



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:14 PM UTC

PDB ID : 9X3M / pdb_00009x3m
Title : Crystal structure of Pseudopedobacter saltans GH43 beta-xylosidase in complex with xylose.
Authors : Vishwakarma, P.; Sachdeva, E.; Ethayathulla, A.S.; Goyal, A.; Singh, T.P.; Kaur, P.
Deposited on : 2025-10-09
Resolution : 2.80 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

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Mol	Chain	Length	Quality of chain
1	E	432	
1	F	432	
1	G	432	
1	H	432	

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	XLS	C	503	-	-	X	-
3	XLS	D	503	-	X	-	-
3	XLS	E	503	-	-	X	-
3	XLS	F	503	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27742 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 Xylan 1,4-beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			
1	B	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			
1	C	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			
1	D	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			
1	E	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			
1	F	432	Total	C	N	O	S	0	1	0
			3431	2209	564	643	15			
1	G	432	Total	C	N	O	S	0	0	0
			3421	2203	562	641	15			
1	H	432	Total	C	N	O	S	0	0	0
			3425	2205	563	642	15			

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

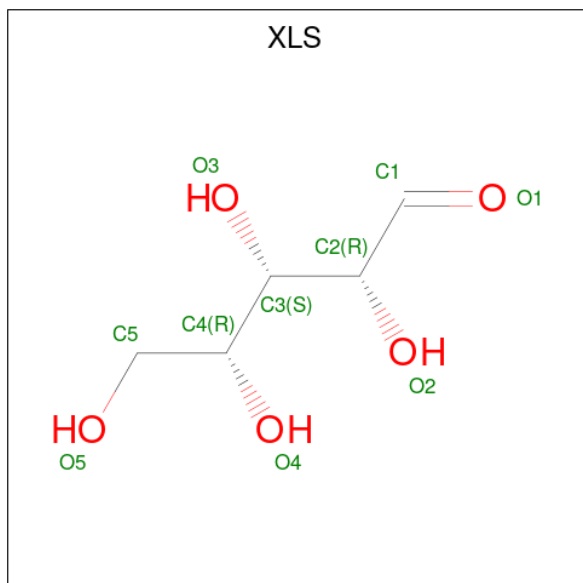
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	F	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Ca	0	0
			2	2		
2	H	2	Total	Ca	0	0
			2	2		

- Molecule 3 is D-xylose (CCD ID: XLS) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		
3	G	1	Total	C	O	0	0
			10	5	5		
3	H	1	Total	C	O	0	0
			10	5	5		

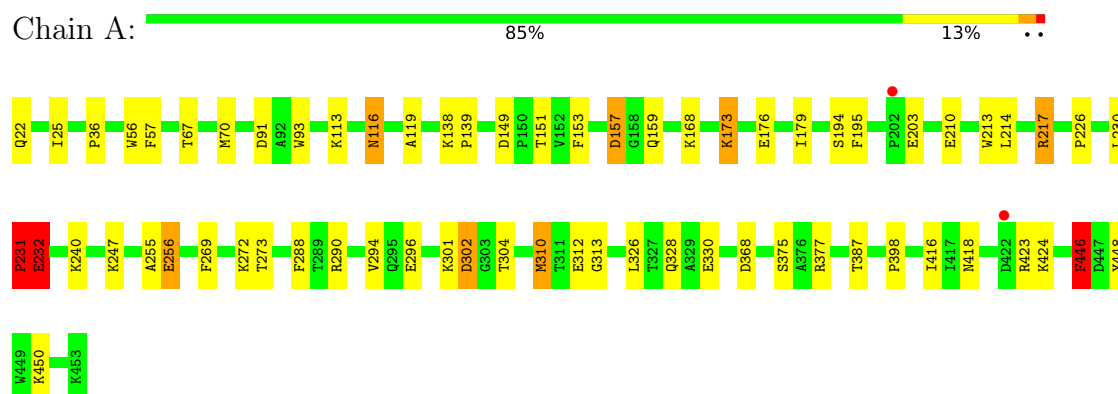
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total 32	O 32	0	0
4	B	29	Total 29	O 29	0	0
4	C	31	Total 31	O 31	0	0
4	D	28	Total 28	O 28	0	0
4	E	36	Total 36	O 36	0	0
4	F	34	Total 34	O 34	0	0
4	G	30	Total 30	O 30	0	0
4	H	24	Total 24	O 24	0	0

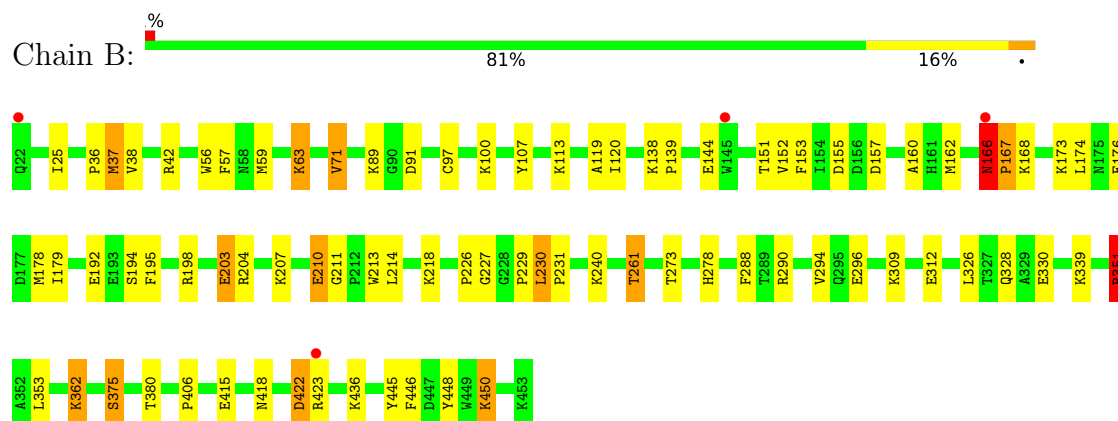
3 Residue-property plots

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.

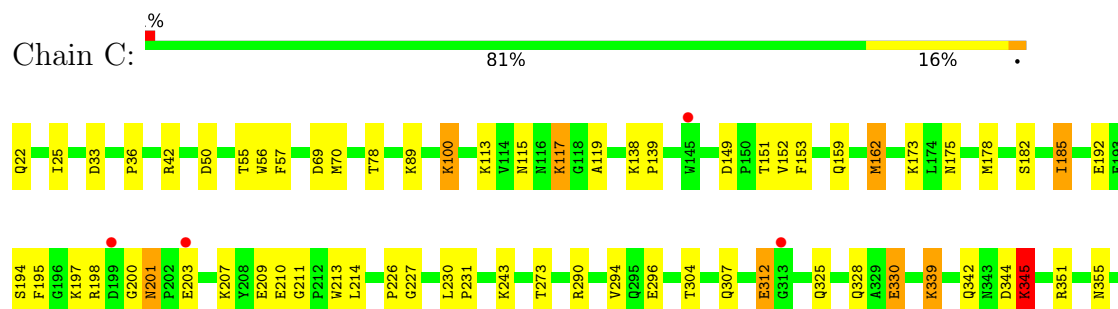
• Molecule 1: Xylan 1,4-beta-xylosidase

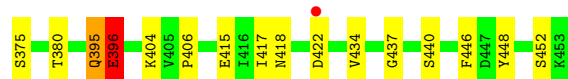


• Molecule 1: Xylan 1,4-beta-xylosidase



• Molecule 1: Xylan 1,4-beta-xylosidase





- Molecule 1: Xylan 1,4-beta-xylosidase

Chain D: 82% 16% .



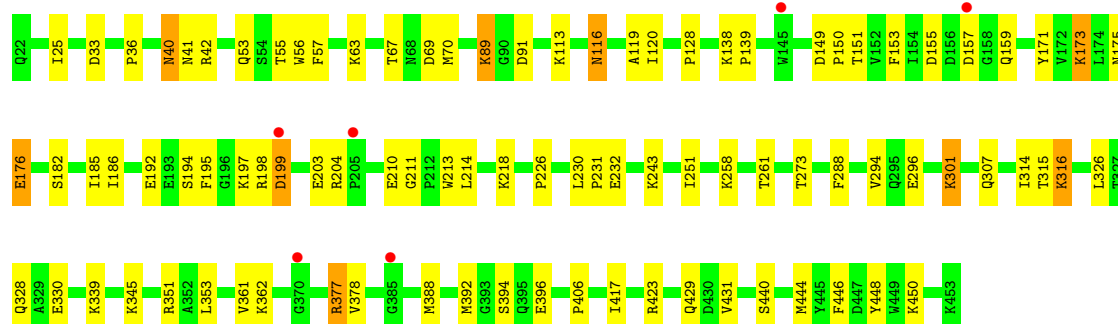
- Molecule 1: Xylan 1,4-beta-xylosidase

Chain E: 81% 17% .



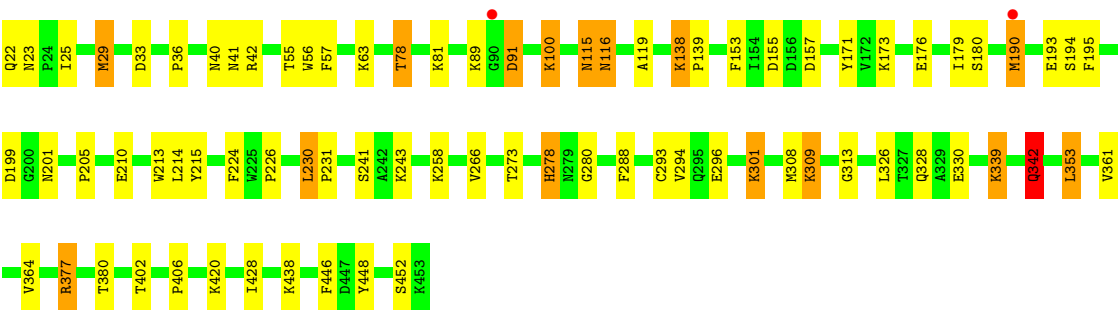
- Molecule 1: Xylan 1,4-beta-xylosidase

Chain F: 79% 19% .

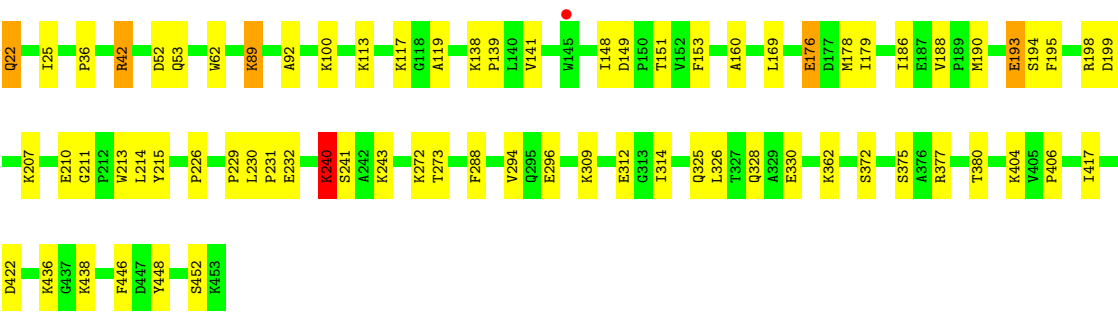
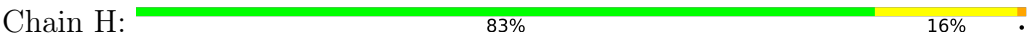


- Molecule 1: Xylan 1,4-beta-xylosidase

Chain G: 82% 15% .



● Molecule 1: Xylan 1,4-beta-xylosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.58Å 89.44Å 138.44Å 102.82° 94.02° 97.88°	Depositor
Resolution (Å)	47.84 – 2.80 47.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.84-2.80) 93.8 (47.84-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.218 , 0.273 0.227 , 0.283	Depositor DCC
R_{free} test set	3996 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27742	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.13% 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, XLS

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	0.81	1/3528 (0.0%)	1.47	32/4791 (0.7%)
1	B	0.81	0/3528	1.43	28/4791 (0.6%)
1	C	0.80	0/3528	1.39	28/4791 (0.6%)
1	D	0.80	1/3528 (0.0%)	1.40	34/4791 (0.7%)
1	E	0.79	0/3528	1.43	36/4791 (0.8%)
1	F	0.80	1/3537 (0.0%)	1.41	36/4803 (0.7%)
1	G	0.80	1/3524 (0.0%)	1.47	45/4786 (0.9%)
1	H	0.81	0/3528	1.42	29/4791 (0.6%)
All	All	0.80	4/28229 (0.0%)	1.43	268/38335 (0.7%)

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	2
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	3
1	G	0	1
1	H	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	440	SER	CA-CB	-6.60	1.42	1.53
1	D	440	SER	CA-CB	-6.06	1.44	1.53
1	A	217	ARG	NE-CZ	5.32	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	SER	CA-CB	-5.05	1.45	1.53

