3	1PE	E	304	-	-	8/13/13/13	-
5	GOL	C	305	-	-	2/4/4/4	-
3	1PE	F	303	-	-	10/13/13/13	-
5	GOL	D	309	-	-	0/4/4/4	-
3	1PE	E	305	-	-	9/13/13/13	-
3	1PE	A	303	-	-	8/13/13/13	-
5	GOL	B	308	-	-	1/4/4/4	-
4	PEG	F	306	-	-	2/4/4/4	-
5	GOL	F	310	-	-	2/4/4/4	-
5	GOL	E	308	-	-	2/4/4/4	-
5	GOL	A	308	-	-	4/4/4/4	-
3	1PE	B	305	-	-	7/13/13/13	-
4	PEG	A	306	-	-	1/4/4/4	-
5	GOL	F	309	-	-	2/4/4/4	-
3	1PE	D	304	-	-	4/13/13/13	-
5	GOL	D	307	-	-	4/4/4/4	-
3	1PE	A	305	-	-	6/13/13/13	-
4	PEG	E	307	-	-	1/4/4/4	-
3	1PE	F	305	-	-	5/13/13/13	-
3	1PE	C	302	-	-	4/13/13/13	-
3	1PE	E	306	-	-	3/13/13/13	-
3	1PE	A	304	-	-	8/13/13/13	-
3	1PE	C	303	-	-	9/13/13/13	-
3	1PE	B	306	-	-	9/13/13/13	-
3	1PE	F	304	-	-	9/13/13/13	-
3	1PE	D	303	-	-	6/13/13/13	-
4	PEG	F	307	-	-	1/4/4/4	-
5	GOL	D	308	-	-	2/4/4/4	-
3	1PE	C	304	-	-	10/13/13/13	-
4	PEG	D	306	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	D	305	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	308	GOL	O1-C1-C2-C3
5	A	308	GOL	C1-C2-C3-O3
5	C	305	GOL	C1-C2-C3-O3
5	D	307	GOL	O1-C1-C2-C3
5	D	307	GOL	C1-C2-C3-O3
5	E	310	GOL	O1-C1-C2-C3
5	F	308	GOL	C1-C2-C3-O3
5	F	309	GOL	O1-C1-C2-O2
5	F	309	GOL	O1-C1-C2-C3
3	F	304	1PE	C24-C14-OH5-C25
3	B	306	1PE	C15-C25-OH5-C14
3	B	304	1PE	OH7-C16-C26-OH6
3	B	305	1PE	OH4-C13-C23-OH3
3	C	302	1PE	OH4-C13-C23-OH3
3	C	303	1PE	OH5-C14-C24-OH4
3	E	306	1PE	OH5-C14-C24-OH4
3	F	303	1PE	C14-C24-OH4-C13
3	B	305	1PE	OH5-C14-C24-OH4
3	F	305	1PE	OH7-C16-C26-OH6
3	D	304	1PE	C13-C23-OH3-C22
3	C	304	1PE	OH6-C15-C25-OH5
3	A	303	1PE	OH4-C13-C23-OH3
3	B	304	1PE	OH6-C15-C25-OH5
3	F	305	1PE	OH5-C14-C24-OH4
3	B	305	1PE	OH6-C15-C25-OH5
3	B	306	1PE	OH4-C13-C23-OH3
3	E	305	1PE	OH6-C15-C25-OH5
3	D	305	1PE	OH4-C13-C23-OH3
6	C	306	PGE	O2-C3-C4-O3
3	B	304	1PE	OH4-C13-C23-OH3
5	D	307	GOL	O1-C1-C2-O2
3	E	305	1PE	OH4-C13-C23-OH3
3	C	303	1PE	OH2-C12-C22-OH3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	303	1PE	OH2-C12-C22-OH3
3	F	303	1PE	OH7-C16-C26-OH6
3	C	302	1PE	C25-C15-OH6-C26
3	B	306	1PE	OH5-C14-C24-OH4
3	A	303	1PE	OH6-C15-C25-OH5
3	F	304	1PE	OH5-C14-C24-OH4
3	B	304	1PE	OH5-C14-C24-OH4
3	C	304	1PE	OH7-C16-C26-OH6
3	D	305	1PE	OH7-C16-C26-OH6
4	B	307	PEG	O1-C1-C2-O2
4	D	306	PEG	O2-C3-C4-O4
3	E	304	1PE	C12-C22-OH3-C23
3	C	303	1PE	OH6-C15-C25-OH5
3	A	304	1PE	OH6-C15-C25-OH5
3	C	303	1PE	OH4-C13-C23-OH3
3	C	303	1PE	C25-C15-OH6-C26
5	D	308	GOL	O1-C1-C2-C3
5	E	308	GOL	C1-C2-C3-O3
5	F	308	GOL	O1-C1-C2-C3
5	F	310	GOL	O1-C1-C2-C3
3	A	305	1PE	C15-C25-OH5-C14
3	F	303	1PE	OH6-C15-C25-OH5
5	A	308	GOL	O1-C1-C2-O2
5	A	308	GOL	O2-C2-C3-O3
5	C	305	GOL	O2-C2-C3-O3
5	D	307	GOL	O2-C2-C3-O3
5	E	308	GOL	O2-C2-C3-O3
5	E	310	GOL	O1-C1-C2-O2
5	F	308	GOL	O1-C1-C2-O2
5	F	310	GOL	O1-C1-C2-O2
3	D	304	1PE	OH2-C12-C22-OH3
3	F	304	1PE	OH4-C13-C23-OH3
3	B	304	1PE	C15-C25-OH5-C14
3	E	304	1PE	OH6-C15-C25-OH5
3	D	303	1PE	OH4-C13-C23-OH3
3	C	303	1PE	OH7-C16-C26-OH6
3	C	304	1PE	OH2-C12-C22-OH3
3	E	303	1PE	OH7-C16-C26-OH6
4	B	307	PEG	O2-C3-C4-O4
3	E	303	1PE	OH5-C14-C24-OH4
5	D	308	GOL	O1-C1-C2-O2
3	F	305	1PE	OH4-C13-C23-OH3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	304	1PE	OH5-C14-C24-OH4
3	A	305	1PE	OH7-C16-C26-OH6
3	B	304	1PE	OH2-C12-C22-OH3
3	B	306	1PE	C25-C15-OH6-C26
5	F	308	GOL	O2-C2-C3-O3
3	A	304	1PE	OH2-C12-C22-OH3
3	A	304	1PE	OH7-C16-C26-OH6
3	E	304	1PE	OH4-C13-C23-OH3
5	A	307	GOL	O1-C1-C2-O2
3	D	304	1PE	C12-C22-OH3-C23
3	E	304	1PE	OH7-C16-C26-OH6
6	C	306	PGE	O3-C5-C6-O4
3	E	305	1PE	C14-C24-OH4-C13
3	E	306	1PE	C12-C22-OH3-C23
4	D	306	PEG	C1-C2-O2-C3
3	C	302	1PE	C14-C24-OH4-C13
3	C	303	1PE	C23-C13-OH4-C24
3	D	305	1PE	C15-C25-OH5-C14
3	F	303	1PE	C24-C14-OH5-C25
3	B	304	1PE	C23-C13-OH4-C24
3	F	303	1PE	C23-C13-OH4-C24
3	A	304	1PE	C24-C14-OH5-C25
3	F	303	1PE	C13-C23-OH3-C22
3	E	304	1PE	C13-C23-OH3-C22
3	A	304	1PE	C16-C26-OH6-C15
3	C	302	1PE	C16-C26-OH6-C15
3	D	303	1PE	C16-C26-OH6-C15
3	E	306	1PE	C13-C23-OH3-C22
3	A	303	1PE	C15-C25-OH5-C14
3	F	304	1PE	C16-C26-OH6-C15
4	D	306	PEG	C4-C3-O2-C2
3	C	304	1PE	C12-C22-OH3-C23
3	F	303	1PE	C16-C26-OH6-C15
3	A	303	1PE	OH7-C16-C26-OH6
3	B	306	1PE	OH2-C12-C22-OH3
4	F	307	PEG	O1-C1-C2-O2
3	A	304	1PE	C23-C13-OH4-C24
3	A	305	1PE	C16-C26-OH6-C15
3	F	304	1PE	C25-C15-OH6-C26
3	B	304	1PE	C12-C22-OH3-C23
3	D	305	1PE	C25-C15-OH6-C26
4	F	306	PEG	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	303	1PE	C13-C23-OH3-C22
3	E	305	1PE	OH7-C16-C26-OH6
3	A	303	1PE	C23-C13-OH4-C24
3	A	303	1PE	C24-C14-OH5-C25
3	B	304	1PE	C24-C14-OH5-C25
3	D	303	1PE	C14-C24-OH4-C13
3	D	305	1PE	OH2-C12-C22-OH3
3	A	305	1PE	C12-C22-OH3-C23
3	B	304	1PE	C14-C24-OH4-C13
3	C	303	1PE	C14-C24-OH4-C13
3	F	305	1PE	C23-C13-OH4-C24
3	E	303	1PE	C15-C25-OH5-C14
4	F	306	PEG	O1-C1-C2-O2
3	B	306	1PE	OH6-C15-C25-OH5
3	F	304	1PE	OH7-C16-C26-OH6
3	A	304	1PE	C25-C15-OH6-C26
3	E	304	1PE	C16-C26-OH6-C15
3	B	306	1PE	C14-C24-OH4-C13
3	E	305	1PE	C16-C26-OH6-C15
3	C	304	1PE	C13-C23-OH3-C22
3	C	304	1PE	C24-C14-OH5-C25
3	F	303	1PE	C15-C25-OH5-C14
3	B	305	1PE	C13-C23-OH3-C22
3	F	305	1PE	C13-C23-OH3-C22
3	A	303	1PE	C13-C23-OH3-C22
3	F	304	1PE	C23-C13-OH4-C24
3	C	304	1PE	C15-C25-OH5-C14
3	E	305	1PE	C25-C15-OH6-C26
3	E	305	1PE	OH5-C14-C24-OH4
3	B	306	1PE	C16-C26-OH6-C15
3	C	303	1PE	C12-C22-OH3-C23
3	C	304	1PE	C14-C24-OH4-C13
3	B	305	1PE	C23-C13-OH4-C24
3	A	305	1PE	C25-C15-OH6-C26
3	E	303	1PE	C23-C13-OH4-C24
3	E	305	1PE	C12-C22-OH3-C23
3	B	306	1PE	C24-C14-OH5-C25
3	E	303	1PE	C24-C14-OH5-C25
3	A	305	1PE	OH2-C12-C22-OH3
3	F	303	1PE	C12-C22-OH3-C23
3	E	304	1PE	C23-C13-OH4-C24
3	B	305	1PE	C25-C15-OH6-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	308	GOL	C1-C2-C3-O3
4	E	307	PEG	O2-C3-C4-O4
4	A	306	PEG	C4-C3-O2-C2
3	B	305	1PE	C16-C26-OH6-C15
3	D	305	1PE	C12-C22-OH3-C23
3	F	304	1PE	C14-C24-OH4-C13
3	D	304	1PE	C23-C13-OH4-C24
3	C	304	1PE	OH5-C14-C24-OH4
3	D	303	1PE	C25-C15-OH6-C26
3	F	304	1PE	C12-C22-OH3-C23
3	C	304	1PE	OH4-C13-C23-OH3
3	A	303	1PE	C12-C22-OH3-C23
3	F	303	1PE	C25-C15-OH6-C26
3	D	305	1PE	C14-C24-OH4-C13
3	E	304	1PE	C14-C24-OH4-C13
3	E	305	1PE	C13-C23-OH3-C22