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	PHE	CA-CB-CG	17.79	131.59	113.80
1	A	446	PHE	CB-CA-C	-14.32	81.32	109.68
1	D	315	THR	CA-CB-OG1	-13.96	88.65	109.60
1	E	22	GLN	CB-CA-C	12.51	133.87	110.10
1	A	157	ASP	CB-CA-C	-12.35	86.50	110.46
1	G	115	ASN	CB-CA-C	-12.22	88.74	109.75
1	B	351	ARG	CB-CG-CD	12.12	139.18	111.30
1	G	278	HIS	CB-CG-CD2	-11.74	115.93	131.20
1	G	278	HIS	CB-CG-ND1	11.21	139.52	122.70
1	E	22	GLN	N-CA-CB	-11.19	91.48	110.50
1	C	100	LYS	CG-CD-CE	11.03	136.66	111.30
1	A	173	LYS	CB-CG-CD	10.99	136.59	111.30
1	E	396	GLU	CB-CG-CD	10.99	131.28	112.60
1	A	232	GLU	CB-CG-CD	10.95	131.22	112.60
1	A	310	MET	CG-SD-CE	-10.77	77.21	100.90
1	G	342	GLN	N-CA-CB	-10.45	94.22	111.66
1	H	312	GLU	CB-CG-CD	10.45	130.36	112.60
1	H	22	GLN	CB-CA-C	10.35	129.76	110.10
1	A	272	LYS	CB-CG-CD	10.27	134.92	111.30
1	G	176	GLU	CB-CG-CD	-9.99	95.62	112.60
1	B	42	ARG	CG-CD-NE	-9.83	90.37	112.00
1	E	110	VAL	N-CA-CB	-9.77	96.43	112.06
1	F	176	GLU	CB-CG-CD	-9.69	96.13	112.60
1	H	22	GLN	N-CA-CB	-9.69	94.03	110.50
1	G	190	MET	CG-SD-CE	9.63	122.08	100.90
1	G	23	ASN	CB-CA-C	9.61	129.11	110.17
1	E	42	ARG	CG-CD-NE	-9.36	91.40	112.00
1	G	91	ASP	CA-CB-CG	9.11	121.71	112.60
1	B	203	GLU	CB-CG-CD	9.09	128.05	112.60
1	C	422	ASP	CA-CB-CG	9.04	121.64	112.60
1	H	446	PHE	CA-CB-CG	8.96	122.76	113.80
1	H	243	LYS	CB-CG-CD	8.84	131.63	111.30
1	H	272	LYS	CG-CD-CE	-8.83	90.98	111.30
1	F	446	PHE	CA-CB-CG	8.78	122.58	113.80
1	F	199	ASP	N-CA-C	8.75	120.75	111.03
1	E	144	GLU	N-CA-CB	8.75	122.75	110.07
1	B	446	PHE	CA-CB-CG	8.70	122.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	446	PHE	CA-CB-CG	8.69	122.49	113.80
1	G	309	LYS	CG-CD-CE	8.53	130.91	111.30
1	F	316	LYS	CA-CB-CG	8.52	131.14	114.10
1	C	446	PHE	CA-CB-CG	8.52	122.31	113.80
1	D	315	THR	N-CA-CB	8.48	122.86	110.47
1	A	301	LYS	CB-CG-CD	8.44	130.71	111.30
1	D	446	PHE	CA-CB-CG	8.36	122.16	113.80
1	D	22	GLN	CB-CA-C	8.25	125.77	110.10
1	B	422	ASP	CA-CB-CG	8.25	120.85	112.60
1	C	396	GLU	CB-CG-CD	8.10	126.37	112.60
1	G	41	ASN	CB-CA-C	8.08	126.51	110.42
1	D	312	GLU	CB-CG-CD	8.06	126.30	112.60
1	F	396	GLU	CB-CG-CD	8.05	126.28	112.60
1	A	176	GLU	CB-CG-CD	-7.97	99.06	112.60
1	A	113	LYS	CG-CD-CE	7.93	129.55	111.30
1	E	446	PHE	CA-CB-CG	7.93	121.73	113.80
1	G	78	THR	CA-CB-OG1	-7.87	97.79	109.60
1	D	422	ASP	CA-CB-CG	7.86	120.46	112.60
1	G	199	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	450	LYS	CB-CG-CD	7.77	129.17	111.30
1	F	243	LYS	CB-CG-CD	7.74	129.10	111.30
1	A	217	ARG	N-CA-CB	7.66	126.09	111.15
1	A	312	GLU	N-CA-C	-7.66	98.98	110.24
1	A	231	PRO	CA-CB-CG	-7.65	89.46	104.00
1	E	438	LYS	CB-CG-CD	7.65	128.89	111.30
1	D	199	ASP	CB-CA-C	7.51	123.21	110.81
1	G	377	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	G	115	ASN	CA-CB-CG	7.47	120.07	112.60
1	G	173	LYS	CA-CB-CG	7.39	128.88	114.10
1	C	117	LYS	CA-CB-CG	7.37	128.83	114.10
1	H	436	LYS	CB-CG-CD	7.34	128.19	111.30
1	E	170	LYS	CG-CD-CE	7.31	128.11	111.30
1	D	176	GLU	CB-CG-CD	-7.25	100.27	112.60
1	G	138	LYS	CG-CD-CE	7.21	127.88	111.30
1	B	144	GLU	N-CA-CB	7.21	120.82	110.16
1	F	301	LYS	CB-CA-C	7.20	123.95	110.63
1	F	40	ASN	CA-C-N	-7.19	107.81	121.54
1	F	40	ASN	C-N-CA	-7.19	107.81	121.54
1	F	199	ASP	CA-C-O	-7.18	113.50	120.90
1	F	41	ASN	CB-CA-C	7.18	124.70	110.42
1	C	395	GLN	N-CA-C	-7.16	96.88	108.41
1	G	288	PHE	N-CA-CB	7.10	121.08	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	288	PHE	N-CA-CB	7.08	121.06	110.65
1	F	63	LYS	CD-CE-NZ	7.05	134.46	111.90
1	G	193	GLU	CB-CG-CD	7.03	124.55	112.60
1	A	301	LYS	CB-CA-C	7.03	122.45	110.79
1	H	422	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	100	LYS	CB-CG-CD	-6.96	95.30	111.30
1	F	91	ASP	CA-CB-CG	6.95	119.55	112.60
1	D	199	ASP	CA-CB-CG	6.94	119.54	112.60
1	G	23	ASN	CA-CB-CG	6.84	119.44	112.60
1	C	345	LYS	CG-CD-CE	6.83	127.01	111.30
1	B	167	PRO	N-CA-CB	6.83	110.76	103.39
1	G	29	MET	CG-SD-CE	-6.79	85.95	100.90
1	H	272	LYS	CB-CG-CD	6.77	126.86	111.30
1	B	176	GLU	CB-CG-CD	-6.75	101.12	112.60
1	G	339	LYS	CB-CG-CD	6.75	126.81	111.30
1	C	42	ARG	CB-CA-C	6.72	122.66	109.35
1	F	42	ARG	CG-CD-NE	-6.72	97.22	112.00
1	C	178	MET	CG-SD-CE	6.71	115.67	100.90
1	A	288	PHE	N-CA-CB	6.70	120.50	110.65
1	B	166	ASN	CA-CB-CG	-6.68	105.92	112.60
1	E	151	THR	CA-CB-OG1	-6.67	99.59	109.60
1	E	298	ASN	CA-CB-CG	-6.66	105.94	112.60
1	E	116	ASN	CB-CA-C	6.66	122.03	111.51
1	G	190	MET	CB-CG-SD	-6.56	93.01	112.70
1	G	402	THR	CA-CB-OG1	-6.55	99.78	109.60
1	D	103	LYS	CB-CG-CD	6.49	126.23	111.30
1	C	396	GLU	N-CA-CB	6.48	121.44	110.49
1	E	55	THR	OG1-CB-CG2	6.45	122.19	109.30
1	G	339	LYS	CA-CB-CG	6.43	126.96	114.10
1	E	197	LYS	CB-CG-CD	6.41	126.04	111.30
1	G	309	LYS	CB-CG-CD	6.40	126.02	111.30
1	F	288	PHE	N-CA-CB	6.40	120.06	110.65
1	G	91	ASP	N-CA-C	-6.34	97.29	110.80
1	F	89	LYS	CD-CE-NZ	-6.34	91.62	111.90
1	A	151	THR	CA-CB-OG1	-6.31	100.14	109.60
1	E	288	PHE	N-CA-CB	6.29	119.90	110.65
1	G	42	ARG	CB-CA-C	6.22	121.66	109.35
1	C	151	THR	CA-CB-OG1	-6.22	100.28	109.60
1	A	312	GLU	CB-CG-CD	6.18	123.11	112.60
1	D	151	THR	CA-CB-OG1	-6.16	100.36	109.60
1	D	81	LYS	CG-CD-CE	6.15	125.45	111.30
1	H	207	LYS	CG-CD-CE	6.15	125.45	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	55	THR	OG1-CB-CG2	6.13	121.56	109.30
1	C	100	LYS	CD-CE-NZ	-6.13	92.28	111.90
1	H	243	LYS	CB-CA-C	6.12	121.73	110.11
1	H	151	THR	CA-CB-OG1	-6.11	100.44	109.60
1	D	42	ARG	CB-CA-C	6.10	121.43	109.35
1	E	361	VAL	N-CA-CB	-6.10	102.99	111.41
1	H	89	LYS	CD-CE-NZ	-6.10	92.39	111.90
1	A	240	LYS	CG-CD-CE	6.09	125.31	111.30
1	F	258	LYS	CB-CG-CD	6.08	125.28	111.30
1	C	162	MET	CG-SD-CE	-6.07	87.56	100.90
1	H	42	ARG	CB-CA-C	6.05	121.34	109.35
1	C	304	THR	OG1-CB-CG2	6.04	121.38	109.30
1	E	176	GLU	CG-CD-OE2	-6.04	104.51	118.40
1	F	151	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	273	THR	CA-CB-OG1	-6.03	100.56	109.60
1	D	215	TYR	N-CA-CB	-6.02	101.07	111.55
1	B	210	GLU	N-CA-C	6.02	123.62	110.80
1	B	166	ASN	N-CA-CB	6.01	121.07	110.37
1	A	116	ASN	CA-CB-CG	-6.00	106.60	112.60
1	D	273	THR	CA-CB-OG1	-5.98	100.63	109.60
1	G	40	ASN	N-CA-C	-5.96	98.10	110.80
1	B	91	ASP	CA-CB-CG	5.95	118.55	112.60
1	H	141	VAL	CA-CB-CG2	5.95	120.51	110.40
1	F	273	THR	CA-CB-OG1	-5.94	100.70	109.60
1	G	40	ASN	CB-CA-C	5.93	122.22	110.42
1	C	296	GLU	CB-CA-C	5.91	119.75	109.65
1	C	339	LYS	CG-CD-CE	5.90	124.88	111.30
1	B	296	GLU	CB-CA-C	5.88	120.37	109.54
1	F	203	GLU	CB-CG-CD	-5.87	102.63	112.60
1	H	438	LYS	N-CA-CB	5.86	119.95	110.40
1	F	296	GLU	CB-CA-C	5.86	120.31	109.54
1	H	296	GLU	CB-CA-C	5.85	119.66	109.65
1	D	424	LYS	CD-CE-NZ	5.83	130.55	111.90
1	A	231	PRO	CA-N-CD	-5.83	103.34	111.50
1	E	182	SER	N-CA-CB	5.81	118.32	110.59
1	H	193	GLU	CB-CG-CD	5.79	122.44	112.60
1	B	151	THR	CA-CB-OG1	-5.79	100.92	109.60
1	F	204	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	E	296	GLU	CB-CA-C	5.76	120.14	109.54
1	E	143	SER	CA-CB-OG	-5.76	99.58	111.10
1	G	243	LYS	CB-CG-CD	5.75	124.53	111.30
1	F	42	ARG	CB-CA-C	5.75	121.04	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	309	LYS	CB-CG-CD	5.74	124.50	111.30
1	D	272	LYS	CG-CD-CE	-5.74	98.11	111.30
1	D	173	LYS	N-CA-CB	-5.72	101.12	110.21
1	A	424	LYS	CA-CB-CG	5.70	125.51	114.10
1	H	288	PHE	N-CA-CB	5.70	119.21	110.61
1	E	173	LYS	N-CA-CB	-5.69	101.17	110.21
1	G	89	LYS	CG-CD-CE	-5.67	98.26	111.30
1	C	50	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	377	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	E	42	ARG	CB-CA-C	5.66	120.56	109.35
1	B	192	GLU	CB-CG-CD	5.66	122.22	112.60
1	G	201	ASN	CB-CA-C	5.65	115.53	110.44
1	F	173	LYS	N-CA-CB	-5.63	101.25	110.21
1	B	210	GLU	CA-C-N	-5.61	113.06	121.87
1	B	210	GLU	C-N-CA	-5.61	113.06	121.87
1	B	362	LYS	CG-CD-CE	5.61	124.20	111.30
1	D	144	GLU	CB-CA-C	5.59	120.35	110.85
1	B	63	LYS	CB-CG-CD	5.58	124.14	111.30
1	E	50	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	415	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	302	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	402	THR	CA-CB-OG1	-5.52	101.31	109.60
1	F	377	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	G	243	LYS	CB-CA-C	5.52	120.93	109.95
1	H	240	LYS	CB-CA-C	5.52	121.84	110.31
1	H	377	ARG	CB-CG-CD	-5.50	98.64	111.30
1	F	40	ASN	N-CA-C	-5.49	99.87	108.00
1	B	288	PHE	N-CA-CB	5.47	118.69	110.65
1	D	138	LYS	CB-CG-CD	5.46	123.87	111.30
1	F	89	LYS	CG-CD-CE	5.46	123.87	111.30
1	G	446	PHE	N-CA-CB	-5.46	101.64	110.71
1	F	199	ASP	CB-CA-C	5.46	119.42	110.95
1	H	176	GLU	CG-CD-OE2	5.46	130.95	118.40
1	G	301	LYS	CB-CG-CD	5.45	123.84	111.30
1	G	296	GLU	CB-CA-C	5.44	119.47	109.46
1	H	273	THR	CA-CB-OG1	-5.43	101.45	109.60
1	C	243	LYS	CB-CG-CD	5.41	123.75	111.30
1	F	204	ARG	NH1-CZ-NH2	5.41	126.34	119.30
1	H	199	ASP	CA-CB-CG	5.41	118.01	112.60
1	E	113	LYS	CG-CD-CE	5.41	123.74	111.30
1	F	218	LYS	CB-CG-CD	5.41	123.74	111.30
1	A	368	ASP	CA-CB-CG	5.40	118.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	THR	CA-CB-OG1	-5.39	101.51	109.60
1	C	330	GLU	CB-CG-CD	5.39	121.77	112.60
1	G	339	LYS	CG-CD-CE	5.38	123.66	111.30
1	A	203	GLU	CB-CG-CD	5.37	121.73	112.60
1	E	272	LYS	CD-CE-NZ	-5.37	94.72	111.90
1	C	173	LYS	N-CA-CB	-5.36	101.68	110.21
1	D	159	GLN	CA-CB-CG	-5.35	103.41	114.10
1	B	167	PRO	CA-CB-CG	-5.35	94.34	104.50
1	C	55	THR	OG1-CB-CG2	5.34	119.98	109.30
1	E	117	LYS	CA-CB-CG	5.33	124.77	114.10
1	E	330	GLU	CB-CG-CD	5.31	121.62	112.60
1	D	301	LYS	CB-CG-CD	5.30	123.50	111.30
1	F	301	LYS	CG-CD-CE	5.29	123.48	111.30
1	A	387	THR	CA-CB-OG1	-5.29	101.66	109.60
1	E	301	LYS	CB-CA-C	5.28	119.56	110.79
1	H	362	LYS	CG-CD-CE	5.28	123.45	111.30
1	B	42	ARG	CB-CA-C	5.27	119.79	109.35
1	B	166	ASN	CA-C-N	-5.27	113.48	119.28
1	B	166	ASN	C-N-CA	-5.27	113.48	119.28
1	F	67	THR	CA-CB-OG1	-5.26	101.71	109.60
1	G	420	LYS	CG-CD-CE	5.26	123.39	111.30
1	G	100	LYS	CB-CA-C	5.25	118.23	110.14
1	E	422	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	273	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	231	PRO	CB-CA-C	-5.23	98.92	112.00
1	C	395	GLN	CA-C-O	-5.22	115.00	120.58
1	G	215	TYR	N-CA-CB	-5.22	101.88	111.37
1	E	113	LYS	CB-CG-CD	5.21	123.29	111.30
1	C	395	GLN	N-CA-CB	5.21	118.50	110.21
1	E	117	LYS	N-CA-CB	-5.21	102.62	111.69
1	B	339	LYS	CB-CG-CD	5.21	123.28	111.30
1	G	81	LYS	CD-CE-NZ	-5.20	95.27	111.90
1	D	89	LYS	CB-CG-CD	5.19	123.24	111.30
1	D	272	LYS	CB-CG-CD	5.19	123.24	111.30
1	F	55	THR	OG1-CB-CG2	5.19	119.67	109.30
1	D	55	THR	OG1-CB-CG2	5.18	119.67	109.30
1	D	296	GLU	CB-CA-C	5.18	119.08	109.54
1	C	339	LYS	CA-CB-CG	5.18	124.46	114.10
1	E	308	MET	CB-CG-SD	5.17	128.22	112.70
1	D	114	VAL	N-CA-CB	5.17	117.57	110.54
1	B	273	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	256	GLU	N-CA-CB	-5.16	103.04	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	362	LYS	CG-CD-CE	5.16	123.16	111.30
1	A	67	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	296	GLU	CB-CA-C	5.12	118.96	109.54
1	D	105	TYR	N-CA-CB	-5.12	102.52	110.55
1	E	446	PHE	N-CA-CB	-5.12	102.22	110.71
1	D	387	THR	CA-CB-OG1	-5.11	101.93	109.60
1	D	207	LYS	CG-CD-CE	5.11	123.05	111.30
1	D	453	LYS	CB-CG-CD	5.09	123.01	111.30
1	A	91	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	210	GLU	O-C-N	-5.08	115.84	122.59
1	G	116	ASN	CA-CB-CG	-5.08	107.53	112.60
1	F	361	VAL	N-CA-CB	-5.07	102.56	111.39
1	H	117	LYS	N-CA-CB	-5.03	102.94	111.69
1	H	438	LYS	CA-CB-CG	5.03	124.16	114.10
1	F	116	ASN	CB-CA-C	5.02	119.17	111.39
1	H	215	TYR	N-CA-CB	-5.02	102.23	111.37
1	E	91	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	117	LYS	CA-C-N	5.02	124.87	120.10
1	C	117	LYS	C-N-CA	5.02	124.87	120.10
1	E	176	GLU	CG-CD-OE1	5.01	129.92	118.40
1	C	273	THR	CA-CB-OG1	-5.01	102.09	109.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ARG	Sidechain
1	A	446	PHE	Sidechain
1	C	351	ARG	Sidechain
1	D	351	ARG	Sidechain
1	D	377	ARG	Sidechain
1	D	42	ARG	Sidechain
1	E	249	GLY	Mainchain
1	F	351	ARG	Sidechain
1	F	377	ARG	Sidechain
1	F	423	ARG	Sidechain
1	G	377	ARG	Sidechain
1	H	42	ARG	Sidechain

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	3425	0	3288	34	0
1	B	3425	0	3288	45	0
1	C	3425	0	3288	49	0
1	D	3425	0	3288	36	0
1	E	3425	0	3288	37	0
1	F	3431	0	3296	51	0
1	G	3421	0	3282	42	0
1	H	3425	0	3288	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	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
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	10	0	10	5	0
3	B	10	0	10	5	0
3	C	10	0	10	9	0
3	D	10	0	10	3	0
3	E	10	0	10	7	0
3	F	10	0	10	1	0
3	G	10	0	10	1	0
3	H	10	0	10	3	0
4	A	32	0	0	0	0
4	B	29	0	0	1	0
4	C	31	0	0	1	0
4	D	28	0	0	0	0
4	E	36	0	0	3	0
4	F	34	0	0	3	0
4	G	30	0	0	2	0
4	H	24	0	0	0	0
All	All	27742	0	26386	325	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 6.

All (325) 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:C:33:ASP:OD2	3:C:503:XLS:H51	1.41	1.18
1:C:290:ARG:HH12	3:C:503:XLS:H52	1.15	1.09
1:F:392:MET:CE	1:F:429:GLN:HB3	1.84	1.08
1:C:290:ARG:NH1	3:C:503:XLS:H52	1.75	1.01
1:D:173:LYS:NZ	1:D:243:LYS:HZ1	1.59	0.99
1:E:159:GLN:HB3	1:E:173:LYS:HZ1	1.25	0.99
1:F:388:MET:HE2	1:F:444:MET:HE1	1.42	0.99
3:E:503:XLS:O1	3:E:503:XLS:H4	1.61	0.99
1:F:392:MET:HE2	1:F:429:GLN:HB3	1.44	0.97
1:F:339:LYS:HD2	1:F:353:LEU:HD11	1.44	0.97
1:E:290:ARG:HH12	3:E:503:XLS:H51	1.26	0.95
1:G:22:GLN:CB	1:G:294:VAL:O	2.17	0.92
1:A:398:PRO:HB2	1:A:423:ARG:NH2	1.84	0.91
1:H:100:LYS:HE2	1:H:178:MET:HE3	1.53	0.88
1:D:173:LYS:HZ3	1:D:243:LYS:NZ	1.72	0.88
1:E:315:THR:HB	1:E:316:LYS:HZ1	1.37	0.88
1:H:240:LYS:NZ	1:H:240:LYS:HB2	1.89	0.88
1:A:231:PRO:O	1:A:232:GLU:HB2	1.73	0.87
1:D:173:LYS:HZ3	1:D:243:LYS:HZ1	0.88	0.87
1:F:392:MET:HE2	1:F:429:GLN:CB	2.03	0.87
1:G:29:MET:HE3	4:G:606:HOH:O	1.74	0.86
1:C:290:ARG:HH12	3:C:503:XLS:C5	1.89	0.85
1:B:59:MET:HE1	3:B:503:XLS:O5	1.76	0.85
1:F:120:ILE:HG12	1:F:150:PRO:HG3	1.60	0.84
1:E:358:TYR:CE2	1:E:395:GLN:OE1	2.32	0.82
1:E:315:THR:HB	1:E:316:LYS:NZ	1.93	0.82
1:G:29:MET:CE	4:G:606:HOH:O	2.28	0.81
1:H:240:LYS:HB2	1:H:240:LYS:HZ2	1.45	0.81
1:A:398:PRO:HB2	1:A:423:ARG:HH21	1.46	0.79
1:A:70:MET:HE1	1:A:269:PHE:CD2	2.16	0.79
1:D:173:LYS:NZ	1:D:243:LYS:NZ	2.28	0.78
1:B:100:LYS:NZ	1:B:178:MET:HE3	2.00	0.77
1:B:261:THR:HG22	1:B:278:HIS:HE2	1.49	0.77
1:C:185:ILE:HD12	1:C:185:ILE:H	1.51	0.75
1:H:160:ALA:HB2	1:H:178:MET:HE1	1.67	0.75
1:F:33:ASP:OD1	3:F:503:XLS:H2	1.88	0.72
1:B:211:GLY:H	1:B:226:PRO:HD2	1.53	0.72
1:F:392:MET:CE	1:F:429:GLN:CB	2.62	0.72
1:G:258:LYS:HD3	1:G:280:GLY:O	1.90	0.72
1:C:210:GLU:CD	3:C:503:XLS:H1	2.15	0.72
1:G:22:GLN:CB	1:G:313:GLY:HA3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:CG2	1:B:162:MET:HE2	2.21	0.71
1:A:70:MET:HE1	1:A:269:PHE:HD2	1.55	0.70
1:F:89:LYS:HE2	1:F:116:ASN:OD1	1.91	0.70
1:F:392:MET:HE2	1:F:429:GLN:CG	2.22	0.70
1:A:326:LEU:HD12	1:B:179:ILE:HD13	1.74	0.69
1:F:171:TYR:HD2	1:F:186:ILE:HD12	1.56	0.69
1:A:290:ARG:HH12	3:A:502:XLS:H52	1.56	0.69
1:E:152:VAL:CG2	1:E:162:MET:HE2	2.23	0.69
1:F:171:TYR:CD2	1:F:186:ILE:HD12	2.28	0.69
1:D:159:GLN:HE22	1:D:173:LYS:CG	2.06	0.68
1:C:395:GLN:O	1:C:395:GLN:HG2	1.92	0.68
1:B:100:LYS:HZ2	1:B:178:MET:HE3	1.59	0.68
1:D:159:GLN:NE2	1:D:173:LYS:CG	2.57	0.67
1:H:148:ILE:HD12	3:H:503:XLS:H1	1.77	0.67
1:F:330:GLU:OE2	4:F:601:HOH:O	2.13	0.67
1:E:290:ARG:HH12	3:E:503:XLS:C5	2.04	0.67
1:G:22:GLN:N	1:G:294:VAL:H	1.93	0.66
1:C:78:THR:HB	1:C:342:GLN:HE22	1.61	0.66
1:A:231:PRO:O	1:A:232:GLU:CB	2.42	0.66
1:A:302:ASP:O	1:A:304:THR:N	2.28	0.66
1:A:149:ASP:OD1	3:A:502:XLS:C1	2.44	0.66
1:B:261:THR:HG22	1:B:278:HIS:NE2	2.12	0.65
1:A:179:ILE:HD13	1:B:326:LEU:HD12	1.79	0.65
3:G:503:XLS:O1	3:G:503:XLS:H4	1.98	0.65
1:C:33:ASP:CG	3:C:503:XLS:H51	2.21	0.64
1:D:263:HIS:ND1	3:D:503:XLS:H4	2.12	0.64
1:C:198:ARG:HH22	1:C:209:GLU:HG2	1.63	0.64
4:E:626:HOH:O	1:F:128:PRO:HD2	1.97	0.64
1:H:52:ASP:O	1:H:53:GLN:HG2	1.98	0.63
1:A:157:ASP:HB2	1:A:159:GLN:H	1.64	0.63
1:C:175:ASN:OD1	1:C:182:SER:HB3	1.98	0.63
1:D:159:GLN:NE2	1:D:173:LYS:HG2	2.12	0.63
1:G:63:LYS:HE2	1:G:78:THR:HG22	1.81	0.62
1:G:326:LEU:HD12	1:H:179:ILE:HD13	1.82	0.62
1:G:63:LYS:NZ	1:G:78:THR:HG22	2.16	0.61
1:H:100:LYS:HE2	1:H:178:MET:CE	2.30	0.60
1:G:190:MET:HE2	1:G:205:PRO:HD2	1.84	0.60
1:C:89:LYS:HB2	1:C:113:LYS:HG2	1.83	0.59
1:F:36:PRO:HD2	1:F:213:TRP:CH2	2.38	0.59
1:A:210:GLU:O	1:A:226:PRO:HD2	2.03	0.59
1:A:231:PRO:HB3	1:A:255:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:PRO:HD2	1:G:213:TRP:CH2	2.39	0.58
3:H:503:XLS:H4	3:H:503:XLS:O1	1.98	0.58
1:G:339:LYS:HG2	1:G:353:LEU:HD21	1.85	0.58
1:B:160:ALA:HB2	1:B:178:MET:HE1	1.85	0.58
1:C:355:ASN:ND2	1:C:437:GLY:O	2.37	0.58
1:D:159:GLN:HE22	1:D:173:LYS:HG3	1.69	0.58
1:B:36:PRO:HD2	1:B:213:TRP:CH2	2.38	0.58
1:C:36:PRO:HD2	1:C:213:TRP:CH2	2.38	0.58
1:E:36:PRO:HD2	1:E:213:TRP:CH2	2.39	0.58
1:G:22:GLN:N	1:G:293:CYS:HA	2.18	0.58
1:H:36:PRO:HD2	1:H:213:TRP:CH2	2.39	0.57
1:F:251:ILE:HB	1:F:307:GLN:HE21	1.69	0.57
1:H:100:LYS:CE	1:H:178:MET:HE3	2.28	0.57
1:H:169:LEU:HB3	1:H:190:MET:HE1	1.86	0.57
1:F:138:LYS:HB2	1:F:139:PRO:HD2	1.86	0.57
1:D:36:PRO:HD2	1:D:213:TRP:CH2	2.39	0.57
1:G:100:LYS:HE3	1:H:325:GLN:NE2	2.20	0.57
1:A:36:PRO:HD2	1:A:213:TRP:CH2	2.40	0.57
1:B:138:LYS:HB2	1:B:139:PRO:HD2	1.87	0.57
1:C:185:ILE:H	1:C:185:ILE:CD1	2.17	0.57
1:F:388:MET:CE	1:F:444:MET:HE1	2.26	0.57
1:H:294:VAL:HG13	1:H:314:ILE:CD1	2.34	0.57
1:E:290:ARG:NH1	3:E:503:XLS:H51	2.08	0.57
1:E:210:GLU:O	1:E:226:PRO:HD2	2.05	0.56
1:B:71:VAL:CG1	1:B:362:LYS:HB2	2.36	0.56
1:C:200:GLY:O	1:C:201:ASN:C	2.48	0.56
1:D:138:LYS:HB2	1:D:139:PRO:HD2	1.88	0.56
1:E:89:LYS:HB2	1:E:113:LYS:HG2	1.87	0.56
1:A:377:ARG:HB2	1:A:416:ILE:HD13	1.86	0.56
1:A:70:MET:HE1	1:A:269:PHE:CE2	2.41	0.56
1:D:315:THR:CG2	1:D:315:THR:O	2.54	0.56
1:F:314:ILE:HD13	4:F:620:HOH:O	2.05	0.56
1:G:22:GLN:HA	1:G:293:CYS:HB3	1.86	0.56
1:G:171:TYR:CD1	1:G:171:TYR:C	2.83	0.56
1:H:210:GLU:O	1:H:226:PRO:HD2	2.05	0.56
1:H:89:LYS:HB2	1:H:113:LYS:HG2	1.88	0.55
1:F:185:ILE:H	1:F:185:ILE:HD12	1.71	0.55
1:B:375:SER:OG	1:B:418:ASN:ND2	2.40	0.55
1:A:290:ARG:NH1	3:A:502:XLS:H52	2.22	0.55
1:B:375:SER:HB2	1:B:450:LYS:HE2	1.88	0.55
1:C:192:GLU:OE2	1:C:197:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ASP:OD1	1:C:345:LYS:HE3	2.07	0.55
1:D:362:LYS:HA	1:D:430:ASP:OD1	2.06	0.55
1:G:63:LYS:CE	1:G:78:THR:HG22	2.36	0.55
1:D:315:THR:O	1:D:315:THR:HG22	2.05	0.55
1:G:78:THR:HG23	1:G:342:GLN:OE1	2.07	0.55
1:F:210:GLU:O	1:F:226:PRO:HD2	2.07	0.55
1:F:261:THR:HG23	4:F:603:HOH:O	2.08	0.54
1:C:149:ASP:OD2	3:C:503:XLS:C1	2.55	0.54
1:C:210:GLU:O	1:C:226:PRO:HD2	2.08	0.54
1:C:375:SER:OG	1:C:418:ASN:ND2	2.40	0.54
1:E:94:ALA:HB2	3:E:503:XLS:H1	1.90	0.54
1:F:392:MET:HE1	1:F:431:VAL:HG22	1.89	0.54
1:G:210:GLU:O	1:G:226:PRO:HD2	2.07	0.54
1:C:325:GLN:HB2	4:C:611:HOH:O	2.08	0.53
1:D:210:GLU:O	1:D:226:PRO:HD2	2.09	0.53
1:F:157:ASP:OD2	1:F:159[A]:GLN:HG3	2.08	0.53
1:A:230:LEU:HA	1:A:231:PRO:C	2.32	0.53
1:E:141:VAL:HG11	1:E:164:TRP:CZ2	2.44	0.53
1:F:339:LYS:HD2	1:F:353:LEU:CD1	2.30	0.53
1:B:37:MET:CE	1:B:97:CYS:SG	2.97	0.53
1:C:395:GLN:O	1:C:396:GLU:CB	2.57	0.53
1:B:166:ASN:HD21	1:B:204:ARG:HH22	1.56	0.53
1:E:138:LYS:HB2	1:E:139:PRO:HD2	1.91	0.52
1:C:210:GLU:OE1	3:C:503:XLS:H1	2.09	0.52
1:G:22:GLN:CB	1:G:313:GLY:CA	2.87	0.52
1:H:230:LEU:HA	1:H:231:PRO:C	2.34	0.52
1:C:395:GLN:O	1:C:395:GLN:CG	2.58	0.52
1:D:230:LEU:HA	1:D:231:PRO:C	2.35	0.52
1:G:230:LEU:HA	1:G:231:PRO:C	2.35	0.52
1:A:138:LYS:HB2	1:A:139:PRO:HD2	1.91	0.51
1:B:230:LEU:HA	1:B:231:PRO:C	2.36	0.51
1:F:301:LYS:HD2	1:G:428:ILE:HG13	1.93	0.51
1:A:149:ASP:OD1	3:A:502:XLS:H1	2.11	0.51
1:H:188:VAL:O	1:H:190:MET:HE3	2.11	0.51
1:C:138:LYS:HB2	1:C:139:PRO:HD2	1.92	0.51
1:A:375:SER:OG	1:A:418:ASN:ND2	2.44	0.50
1:C:406:PRO:HG2	1:C:415:GLU:HG3	1.93	0.50
1:H:188:VAL:O	1:H:190:MET:CE	2.58	0.50
1:G:138:LYS:HB2	1:G:139:PRO:HD2	1.92	0.50
1:B:153:PHE:HB3	1:B:214:LEU:HD23	1.92	0.50
1:B:351:ARG:HG2	1:B:445:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:HH12	3:B:503:XLS:H51	1.76	0.50
1:F:89:LYS:HB2	1:F:113:LYS:HG2	1.94	0.50
1:H:169:LEU:HB3	1:H:190:MET:CE	2.41	0.50
1:E:168:LYS:HE3	1:E:187:GLU:OE1	2.12	0.49
1:F:392:MET:HE3	1:F:429:GLN:HB3	1.84	0.49
1:B:100:LYS:HZ3	1:B:178:MET:HE3	1.75	0.49
1:G:25:ILE:HG21	1:G:294:VAL:HG12	1.95	0.49
1:B:59:MET:CE	3:B:503:XLS:O5	2.55	0.49
1:E:437:GLY:HA3	4:E:625:HOH:O	2.12	0.49
1:B:229:PRO:HB3	4:B:621:HOH:O	2.13	0.49
1:F:153:PHE:CE1	1:F:155:ASP:HA	2.48	0.49
1:F:378:VAL:HG11	1:F:388:MET:HE1	1.94	0.49
1:B:290:ARG:HH12	3:B:503:XLS:C5	2.25	0.48
1:E:328:GLN:HB3	1:E:330:GLU:CD	2.38	0.48
1:D:119:ALA:HB1	1:D:139:PRO:HB3	1.95	0.48
1:C:203:GLU:O	1:C:203:GLU:HG2	2.14	0.48
1:D:159:GLN:NE2	1:D:173:LYS:HG3	2.26	0.48
1:G:29:MET:HB2	1:G:29:MET:HE2	1.42	0.48
1:D:153:PHE:HB3	1:D:214:LEU:HD23	1.95	0.48
1:H:119:ALA:HB1	1:H:139:PRO:HB3	1.95	0.48
1:C:328:GLN:HB3	1:C:330:GLU:CD	2.39	0.48
1:F:119:ALA:HB1	1:F:139:PRO:HB3	1.95	0.48
1:A:119:ALA:HB1	1:A:139:PRO:HB3	1.95	0.47
1:E:119:ALA:HB1	1:E:139:PRO:HB3	1.96	0.47
1:F:230:LEU:HA	1:F:231:PRO:C	2.39	0.47
1:G:22:GLN:N	1:G:293:CYS:CA	2.77	0.47
1:G:328:GLN:HB3	1:G:330:GLU:CD	2.40	0.47
1:C:395:GLN:O	1:C:396:GLU:HB2	2.15	0.47
1:G:33:ASP:H	1:G:278:HIS:CD2	2.32	0.47
1:G:119:ALA:HB1	1:G:139:PRO:HB3	1.96	0.47
1:D:328:GLN:HB3	1:D:330:GLU:CD	2.40	0.46
1:E:33:ASP:OD2	3:E:503:XLS:O5	2.33	0.46
1:F:25:ILE:HG21	1:F:294:VAL:HG12	1.97	0.46
1:B:328:GLN:HB3	1:B:330:GLU:CD	2.40	0.46
1:E:149:ASP:OD1	3:E:503:XLS:O2	2.27	0.46
1:F:328:GLN:HB3	1:F:330:GLU:CD	2.40	0.46
1:G:361:VAL:HG23	1:G:364:VAL:HG21	1.96	0.46
1:H:149:ASP:OD2	3:H:503:XLS:O2	2.26	0.46
1:E:22:GLN:HA	1:E:312:GLU:O	2.16	0.46
3:B:503:XLS:O1	3:B:503:XLS:O3	2.34	0.46
1:D:297:LEU:HD13	1:D:308:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:ASN:OD1	1:F:182:SER:HB3	2.16	0.46
1:H:153:PHE:HB3	1:H:214:LEU:HD23	1.97	0.46
1:H:328:GLN:HB3	1:H:330:GLU:CD	2.41	0.46
1:C:119:ALA:HB1	1:C:139:PRO:HB3	1.97	0.46
1:C:153:PHE:HB3	1:C:214:LEU:HD23	1.98	0.46
1:E:230:LEU:HA	1:E:231:PRO:C	2.40	0.46
1:B:89:LYS:HB2	1:B:113:LYS:HG2	1.98	0.45
1:B:152:VAL:CG2	1:B:162:MET:CE	2.91	0.45
1:C:152:VAL:CG2	1:C:162:MET:HE3	2.46	0.45
1:B:160:ALA:CB	1:B:178:MET:HE1	2.45	0.45
1:D:353:LEU:O	1:D:441:SER:HA	2.16	0.45
1:A:328:GLN:HB3	1:A:330:GLU:CD	2.41	0.45
1:B:119:ALA:HB1	1:B:139:PRO:HB3	1.97	0.45
3:D:503:XLS:O1	3:D:503:XLS:O3	2.27	0.45
1:H:138:LYS:HB3	1:H:139:PRO:HD2	1.98	0.45
1:D:155:ASP:HB3	1:D:157:ASP:OD1	2.16	0.45
1:D:210:GLU:OE2	3:D:503:XLS:H51	2.17	0.45
1:F:448:TYR:CD1	1:F:448:TYR:C	2.95	0.45
1:F:194:SER:HB2	1:F:195:PHE:CD2	2.52	0.45
1:D:25:ILE:HG21	1:D:294:VAL:HG12	1.98	0.45
1:E:236:TYR:HE1	4:E:620:HOH:O	2.00	0.45
1:H:25:ILE:HG21	1:H:294:VAL:HG12	1.99	0.44
1:A:256:GLU:CD	1:A:310:MET:HE2	2.42	0.44
1:E:162:MET:HE3	1:E:174:LEU:HD11	1.98	0.44
1:A:22:GLN:HG3	1:A:22:GLN:O	2.16	0.44
1:F:406:PRO:HG3	1:F:417:ILE:HD11	1.99	0.44
1:B:37:MET:HG2	1:B:38:VAL:N	2.33	0.44
1:G:339:LYS:HG2	1:G:353:LEU:CD2	2.46	0.44
1:A:25:ILE:HG21	1:A:294:VAL:HG12	1.99	0.44
1:A:302:ASP:C	1:A:304:THR:H	2.23	0.44
1:H:406:PRO:HG3	1:H:417:ILE:HD11	1.99	0.44
1:B:162:MET:HE3	1:B:174:LEU:HD11	1.99	0.44
1:B:198:ARG:HG3	1:B:229:PRO:HD3	1.99	0.44
1:D:194:SER:HB2	1:D:195:PHE:CD2	2.53	0.44
1:F:40:ASN:HD22	1:F:40:ASN:HA	1.56	0.44
1:E:230:LEU:HD22	1:E:232:GLU:HG3	1.99	0.44
1:C:448:TYR:CD1	1:C:448:TYR:C	2.96	0.44
1:E:453:LYS:NZ	1:F:176:GLU:OE1	2.50	0.43
1:F:192:GLU:OE1	1:F:197:LYS:HG3	2.18	0.43
1:B:448:TYR:CD1	1:B:448:TYR:C	2.96	0.43
1:C:395:GLN:O	1:C:396:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:MET:HG2	1:E:38:VAL:N	2.33	0.43
1:B:261:THR:HG22	1:B:278:HIS:CE1	2.53	0.43
1:C:25:ILE:HG21	1:C:294:VAL:HG12	1.99	0.43
1:G:153:PHE:HB3	1:G:214:LEU:HD23	1.99	0.43
1:D:380:THR:HG22	1:D:406:PRO:O	2.18	0.43
1:G:448:TYR:CD1	1:G:448:TYR:C	2.96	0.43
1:H:240:LYS:HB2	1:H:240:LYS:HZ3	1.79	0.43
1:E:78:THR:HB	1:E:342:GLN:HE22	1.83	0.43
1:G:29:MET:HE3	1:G:29:MET:HB3	1.60	0.43
1:C:149:ASP:OD2	3:C:503:XLS:O1	2.37	0.43
1:C:149:ASP:HB3	1:C:211:GLY:HA2	2.00	0.43
1:E:179:ILE:HD13	1:F:326:LEU:HD12	1.99	0.43
1:B:194:SER:HB2	1:B:195:PHE:CD2	2.54	0.43
1:E:155:ASP:HB3	1:E:157:ASP:OD1	2.19	0.43
1:F:210:GLU:OE2	1:F:232:GLU:OE2	2.36	0.43
1:C:230:LEU:HA	1:C:231:PRO:C	2.44	0.43
1:G:56:TRP:CG	1:G:57:PHE:N	2.87	0.43
1:E:380:THR:HG22	1:E:406:PRO:O	2.19	0.43
1:C:194:SER:HB2	1:C:195:PHE:CD2	2.53	0.43
1:F:149:ASP:HB3	1:F:211:GLY:HA2	2.00	0.43
1:H:230:LEU:CD2	1:H:232:GLU:HG3	2.49	0.42
1:C:22:GLN:HA	1:C:312:GLU:O	2.20	0.42
1:D:406:PRO:HG3	1:D:417:ILE:HD11	2.01	0.42
1:E:56:TRP:CG	1:E:57:PHE:N	2.87	0.42
1:F:69:ASP:O	1:F:70:MET:HB2	2.19	0.42
1:G:179:ILE:HD13	1:H:326:LEU:HD12	2.01	0.42
1:A:93:TRP:HB3	3:A:502:XLS:C1	2.48	0.42
1:B:56:TRP:CG	1:B:57:PHE:N	2.88	0.42
1:C:115:ASN:O	1:C:117:LYS:HG2	2.18	0.42
1:E:152:VAL:CG2	1:E:162:MET:CE	2.94	0.42
1:C:185:ILE:HD12	1:C:185:ILE:N	2.28	0.42
1:H:240:LYS:NZ	1:H:240:LYS:CB	2.70	0.42
1:B:380:THR:HG22	1:B:406:PRO:O	2.20	0.42
1:D:69:ASP:O	1:D:70:MET:HB2	2.20	0.42
1:D:159:GLN:HE21	1:D:173:LYS:HG2	1.81	0.42
1:A:230:LEU:HA	1:A:231:PRO:O	2.20	0.42
1:D:448:TYR:CD1	1:D:448:TYR:C	2.97	0.42
1:H:380:THR:HG22	1:H:406:PRO:O	2.19	0.42
1:A:448:TYR:CD1	1:A:448:TYR:C	2.97	0.42
1:B:107:TYR:CD1	1:B:162:MET:HE1	2.55	0.42
1:C:395:GLN:HB2	1:C:434:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ASP:HB3	1:E:211:GLY:HA2	2.02	0.42
1:E:448:TYR:CD1	1:E:448:TYR:C	2.97	0.42
1:G:380:THR:HG22	1:G:406:PRO:O	2.19	0.42
1:B:240:LYS:HD3	1:B:240:LYS:HA	1.93	0.42
1:H:62:TRP:CZ2	1:H:92:ALA:HB1	2.55	0.42
1:H:448:TYR:CD1	1:H:448:TYR:C	2.97	0.42
1:A:194:SER:HB2	1:A:195:PHE:CD2	2.55	0.42
1:B:25:ILE:HG21	1:B:294:VAL:HG12	2.02	0.42
1:C:406:PRO:HG3	1:C:417:ILE:HD11	2.02	0.42
1:D:37:MET:HG2	1:D:38:VAL:N	2.35	0.42
1:G:194:SER:HB2	1:G:195:PHE:CD2	2.54	0.42
1:B:155:ASP:HB3	1:B:157:ASP:OD1	2.20	0.41
1:C:56:TRP:CG	1:C:57:PHE:N	2.88	0.41
1:G:190:MET:CE	1:G:205:PRO:HD2	2.47	0.41
1:C:380:THR:HG22	1:C:406:PRO:O	2.19	0.41
1:F:153:PHE:HB3	1:F:214:LEU:HD23	2.01	0.41
1:F:120:ILE:HG12	1:F:150:PRO:CG	2.41	0.41
1:B:152:VAL:HG23	1:B:162:MET:HE2	2.02	0.41
1:E:339:LYS:HG3	1:E:340:ALA:N	2.35	0.41
1:F:316:LYS:NZ	1:G:301:LYS:HE2	2.36	0.41
1:D:56:TRP:CG	1:D:57:PHE:N	2.88	0.41
1:B:207:LYS:O	1:B:227:GLY:HA2	2.21	0.41
1:C:207:LYS:O	1:C:227:GLY:HA2	2.21	0.41
1:D:149:ASP:HB3	1:D:211:GLY:HA2	2.03	0.41
1:D:210:GLU:OE2	1:D:232:GLU:OE2	2.37	0.41
1:E:69:ASP:O	1:E:70:MET:HB2	2.21	0.41
1:A:56:TRP:CG	1:A:57:PHE:N	2.89	0.41
1:D:438:LYS:HD2	1:F:394:SER:HB2	2.03	0.41
1:F:56:TRP:CG	1:F:57:PHE:N	2.89	0.41
1:A:153:PHE:HB3	1:A:214:LEU:HD23	2.03	0.40
1:C:69:ASP:O	1:C:70:MET:HB2	2.21	0.40
1:F:198:ARG:HG2	1:F:199:ASP:N	2.36	0.40
1:H:194:SER:HB2	1:H:195:PHE:CD2	2.56	0.40
1:H:198:ARG:HG3	1:H:229:PRO:HD3	2.03	0.40
1:G:155:ASP:HB3	1:G:157:ASP:OD1	2.21	0.40
1:H:149:ASP:HB3	1:H:211:GLY:HA2	2.02	0.40
1:G:224:PHE:CE2	1:G:266:VAL:HG21	2.57	0.40
1:B:166:ASN:O	1:B:167:PRO:C	2.62	0.40