There are no ring outliers.

29 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	309	GOL	1	0
3	B	304	1PE	6	0
5	F	308	GOL	1	0
3	E	303	1PE	3	0
5	E	310	GOL	1	0
6	C	306	PGE	2	0
3	E	304	1PE	2	0
3	F	303	1PE	1	0
3	E	305	1PE	8	0
3	A	303	1PE	3	0
3	B	305	1PE	2	0
4	A	306	PEG	1	0
5	F	309	GOL	0	1
3	D	304	1PE	3	0
5	D	307	GOL	2	0
4	E	307	PEG	1	0
3	F	305	1PE	3	0
3	C	302	1PE	4	0
3	E	306	1PE	1	0
3	A	304	1PE	3	0
3	C	303	1PE	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	306	1PE	1	0
3	F	304	1PE	3	0
3	D	303	1PE	2	0
4	F	307	PEG	1	0
5	D	308	GOL	1	0
3	C	304	1PE	8	0
4	D	306	PEG	1	0
3	D	305	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	200/250 (80%)	0.08	8 (4%)	42	44	24, 43, 69, 105	1 (0%)
1	B	198/250 (79%)	0.13	8 (4%)	42	44	19, 44, 82, 114	1 (0%)
1	C	199/250 (79%)	0.07	8 (4%)	42	44	22, 41, 84, 108	1 (0%)
1	D	198/250 (79%)	0.13	3 (1%)	72	74	29, 46, 76, 110	0
1	E	200/250 (80%)	-0.02	4 (2%)	65	67	23, 39, 79, 119	0
1	F	199/250 (79%)	0.07	6 (3%)	52	55	27, 46, 76, 108	0
All	All	1194/1500 (79%)	0.08	37 (3%)	51	54	19, 44, 77, 119	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	THR	3.7
1	C	172	GLY	3.6
1	A	170	THR	3.3
1	D	20	THR	3.3
1	A	141	SER	3.2
1	F	171	LYS	3.2
1	E	22	LEU	3.1
1	B	219	GLU	3.1
1	A	19	THR	3.1
1	B	170	THR	3.0
1	B	174	ALA	2.9
1	D	22	LEU	2.9
1	C	218	GLN	2.7
1	F	138	GLU	2.7
1	B	20	THR	2.6
1	A	217	LEU	2.6
1	A	21	SER	2.6
1	F	170	THR	2.6
1	E	141	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	144	ILE	2.5
1	F	143	ASN	2.5
1	F	144	ILE	2.4
1	F	20	THR	2.4
1	C	220	ASN	2.3
1	B	22	LEU	2.3
1	C	171	LYS	2.3
1	D	219	GLU	2.2
1	B	163	ASN	2.2
1	B	173	THR	2.2
1	C	144	ILE	2.2
1	E	171	LYS	2.2
1	A	57	VAL	2.1
1	A	20	THR	2.1
1	C	141	SER	2.1
1	C	173	THR	2.1
1	B	172	GLY	2.1
1	A	171	LYS	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(Å ²)	Q<0.9
3	1PE	A	305	16/16	0.68	0.15	83,90,106,106	0
3	1PE	B	306	16/16	0.70	0.14	91,98,109,109	0
5	GOL	D	309	6/6	0.70	0.14	71,78,79,80	0
5	GOL	B	308	6/6	0.71	0.18	85,96,98,100	0
5	GOL	D	308	6/6	0.73	0.13	72,91,94,96	0

Continued on next page...

Continued from previous page...