There are no symmetry-related clashes.

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	430/432 (100%)	405 (94%)	22 (5%)	3 (1%)	18	47
1	B	430/432 (100%)	408 (95%)	20 (5%)	2 (0%)	24	55
1	C	430/432 (100%)	411 (96%)	17 (4%)	2 (0%)	24	55
1	D	430/432 (100%)	408 (95%)	22 (5%)	0	100	100
1	E	430/432 (100%)	410 (95%)	20 (5%)	0	100	100
1	F	431/432 (100%)	410 (95%)	21 (5%)	0	100	100
1	G	430/432 (100%)	408 (95%)	21 (5%)	1 (0%)	43	72
1	H	430/432 (100%)	409 (95%)	21 (5%)	0	100	100
All	All	3441/3456 (100%)	3269 (95%)	164 (5%)	8 (0%)	43	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	PRO
1	A	232	GLU
1	B	166	ASN
1	C	396	GLU
1	G	91	ASP
1	B	210	GLU
1	C	201	ASN
1	A	313	GLY

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	363/363 (100%)	357 (98%)	6 (2%)	53	83
1	B	363/363 (100%)	344 (95%)	19 (5%)	21	53
1	C	363/363 (100%)	353 (97%)	10 (3%)	38	73
1	D	363/363 (100%)	357 (98%)	6 (2%)	53	83
1	E	363/363 (100%)	350 (96%)	13 (4%)	31	66
1	F	364/363 (100%)	359 (99%)	5 (1%)	59	85
1	G	362/363 (100%)	352 (97%)	10 (3%)	38	73
1	H	363/363 (100%)	353 (97%)	10 (3%)	38	73
All	All	2904/2904 (100%)	2825 (97%)	79 (3%)	39	74

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	168	LYS
1	A	173	LYS
1	A	231	PRO
1	A	247	LYS
1	A	446	PHE
1	B	37	MET
1	B	63	LYS
1	B	71	VAL
1	B	120	ILE
1	B	168	LYS
1	B	173	LYS
1	B	203	GLU
1	B	218	LYS
1	B	230	LEU
1	B	261	THR
1	B	309	LYS
1	B	312	GLU
1	B	351	ARG
1	B	353	LEU
1	B	375	SER
1	B	422	ASP
1	B	423	ARG
1	B	436	LYS
1	B	450	LYS
1	C	100	LYS
1	C	159	GLN

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Mol	Chain	Res	Type
1	C	185	ILE
1	C	307	GLN
1	C	312	GLU
1	C	339	LYS
1	C	345	LYS
1	C	404	LYS
1	C	440	SER
1	C	452	SER
1	D	22	GLN
1	D	89	LYS
1	D	117	LYS
1	D	241	SER
1	D	251	ILE
1	D	316	LYS
1	E	22	GLN
1	E	141	VAL
1	E	143	SER
1	E	144	GLU
1	E	168	LYS
1	E	172	VAL
1	E	173	LYS
1	E	308	MET
1	E	315	THR
1	E	316	LYS
1	E	325	GLN
1	E	416	ILE
1	E	452	SER
1	F	53	GLN
1	F	173	LYS
1	F	315	THR
1	F	345	LYS
1	F	450	LYS
1	G	115	ASN
1	G	116	ASN
1	G	230	LEU
1	G	241	SER
1	G	308	MET
1	G	309	LYS
1	G	342	GLN
1	G	353	LEU
1	G	438	LYS
1	G	452	SER

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Mol	Chain	Res	Type
1	H	22	GLN
1	H	176	GLU
1	H	186	ILE
1	H	193	GLU
1	H	240	LYS
1	H	241	SER
1	H	372	SER
1	H	375	SER
1	H	404	LYS
1	H	452	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	58	ASN
1	A	116	ASN
1	A	325	GLN
1	A	418	ASN
1	B	53	GLN
1	B	159	GLN
1	B	166	ASN
1	B	325	GLN
1	B	418	ASN
1	C	22	GLN
1	C	40	ASN
1	C	159	GLN
1	C	354	GLN
1	C	418	ASN
1	D	58	ASN
1	D	159	GLN
1	E	58	ASN
1	E	101	ASN
1	E	354	GLN
1	F	40	ASN
1	F	307	GLN
1	F	325	GLN
1	G	23	ASN
1	G	58	ASN
1	G	325	GLN
1	H	101	ASN
1	H	307	GLN

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Mol	Chain	Res	Type
1	H	337	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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$
3	XLS	D	503	-	8,9,9	0.88	1 (12%)	10,11,11	2.61	5 (50%)
3	XLS	A	502	-	8,9,9	0.64	0	10,11,11	1.53	3 (30%)
3	XLS	G	503	-	8,9,9	0.76	0	10,11,11	2.22	3 (30%)
3	XLS	F	503	-	8,9,9	1.31	2 (25%)	10,11,11	2.94	5 (50%)
3	XLS	C	503	-	8,9,9	0.62	0	10,11,11	1.50	2 (20%)
3	XLS	B	503	-	8,9,9	1.28	1 (12%)	10,11,11	2.25	5 (50%)
3	XLS	E	503	-	8,9,9	1.64	1 (12%)	10,11,11	3.44	5 (50%)
3	XLS	H	503	-	8,9,9	0.66	0	10,11,11	2.04	4 (40%)

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
3	XLS	D	503	-	-	9/11/12/12	-
3	XLS	A	502	-	-	8/11/12/12	-
3	XLS	G	503	-	-	6/11/12/12	-
3	XLS	F	503	-	-	9/11/12/12	-
3	XLS	C	503	-	-	5/11/12/12	-
3	XLS	B	503	-	-	5/11/12/12	-
3	XLS	E	503	-	-	4/11/12/12	-
3	XLS	H	503	-	-	5/11/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	XLS	C3-C2	-4.21	1.47	1.53
3	B	503	XLS	C3-C2	-2.56	1.49	1.53
3	F	503	XLS	C4-C3	2.30	1.57	1.53
3	D	503	XLS	O2-C2	-2.17	1.39	1.43
3	F	503	XLS	C3-C2	2.03	1.56	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	XLS	O2-C2-C3	-9.14	88.06	109.46
3	F	503	XLS	O4-C4-C3	5.93	123.12	109.25
3	D	503	XLS	C3-C2-C1	-5.29	94.93	111.03
3	G	503	XLS	C3-C2-C1	-4.94	96.01	111.03
3	F	503	XLS	C4-C3-C2	4.25	122.84	112.70
3	B	503	XLS	O2-C2-C3	-3.67	100.88	109.46
3	D	503	XLS	O2-C2-C3	3.52	117.70	109.46
3	B	503	XLS	C3-C2-C1	-3.42	100.64	111.03
3	H	503	XLS	O2-C2-C3	3.35	117.31	109.46
3	F	503	XLS	C3-C2-C1	3.28	121.03	111.03
3	G	503	XLS	O3-C3-C4	3.25	116.31	108.93
3	E	503	XLS	O3-C3-C4	3.16	116.10	108.93
3	D	503	XLS	O5-C5-C4	3.12	117.72	111.16
3	B	503	XLS	C4-C3-C2	-2.97	105.61	112.70
3	F	503	XLS	O5-C5-C4	-2.95	104.95	111.16
3	H	503	XLS	O4-C4-C5	2.93	115.68	109.03
3	E	503	XLS	C3-C2-C1	-2.89	102.25	111.03
3	E	503	XLS	O2-C2-C1	2.76	116.75	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	XLS	C4-C3-C2	2.69	119.11	112.70
3	B	503	XLS	O4-C4-C3	2.67	115.50	109.25
3	A	502	XLS	C3-C2-C1	-2.58	103.17	111.03
3	G	503	XLS	O3-C3-C2	2.55	113.87	109.13
3	D	503	XLS	O4-C4-C5	2.50	114.71	109.03
3	H	503	XLS	C4-C3-C2	-2.46	106.83	112.70
3	C	503	XLS	O3-C3-C4	2.43	114.44	108.93
3	F	503	XLS	C5-C4-C3	-2.37	107.34	112.17
3	E	503	XLS	O3-C3-C2	-2.25	104.95	109.13
3	B	503	XLS	O4-C4-C5	2.17	113.96	109.03
3	C	503	XLS	C3-C2-C1	-2.16	104.46	111.03
3	H	503	XLS	O3-C3-C2	2.12	113.07	109.13
3	A	502	XLS	O3-C3-C4	2.02	113.51	108.93
3	A	502	XLS	C4-C3-C2	-2.01	107.92	112.70

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	XLS	C1-C2-C3-C4
3	A	502	XLS	C1-C2-C3-O3
3	A	502	XLS	O2-C2-C3-C4
3	A	502	XLS	O2-C2-C3-O3
3	A	502	XLS	O3-C3-C4-C5
3	A	502	XLS	O3-C3-C4-O4
3	B	503	XLS	C2-C3-C4-O4
3	B	503	XLS	O3-C3-C4-C5
3	B	503	XLS	O3-C3-C4-O4
3	C	503	XLS	C2-C3-C4-O4
3	C	503	XLS	O3-C3-C4-C5
3	C	503	XLS	O3-C3-C4-O4
3	D	503	XLS	O1-C1-C2-C3
3	D	503	XLS	C1-C2-C3-C4
3	D	503	XLS	C1-C2-C3-O3
3	D	503	XLS	O2-C2-C3-C4
3	D	503	XLS	O2-C2-C3-O3
3	D	503	XLS	C2-C3-C4-C5
3	D	503	XLS	C2-C3-C4-O4
3	D	503	XLS	O3-C3-C4-C5
3	D	503	XLS	O3-C3-C4-O4
3	E	503	XLS	C2-C3-C4-C5
3	E	503	XLS	C2-C3-C4-O4

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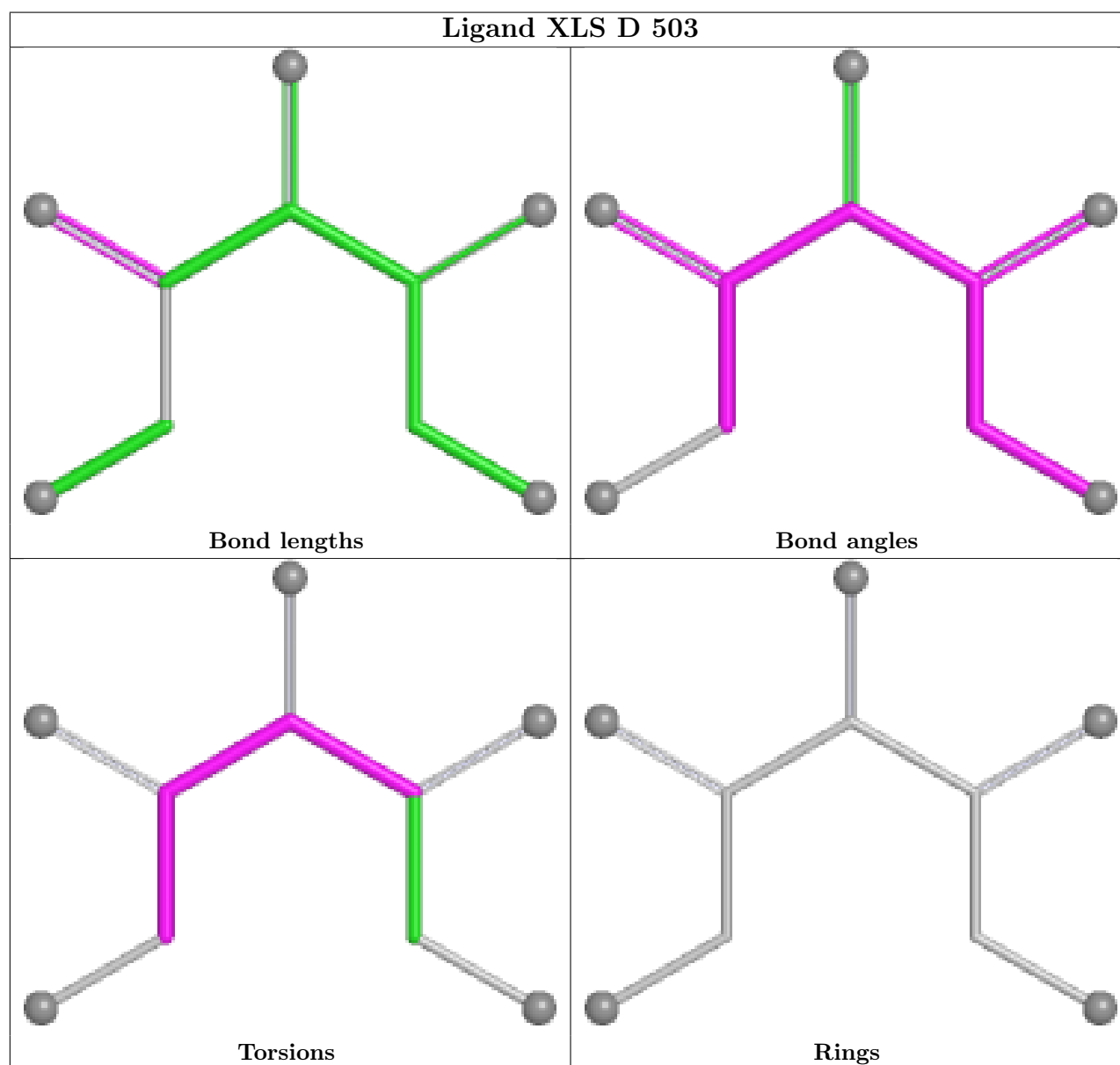
Mol	Chain	Res	Type	Atoms
3	E	503	XLS	O3-C3-C4-C5
3	E	503	XLS	O3-C3-C4-O4
3	F	503	XLS	C1-C2-C3-C4
3	F	503	XLS	C1-C2-C3-O3
3	F	503	XLS	O2-C2-C3-C4
3	F	503	XLS	O2-C2-C3-O3
3	F	503	XLS	C2-C3-C4-O4
3	F	503	XLS	O3-C3-C4-C5
3	F	503	XLS	O3-C3-C4-O4
3	G	503	XLS	C2-C3-C4-C5
3	G	503	XLS	C2-C3-C4-O4
3	G	503	XLS	O3-C3-C4-O4
3	G	503	XLS	C3-C4-C5-O5
3	G	503	XLS	O4-C4-C5-O5
3	H	503	XLS	O4-C4-C5-O5
3	A	502	XLS	C2-C3-C4-O4
3	G	503	XLS	O3-C3-C4-C5
3	A	502	XLS	C2-C3-C4-C5
3	B	503	XLS	C2-C3-C4-C5
3	C	503	XLS	C2-C3-C4-C5
3	F	503	XLS	C2-C3-C4-C5
3	H	503	XLS	C2-C3-C4-C5
3	H	503	XLS	O3-C3-C4-C5
3	F	503	XLS	O4-C4-C5-O5
3	H	503	XLS	C3-C4-C5-O5
3	B	503	XLS	C3-C4-C5-O5
3	C	503	XLS	O4-C4-C5-O5
3	H	503	XLS	C2-C3-C4-O4

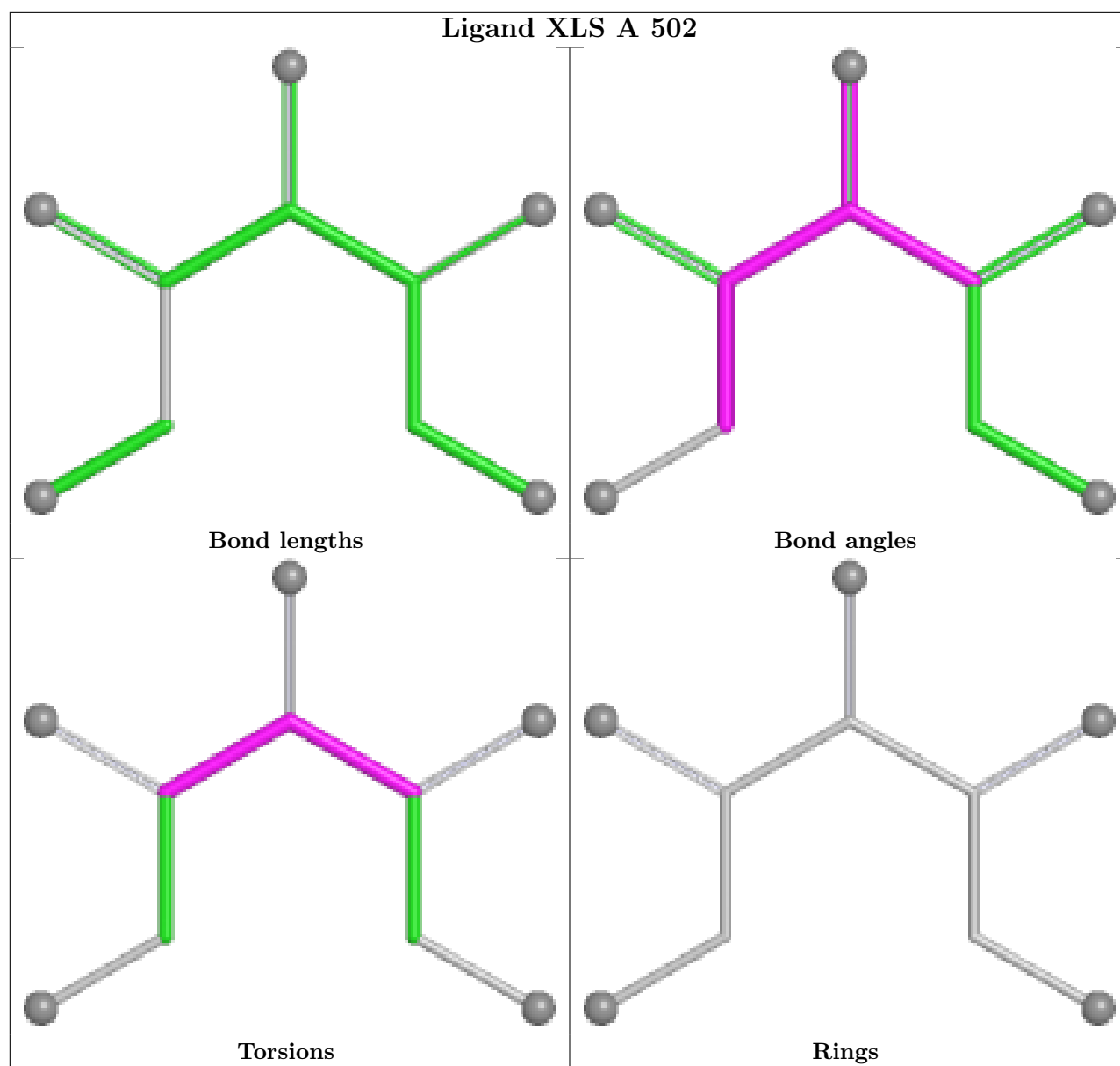
There are no ring outliers.