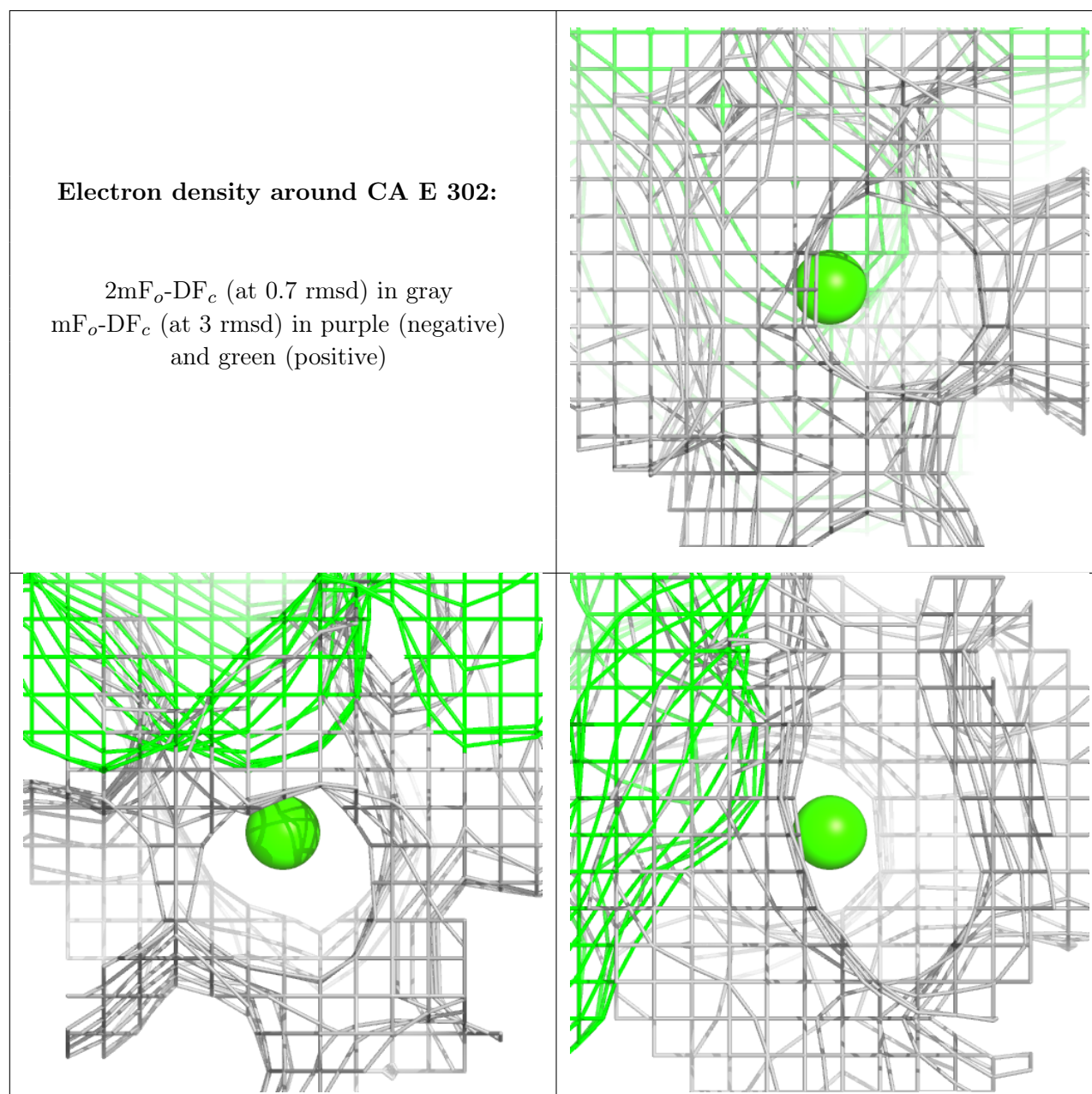
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1PE	E	306	16/16	0.75	0.17	78,95,99,101	0
5	GOL	D	307	6/6	0.75	0.16	55,83,90,92	0
5	GOL	F	308	6/6	0.75	0.17	53,58,65,67	0
3	1PE	D	305	16/16	0.77	0.17	49,85,99,100	0
4	PEG	E	307	7/7	0.78	0.17	64,73,77,78	0
3	1PE	F	303	16/16	0.78	0.22	75,94,126,127	0
5	GOL	A	308	6/6	0.80	0.15	67,79,81,81	0
3	1PE	E	304	16/16	0.81	0.17	59,84,91,94	0
5	GOL	E	309	6/6	0.81	0.17	71,73,77,77	0
4	PEG	F	307	7/7	0.81	0.16	61,64,70,73	0
4	PEG	A	306	7/7	0.82	0.15	62,79,81,81	0
5	GOL	E	310	6/6	0.82	0.20	81,83,84,86	0
3	1PE	F	305	16/16	0.82	0.19	65,80,102,103	0
5	GOL	A	307	6/6	0.83	0.12	62,73,80,85	0
3	1PE	C	302	16/16	0.83	0.17	54,75,87,88	0
3	1PE	E	305	16/16	0.83	0.20	47,79,93,95	0
5	GOL	E	308	6/6	0.84	0.13	82,86,88,91	0
3	1PE	B	304	16/16	0.84	0.17	45,67,82,83	0
6	PGE	C	306	10/10	0.84	0.17	67,76,78,83	0
5	GOL	C	305	6/6	0.85	0.14	50,59,66,67	0
3	1PE	B	305	16/16	0.85	0.15	53,73,90,91	0
3	1PE	D	303	16/16	0.85	0.16	38,70,87,89	0
3	1PE	A	303	16/16	0.86	0.15	41,65,74,76	0
4	PEG	B	307	7/7	0.86	0.14	64,68,75,77	0
3	1PE	C	303	16/16	0.86	0.17	50,69,81,81	0
3	1PE	A	304	16/16	0.86	0.14	56,69,81,84	0
3	1PE	F	304	16/16	0.87	0.13	55,71,87,87	0
5	GOL	F	309	6/6	0.87	0.12	54,62,80,81	0
3	1PE	C	304	16/16	0.87	0.14	66,73,91,97	0
5	GOL	F	310	6/6	0.90	0.12	44,80,82,88	0
4	PEG	F	306	7/7	0.90	0.13	67,71,78,81	0
4	PEG	D	306	7/7	0.91	0.14	47,65,76,79	0
3	1PE	D	304	16/16	0.91	0.12	57,63,89,90	0
3	1PE	E	303	16/16	0.91	0.12	51,64,80,83	0
2	CA	E	302	1/1	0.97	0.03	28,28,28,28	0
2	CA	A	301	1/1	0.98	0.04	31,31,31,31	0
2	CA	F	301	1/1	0.98	0.03	27,27,27,27	0
2	CA	F	302	1/1	0.98	0.03	32,32,32,32	0
2	CA	B	301	1/1	0.98	0.02	29,29,29,29	0
2	CA	B	302	1/1	0.98	0.04	30,30,30,30	0
2	CA	D	301	1/1	0.98	0.03	30,30,30,30	0
2	CA	D	302	1/1	0.98	0.03	32,32,32,32	0

Continued on next page...

Continued from previous page...