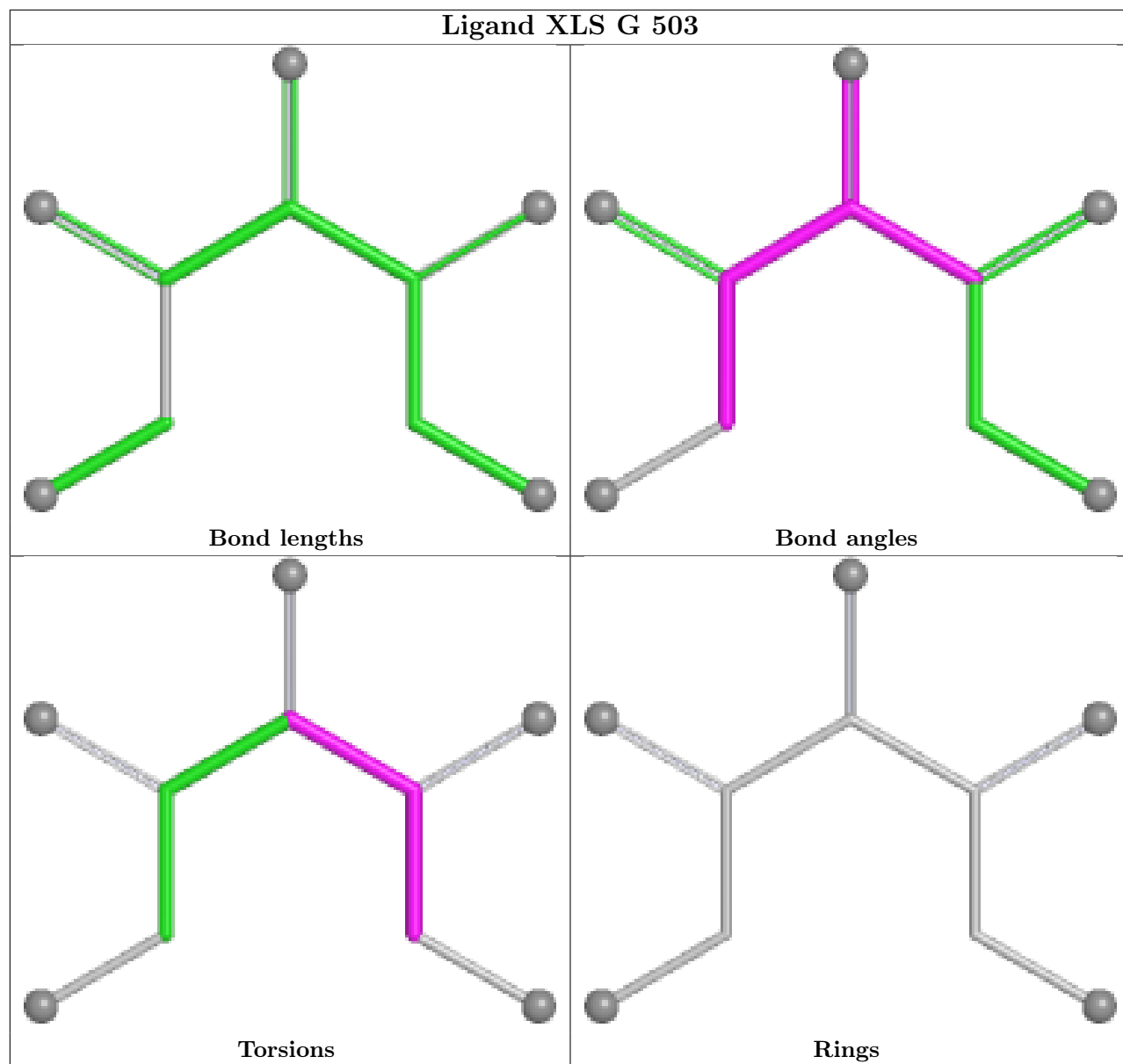
8 monomers are involved in 34 short contacts:

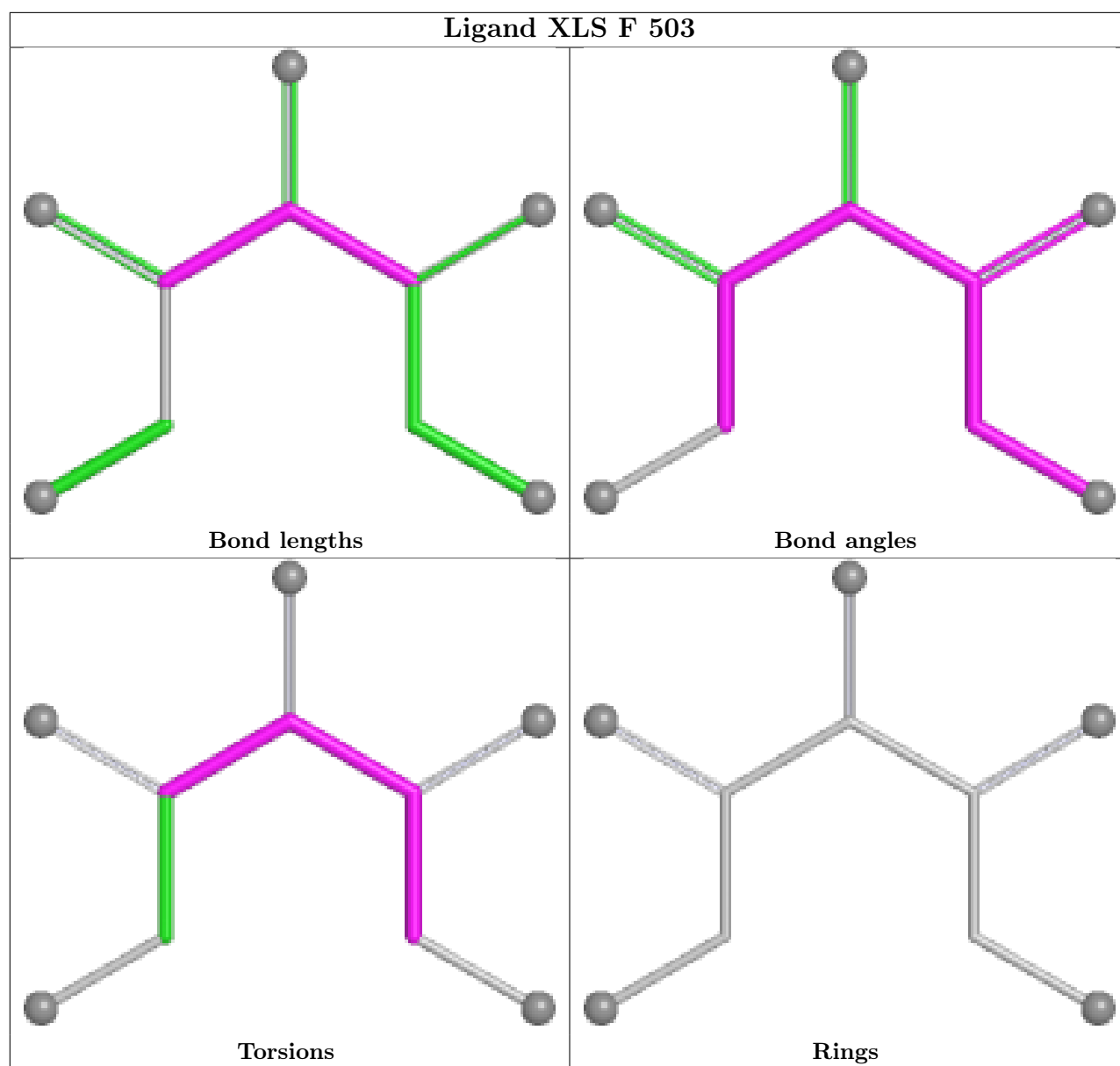
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	XLS	3	0
3	A	502	XLS	5	0
3	G	503	XLS	1	0
3	F	503	XLS	1	0
3	C	503	XLS	9	0
3	B	503	XLS	5	0
3	E	503	XLS	7	0
3	H	503	XLS	3	0

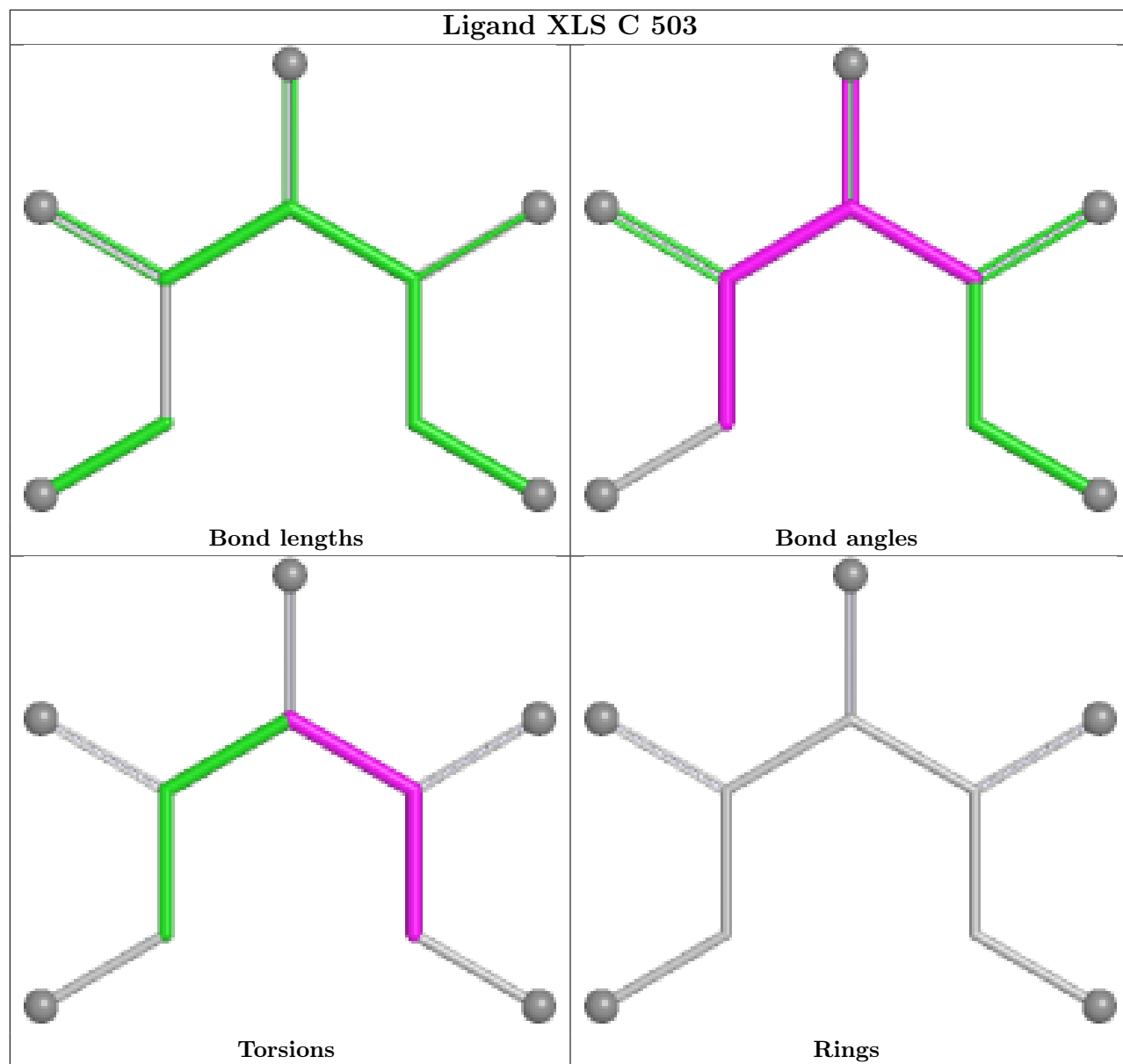
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