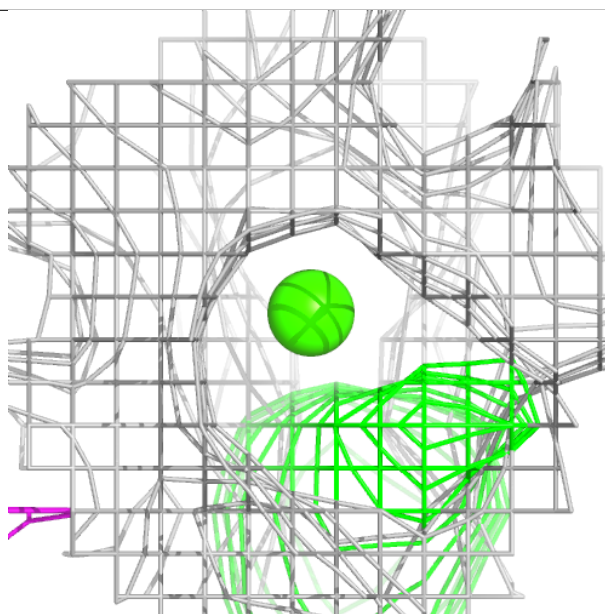
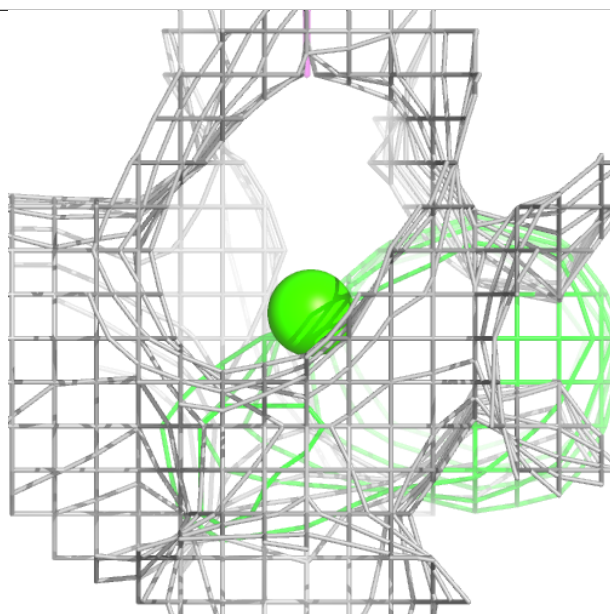
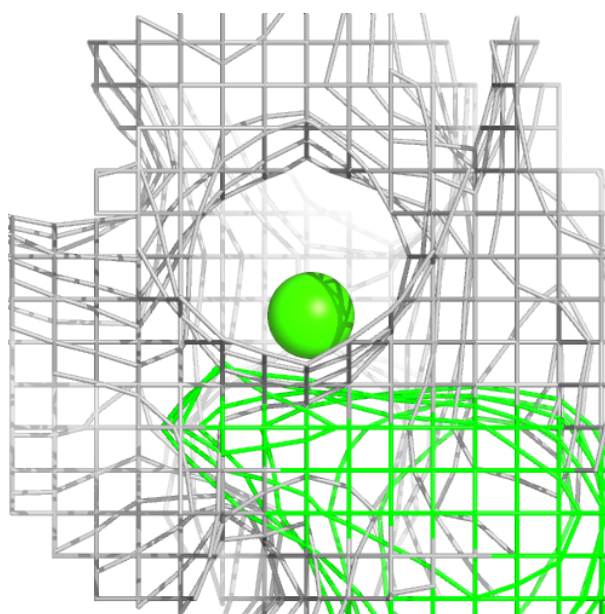
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	C	301	1/1	0.99	0.03	31,31,31,31	0
2	CA	A	302	1/1	0.99	0.02	30,30,30,30	0
2	CA	B	303	1/1	0.99	0.02	32,32,32,32	0
2	CA	E	301	1/1	1.00	0.04	25,25,25,25	0

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.



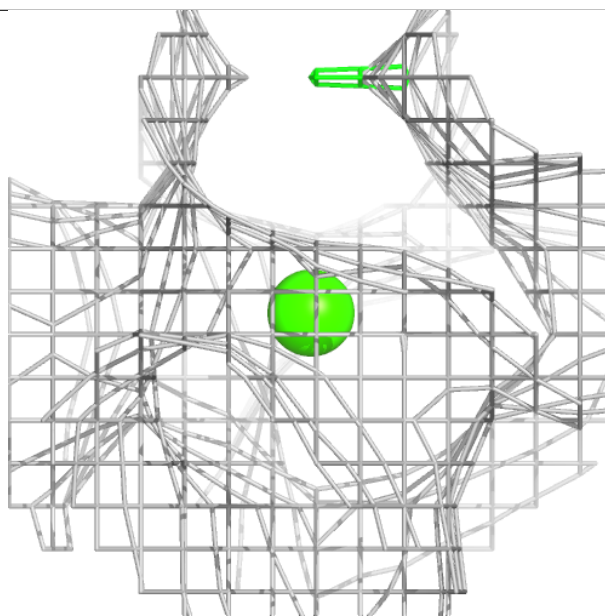
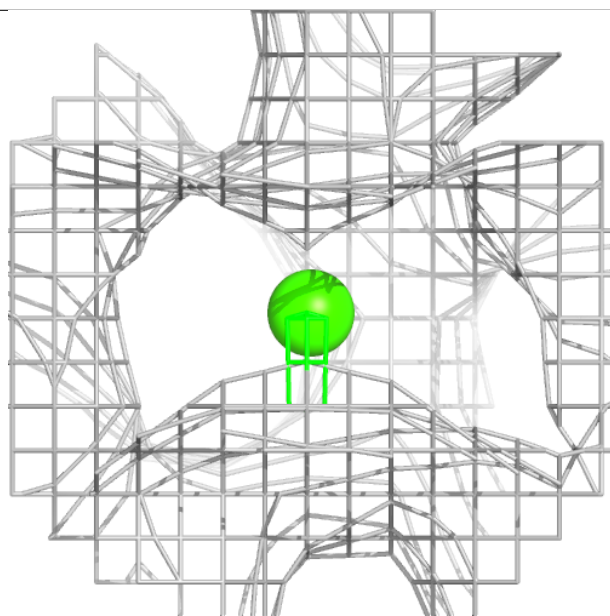
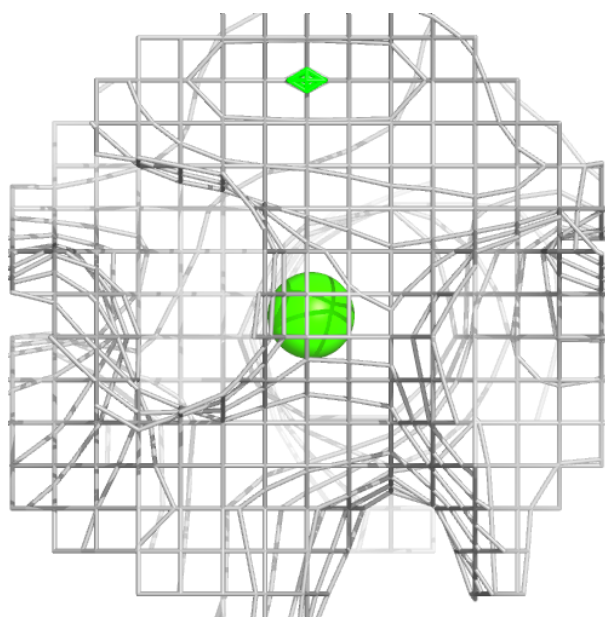
Electron density around CA A 301:

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



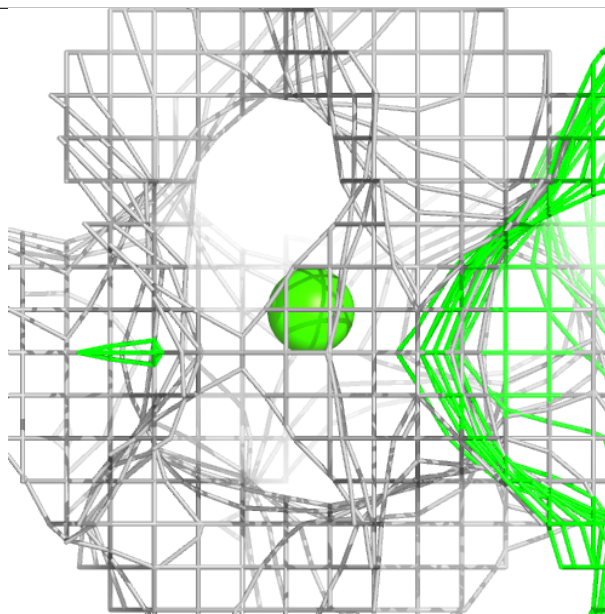
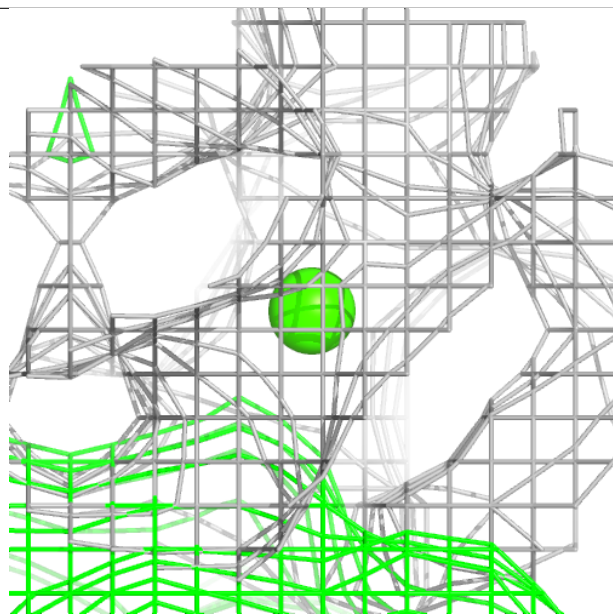
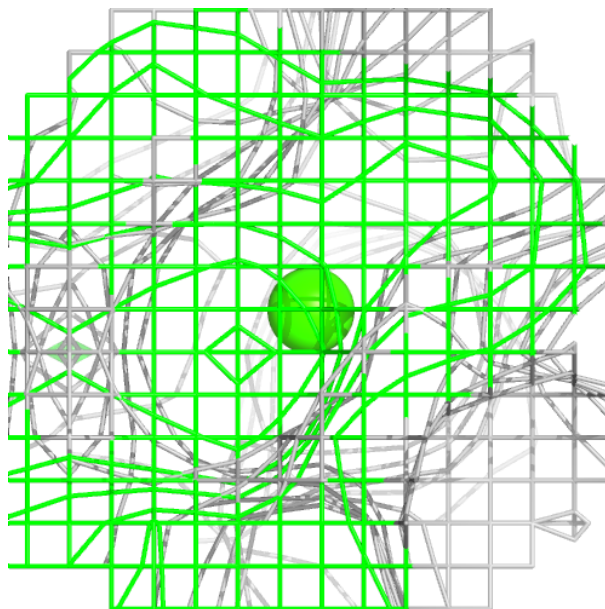
Electron density around CA F 301:

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



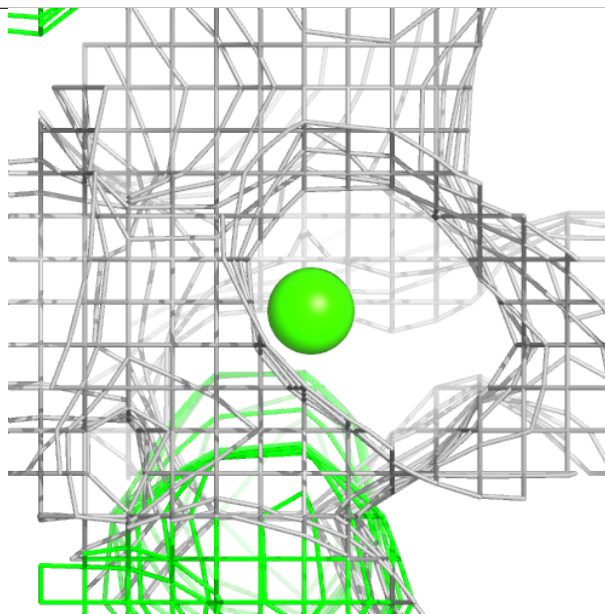
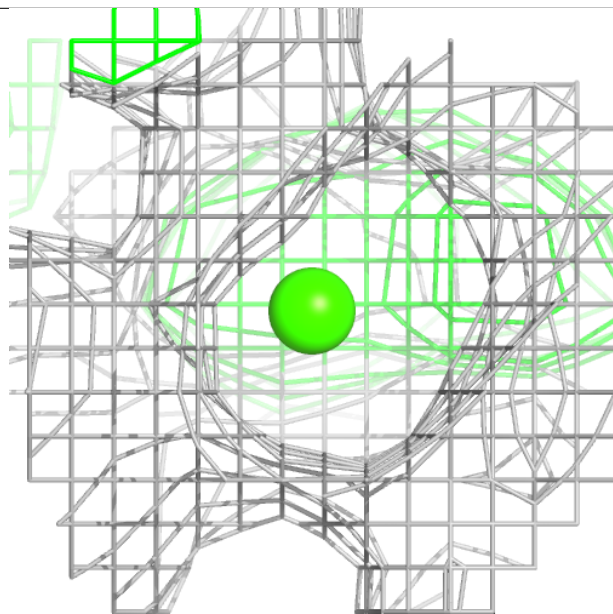
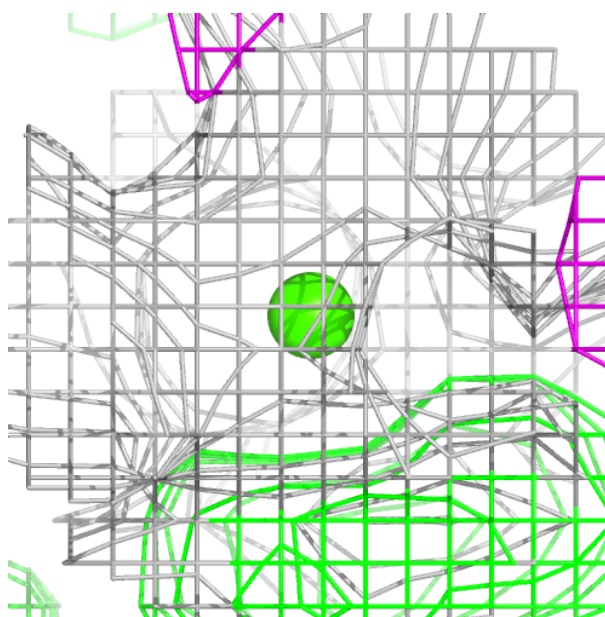
Electron density around CA F 302:

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



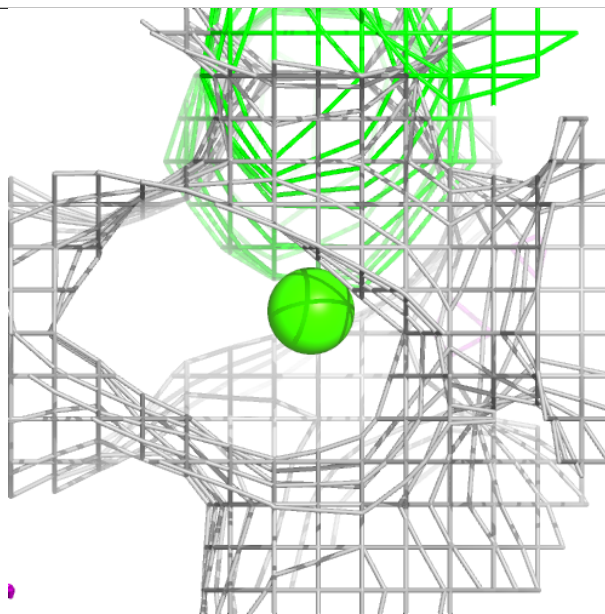
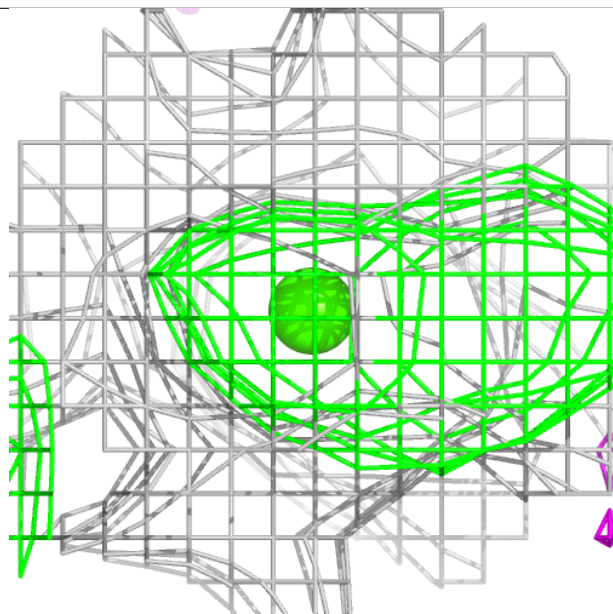
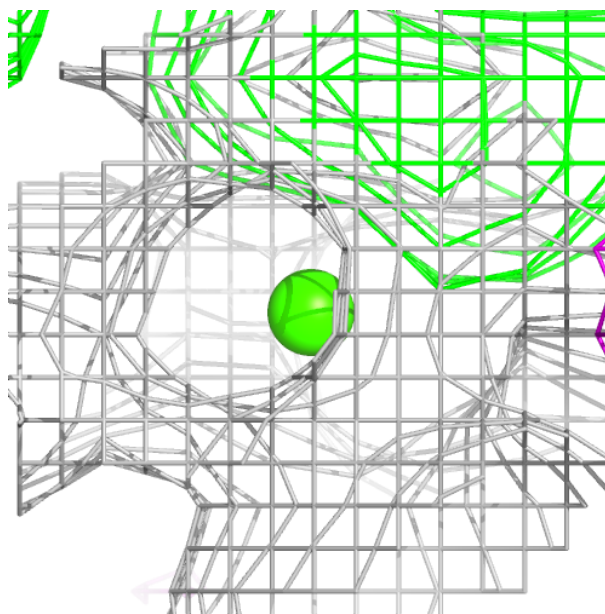
Electron density around CA B 301:

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



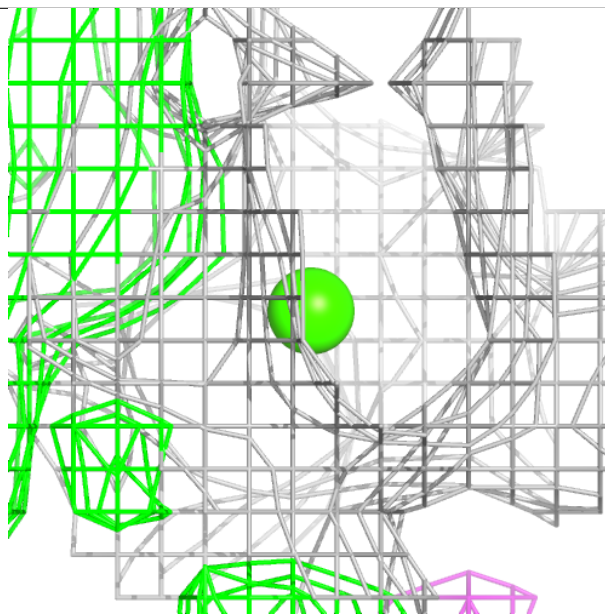
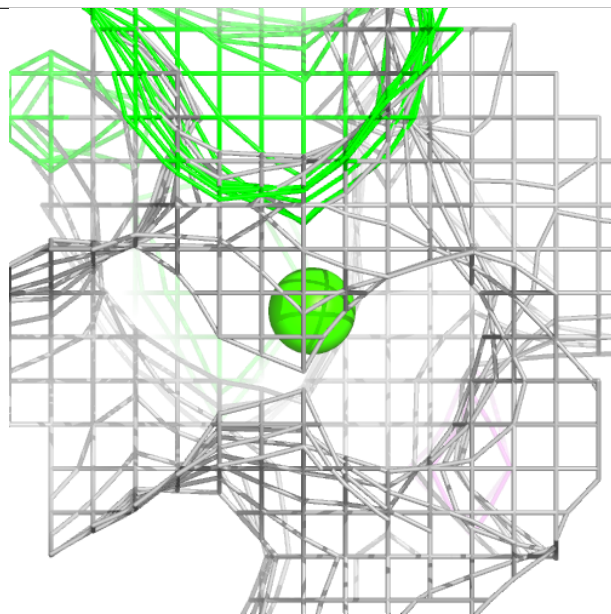
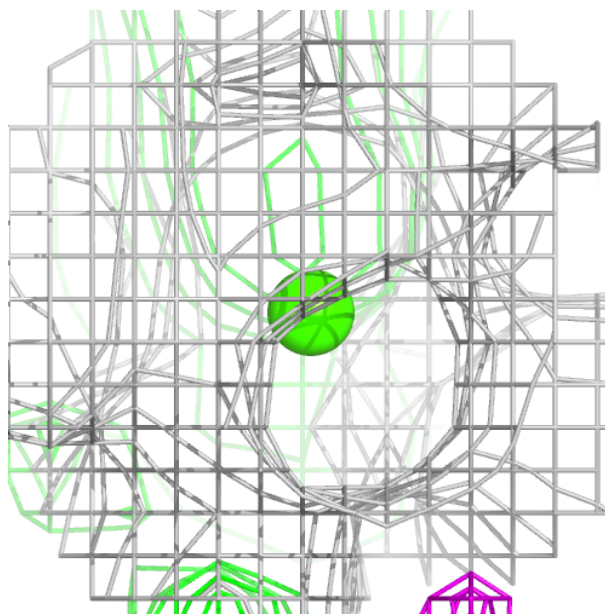
Electron density around CA B 302:

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



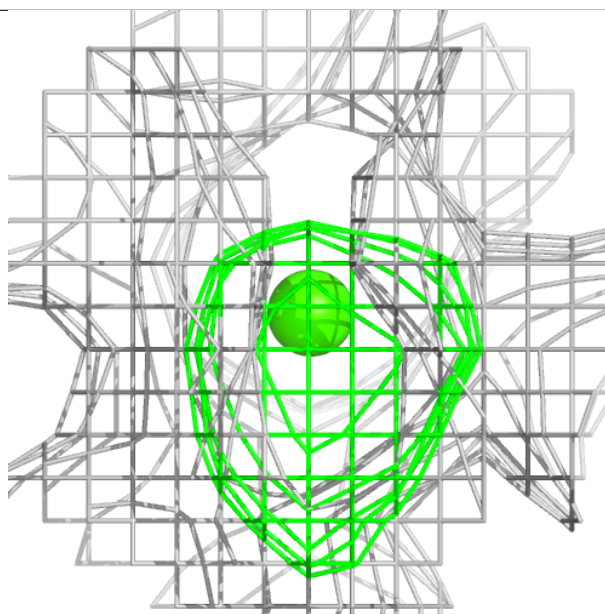
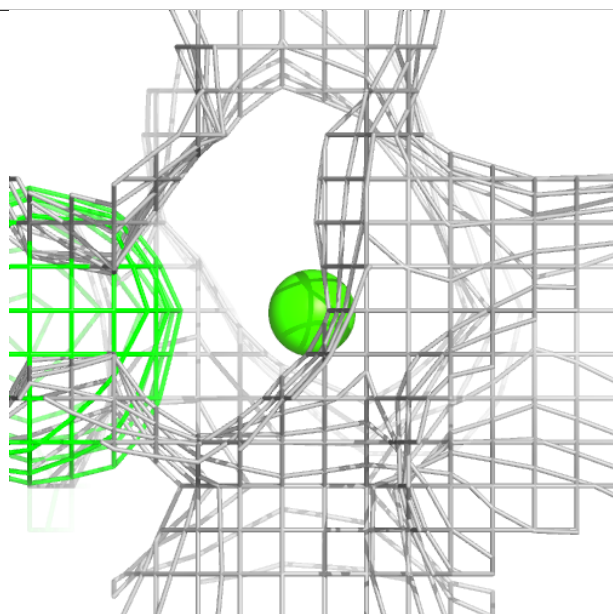
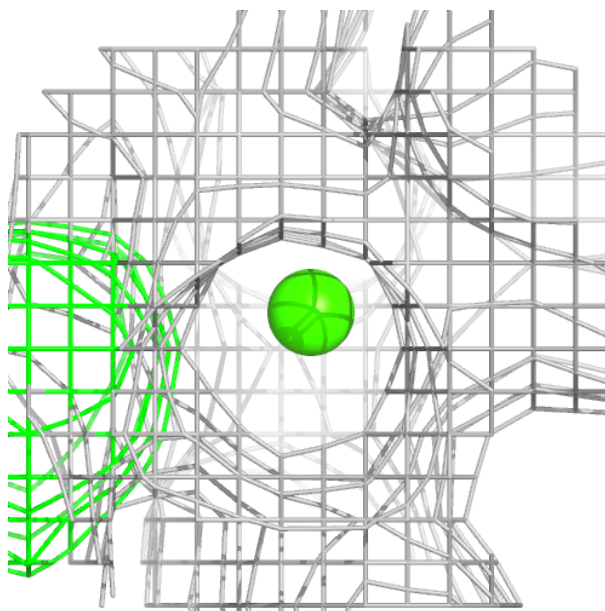
Electron density around CA D 301:

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



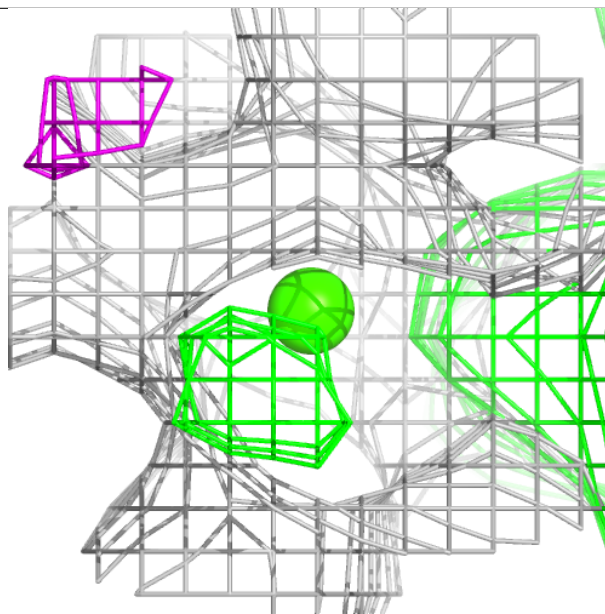
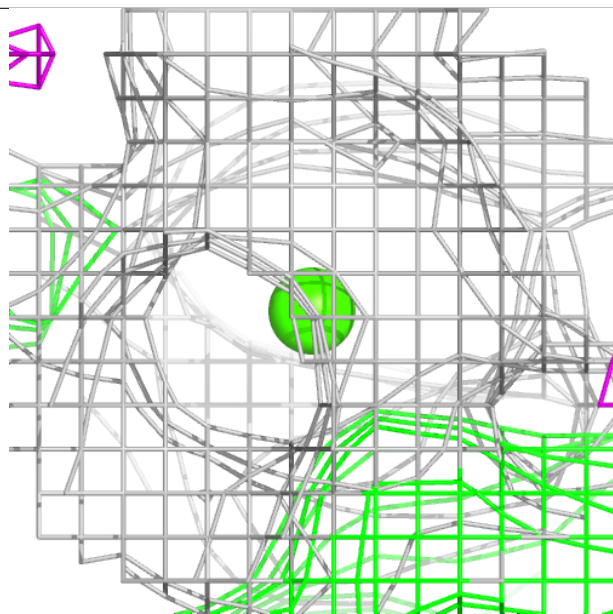
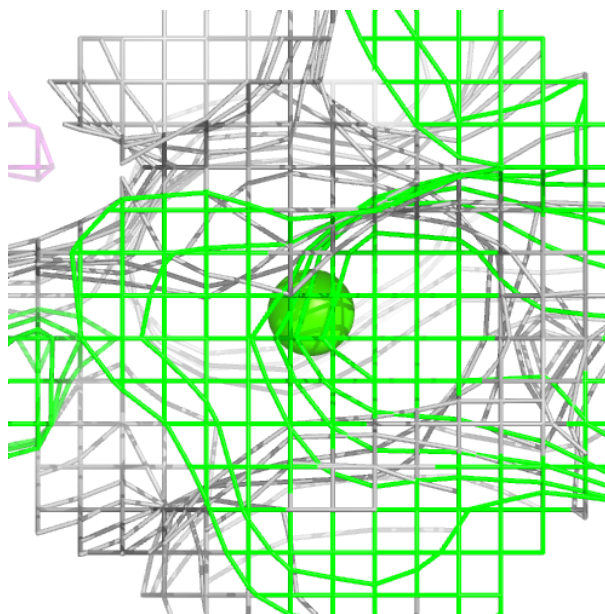
Electron density around CA D 302:

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



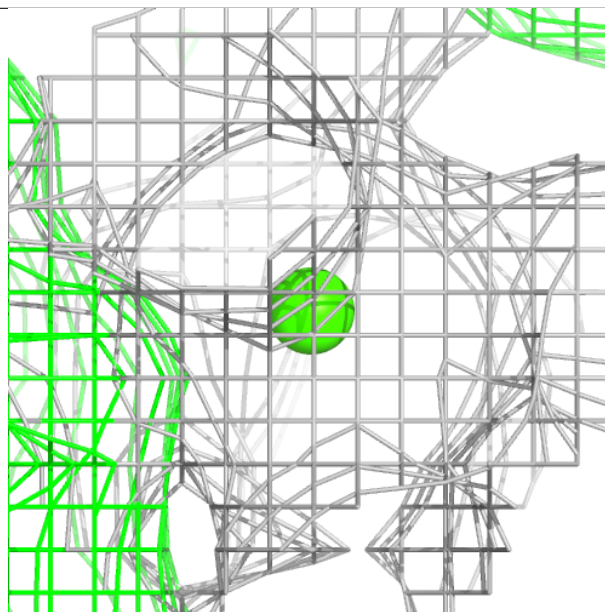
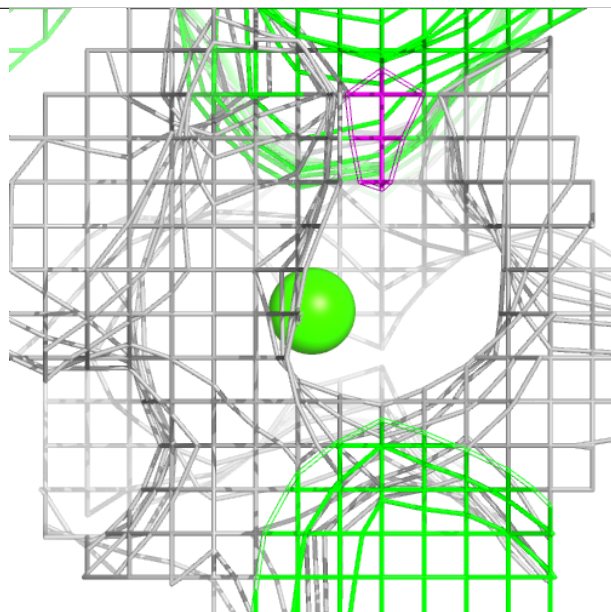
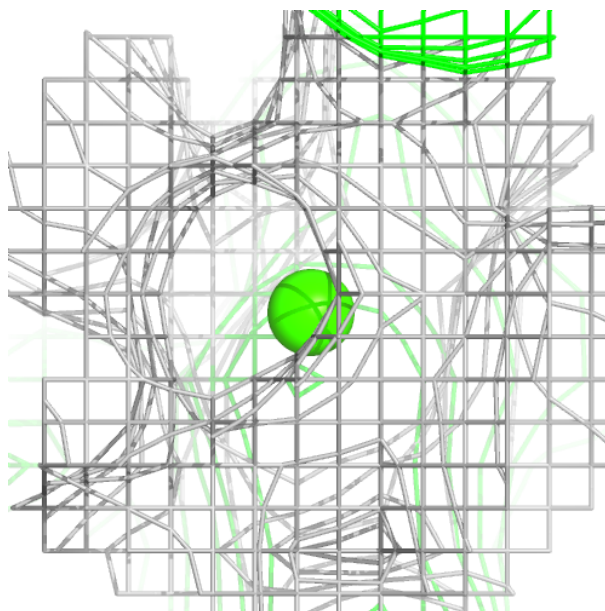
Electron density around CA C 301:

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



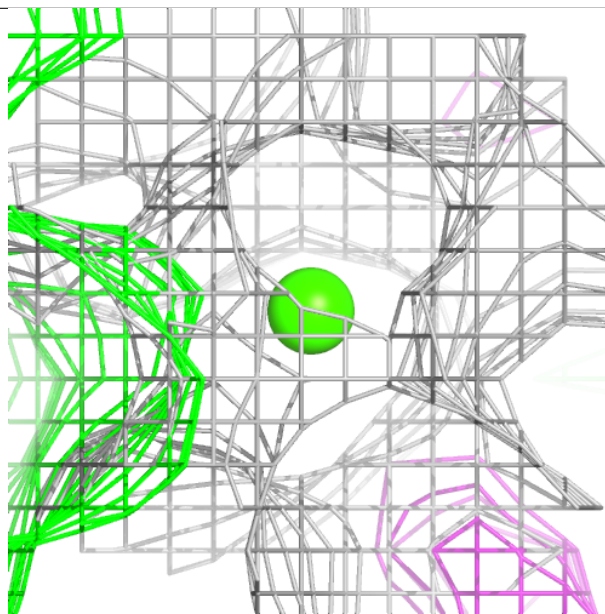
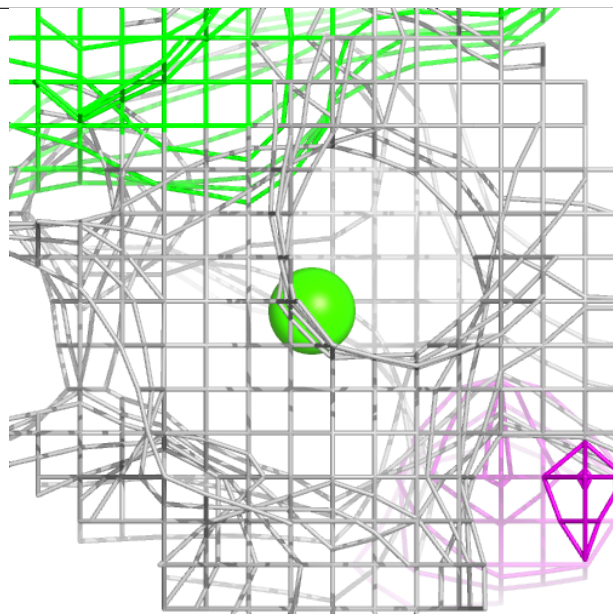
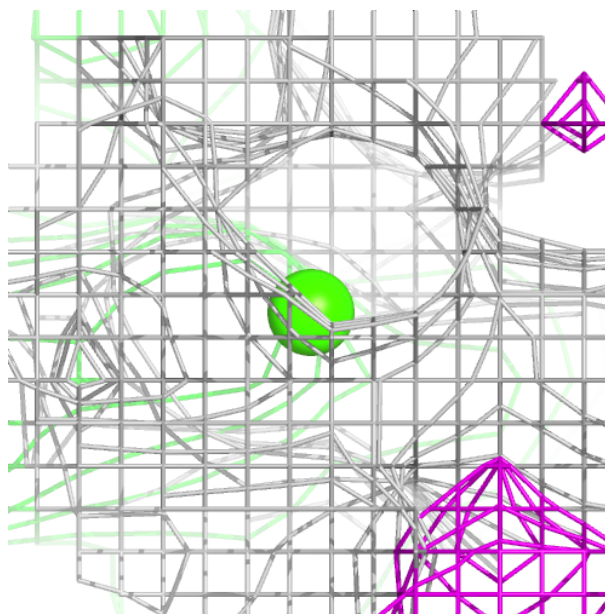
Electron density around CA A 302:

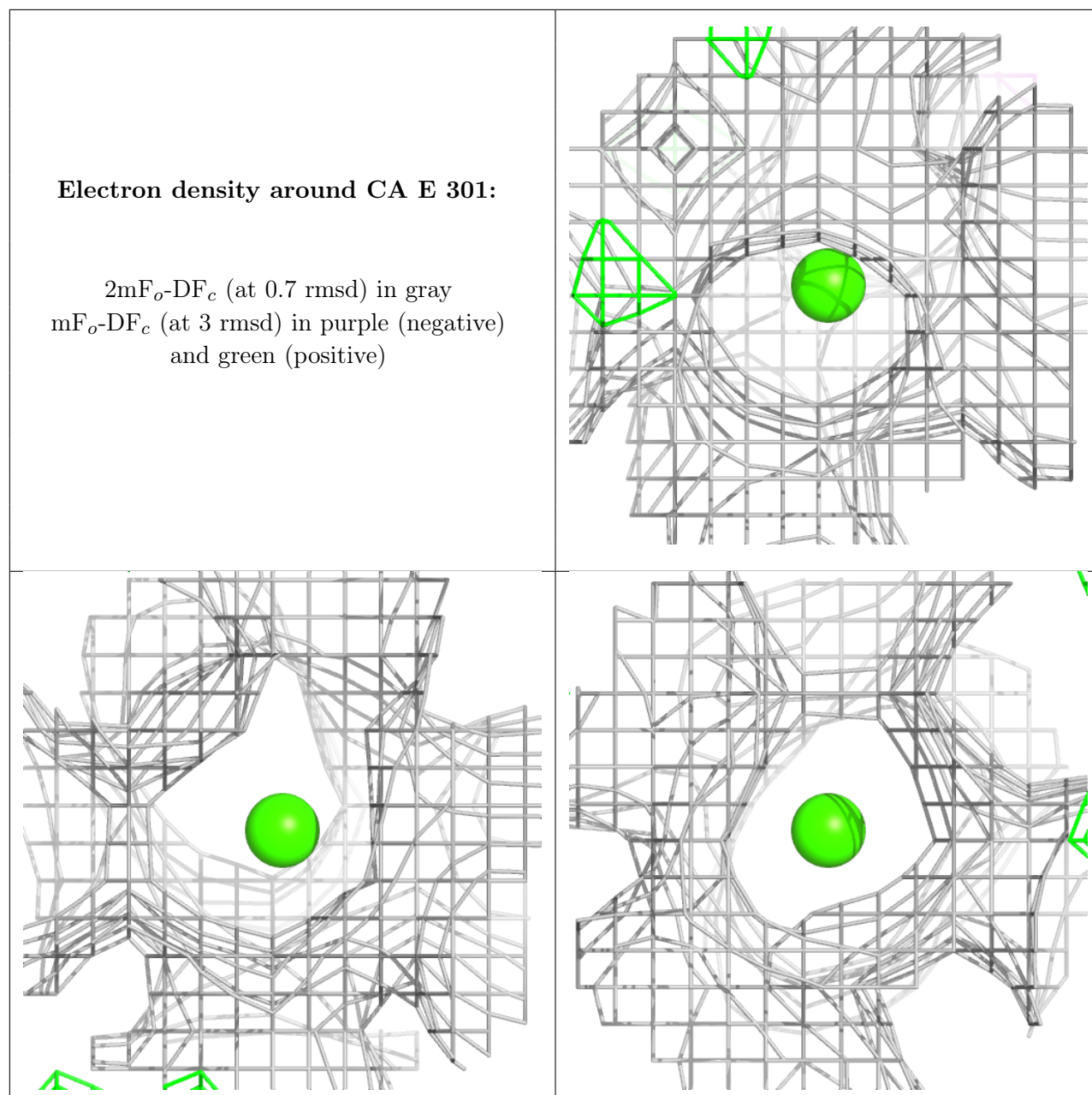
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 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.