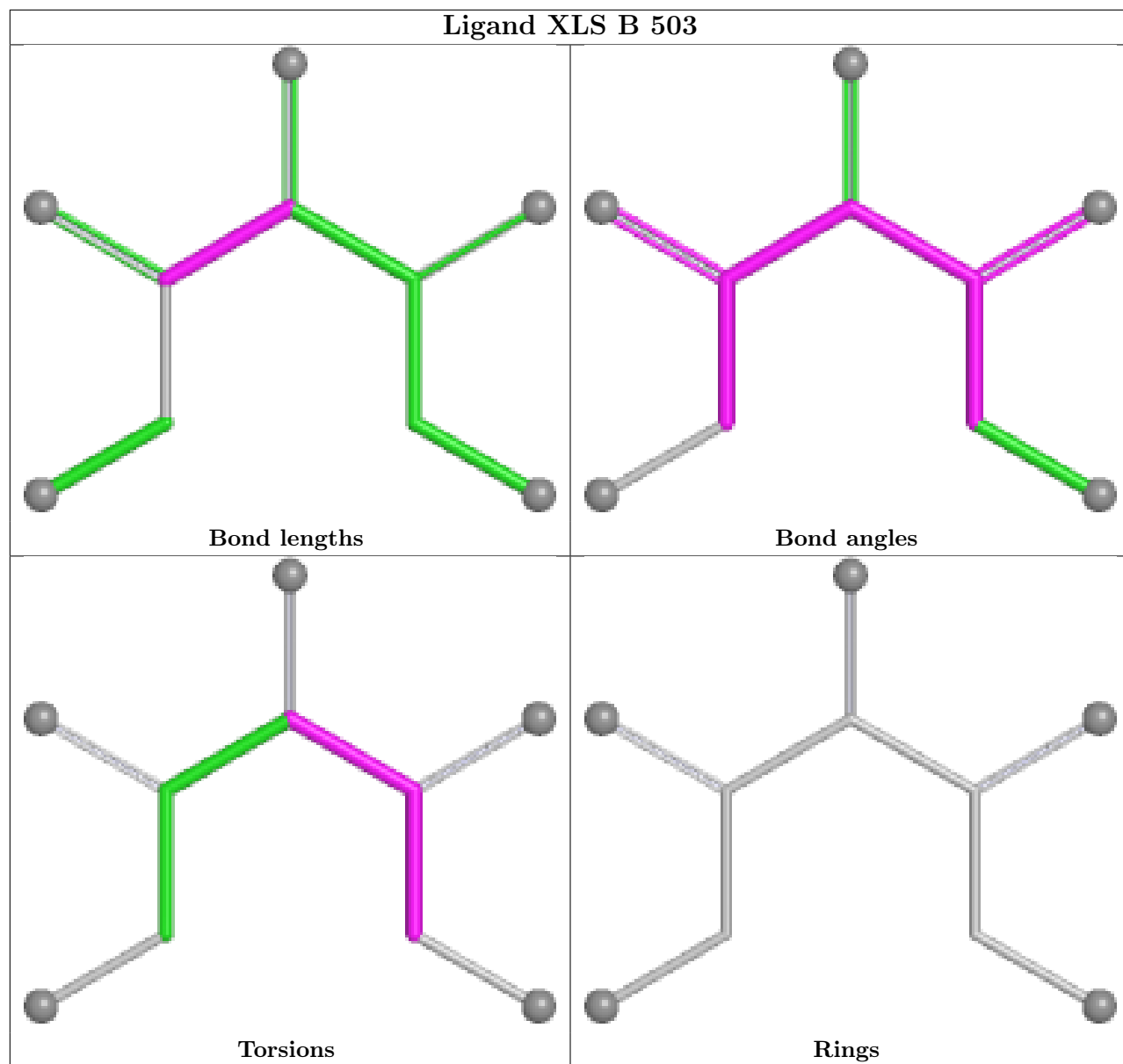


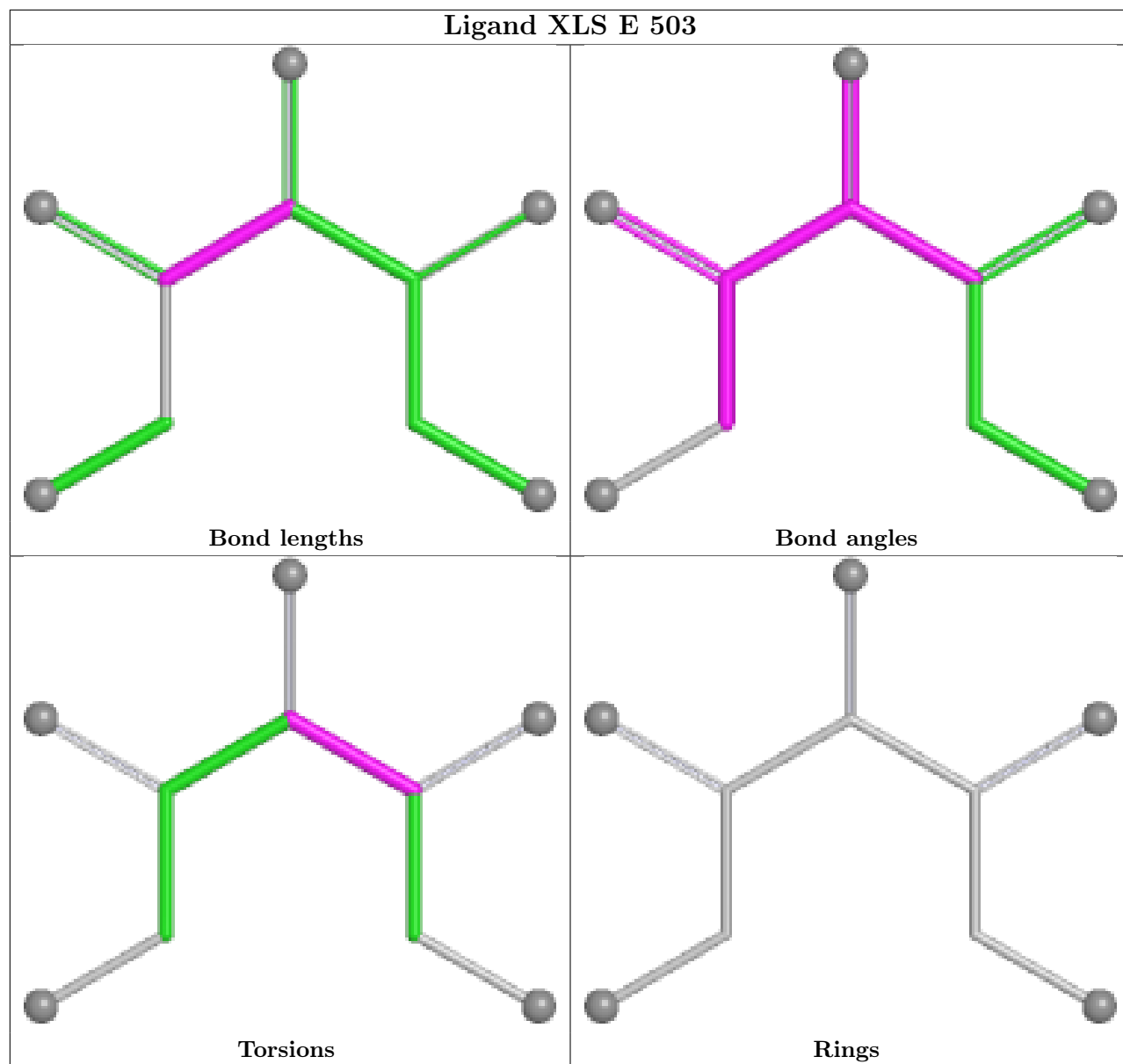


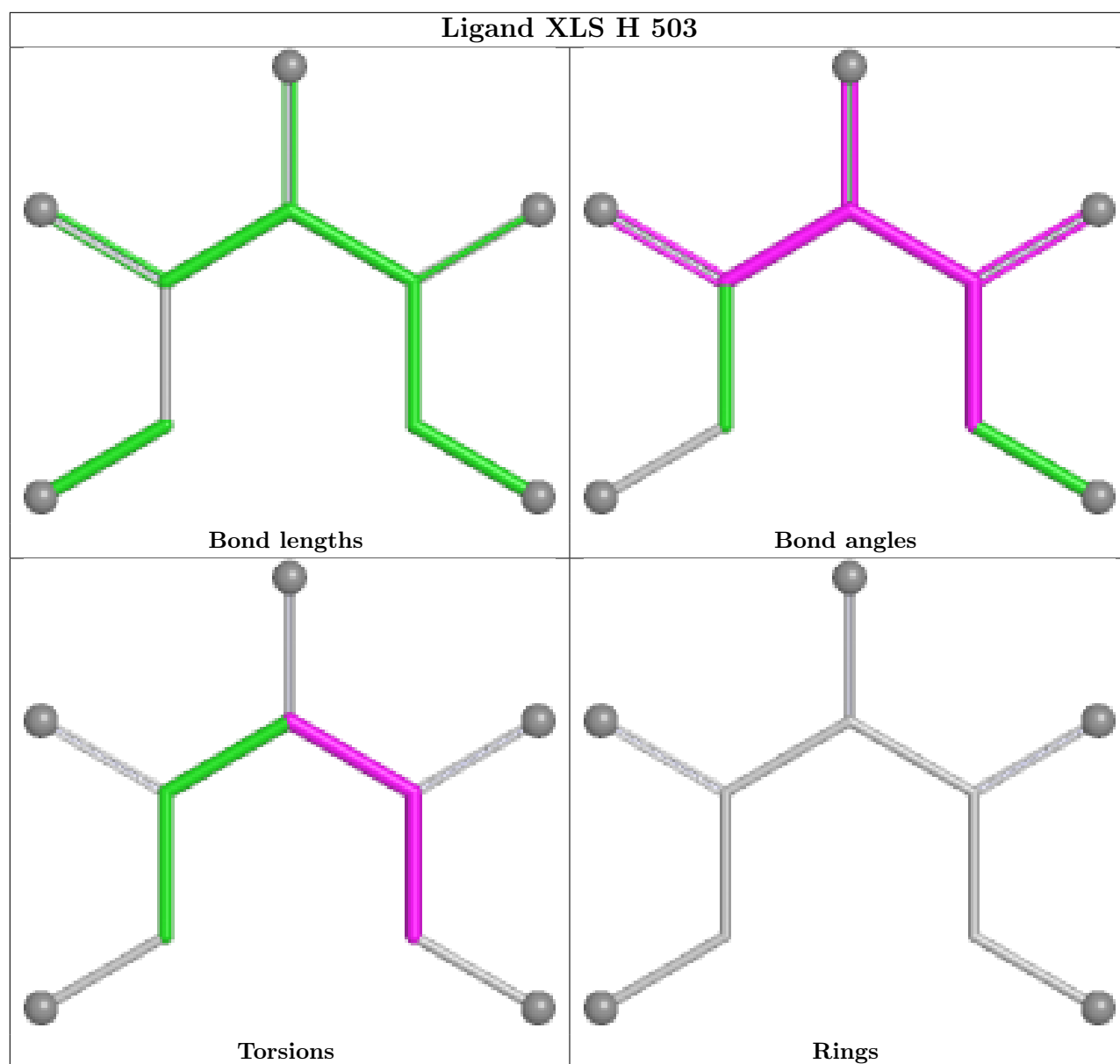












5.7 Other polymers [i](#)

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	432/432 (100%)	0.01	2 (0%) 87 82	13, 22, 41, 82	0
1	B	432/432 (100%)	0.01	4 (0%) 81 74	13, 23, 42, 84	0
1	C	432/432 (100%)	-0.00	5 (1%) 76 68	13, 22, 42, 74	0
1	D	432/432 (100%)	0.00	2 (0%) 87 82	13, 22, 39, 86	0
1	E	432/432 (100%)	-0.11	2 (0%) 87 82	12, 20, 35, 83	0
1	F	432/432 (100%)	0.02	6 (1%) 73 64	12, 22, 39, 62	1 (0%)
1	G	432/432 (100%)	-0.04	2 (0%) 87 82	12, 22, 38, 66	0
1	H	432/432 (100%)	-0.03	1 (0%) 91 88	12, 21, 35, 72	0
All	All	3456/3456 (100%)	-0.02	24 (0%) 84 77	12, 22, 38, 86	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ASN	4.4
1	E	145	TRP	3.6
1	F	370	GLY	3.6
1	F	145	TRP	3.3
1	B	423	ARG	3.1
1	B	145	TRP	3.1
1	D	199	ASP	3.0
1	C	145	TRP	2.8
1	G	190	MET	2.8
1	C	203	GLU	2.7
1	A	202	PRO	2.7
1	G	90	GLY	2.4
1	D	202	PRO	2.4
1	C	313	GLY	2.2
1	F	199	ASP	2.2
1	F	205	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	385	GLY	2.1
1	H	145	TRP	2.1
1	C	422	ASP	2.1
1	F	157	ASP	2.1
1	E	183	GLY	2.0
1	B	22	GLN	2.0
1	A	422	ASP	2.0
1	C	199	ASP	2.0

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 oligosaccharides 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, 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	XLS	F	503	10/10	0.82	0.13	28,35,46,48	0
3	XLS	H	503	10/10	0.82	0.22	26,37,43,44	0
3	XLS	C	503	10/10	0.87	0.14	28,37,48,52	0
3	XLS	E	503	10/10	0.88	0.17	25,35,46,49	0
3	XLS	B	503	10/10	0.88	0.12	20,22,22,23	10
3	XLS	D	503	10/10	0.88	0.14	21,39,52,56	0
3	XLS	A	502	10/10	0.90	0.14	24,33,34,37	0
3	XLS	G	503	10/10	0.92	0.11	26,36,54,57	0
2	CA	B	502	1/1	0.93	0.06	16,16,16,16	0
2	CA	H	502	1/1	0.94	0.04	22,22,22,22	0
2	CA	G	501	1/1	0.95	0.06	36,36,36,36	0
2	CA	H	501	1/1	0.96	0.03	28,28,28,28	0
2	CA	A	501	1/1	0.96	0.04	22,22,22,22	0
2	CA	F	501	1/1	0.96	0.04	22,22,22,22	0
2	CA	A	503	1/1	0.96	0.04	46,46,46,46	0

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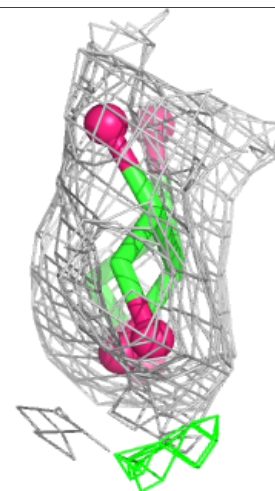
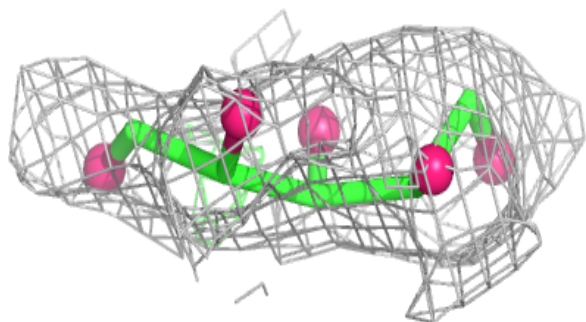
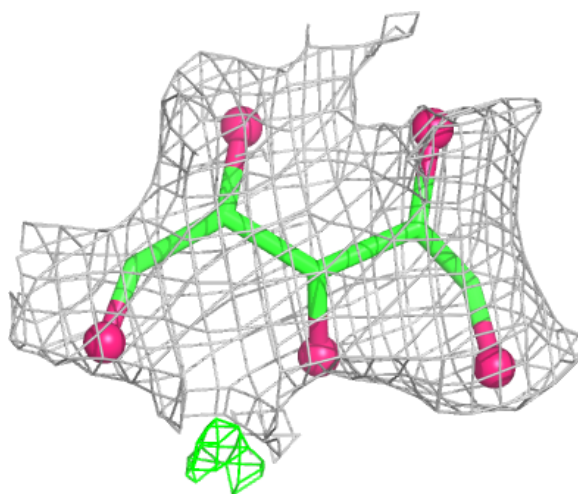
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	G	502	1/1	0.96	0.05	19,19,19,19	0
2	CA	E	501	1/1	0.97	0.04	33,33,33,33	0
2	CA	E	502	1/1	0.97	0.04	16,16,16,16	0
2	CA	B	501	1/1	0.97	0.03	32,32,32,32	0
2	CA	C	502	1/1	0.98	0.06	18,18,18,18	0
2	CA	D	501	1/1	0.98	0.04	36,36,36,36	0
2	CA	D	502	1/1	0.98	0.03	15,15,15,15	0
2	CA	C	501	1/1	0.99	0.02	30,30,30,30	0
2	CA	F	502	1/1	0.99	0.04	10,10,10,10	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.

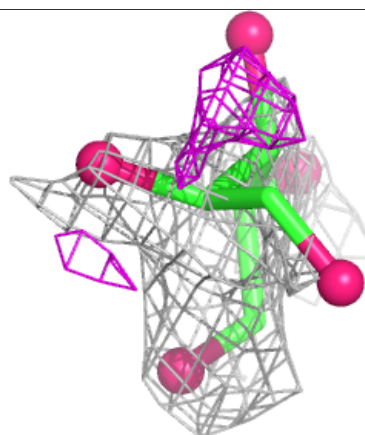
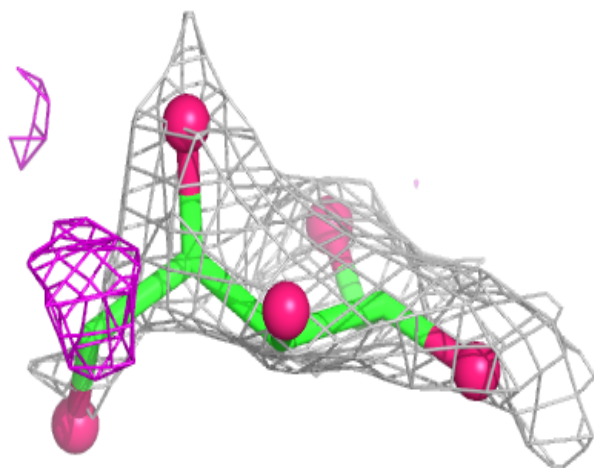
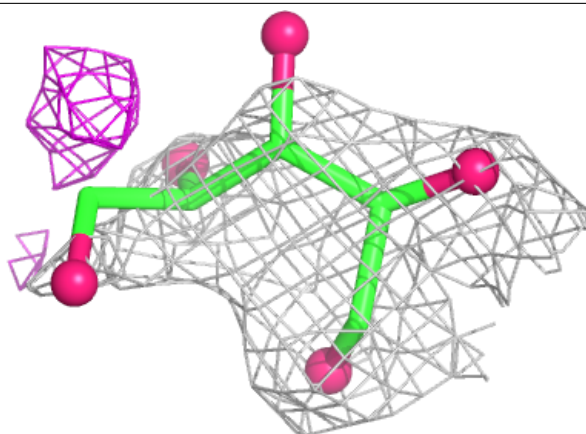
Electron density around XLS F 503:

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



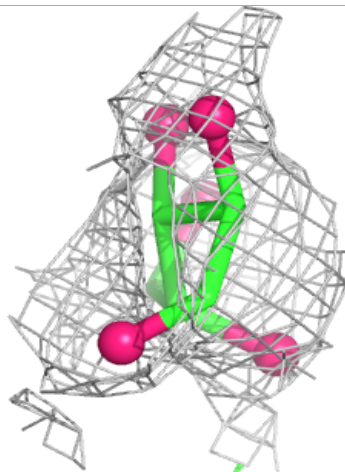
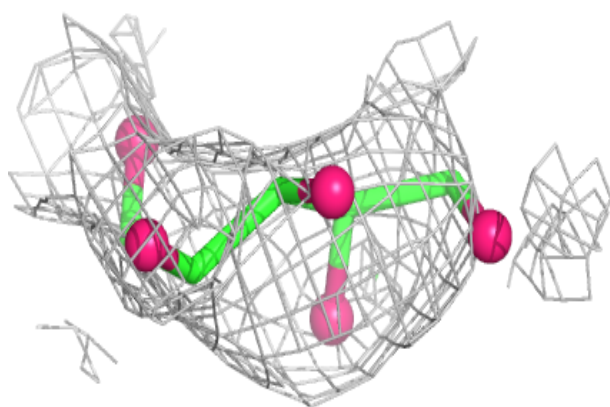
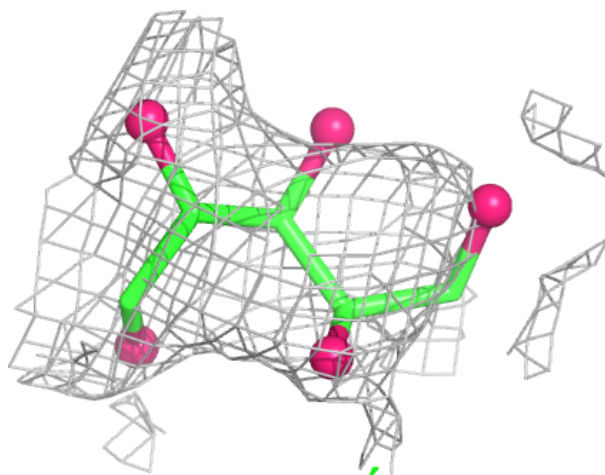
Electron density around XLS H 503:

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



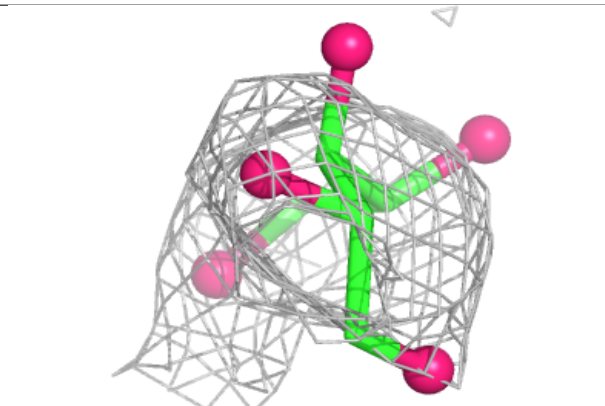
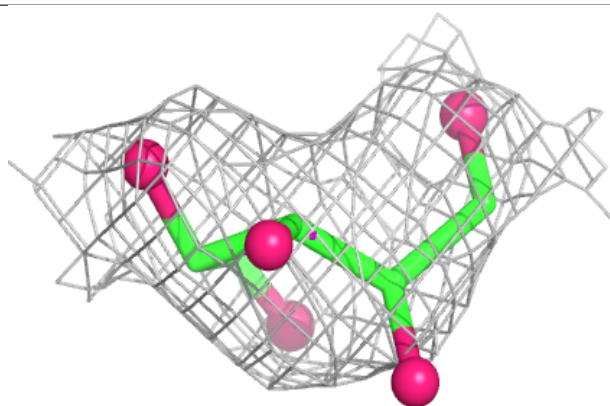
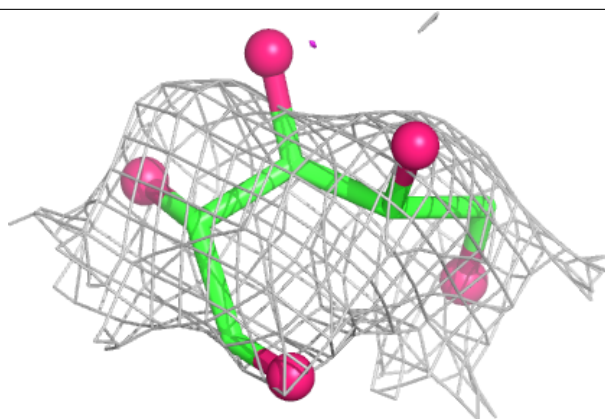
Electron density around XLS C 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

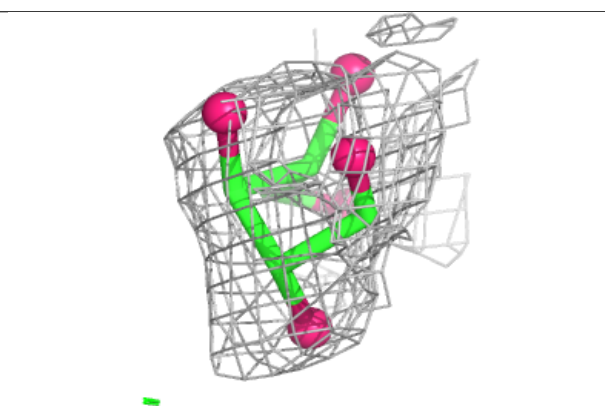
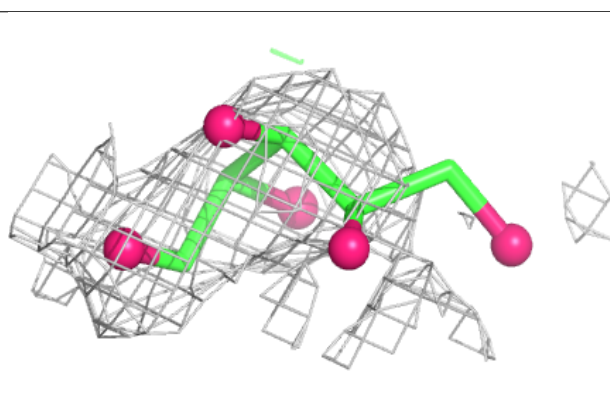
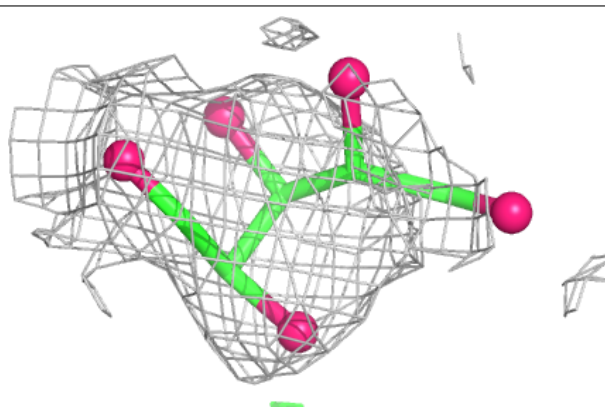


Electron density around XLS E 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

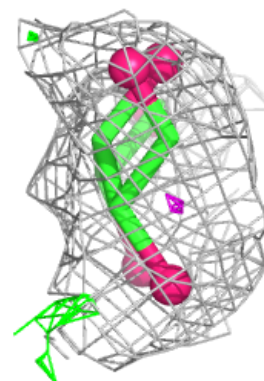
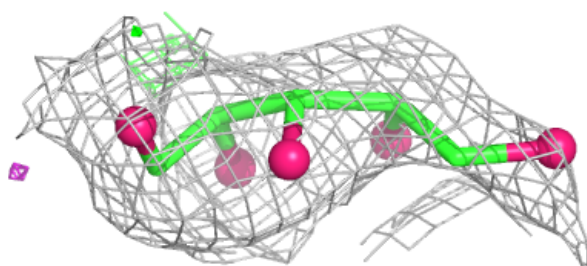
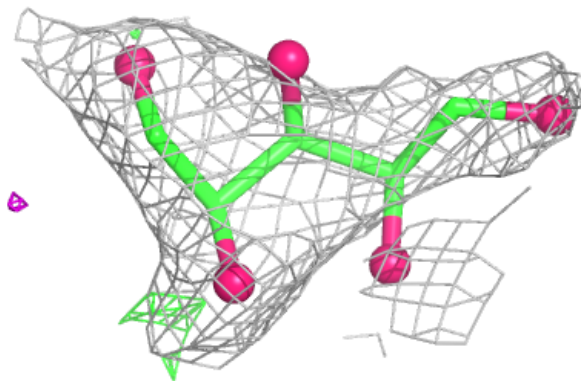
**Electron density around XLS B 503:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



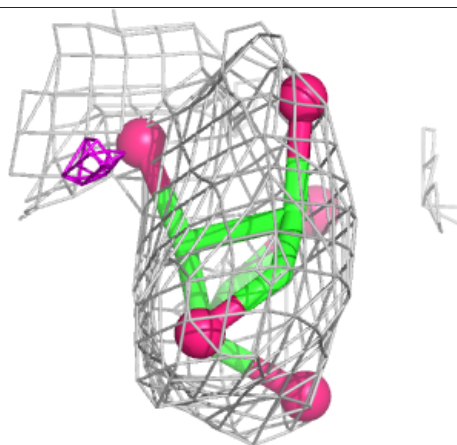
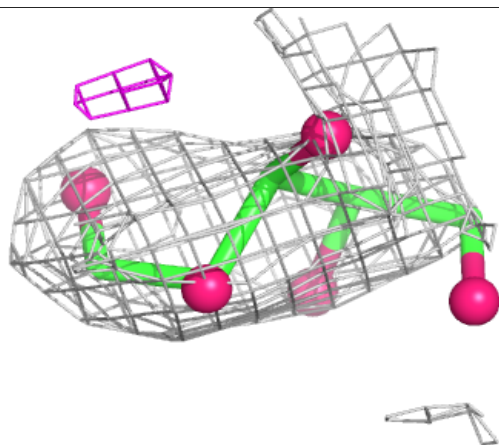
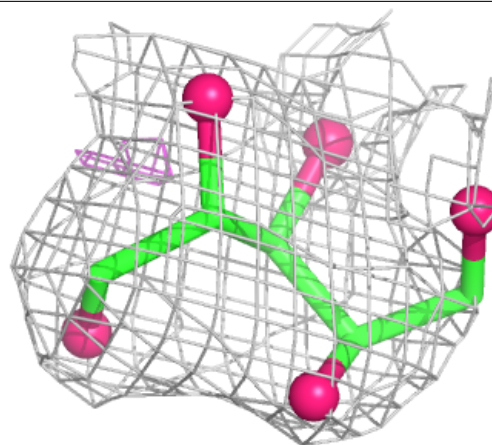
Electron density around XLS D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



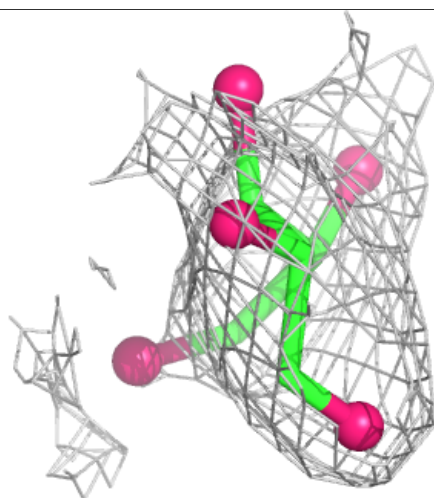
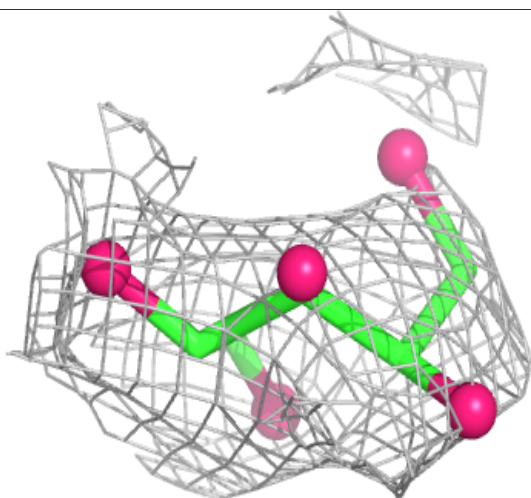
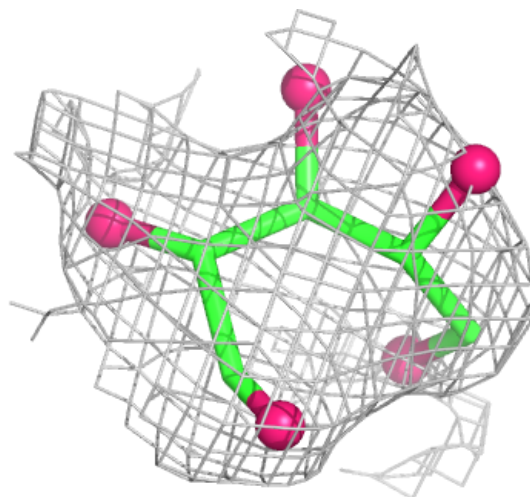
Electron density around XLS A 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



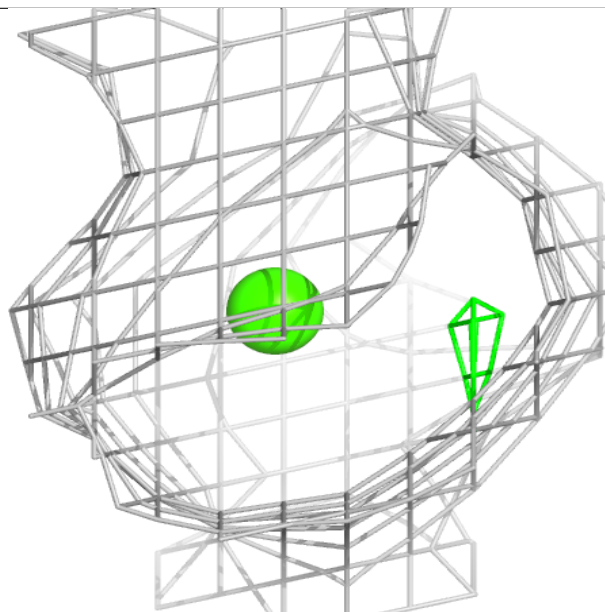
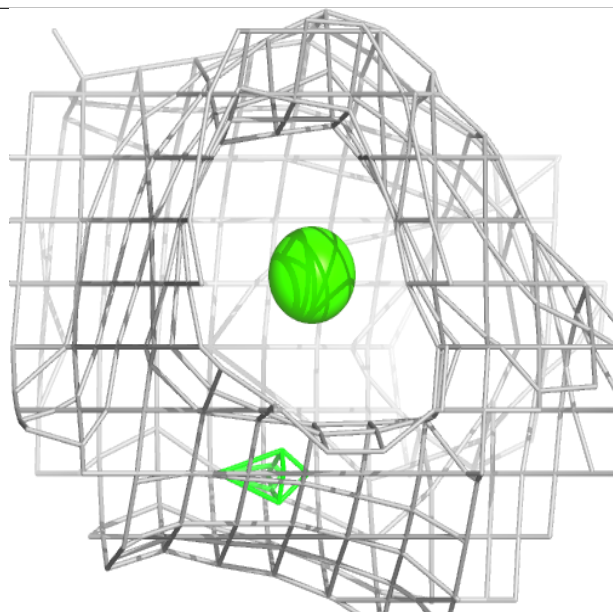
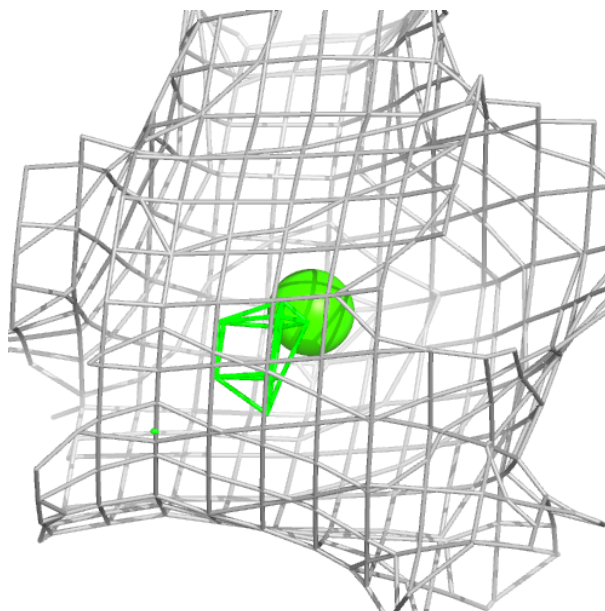
Electron density around XLS G 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



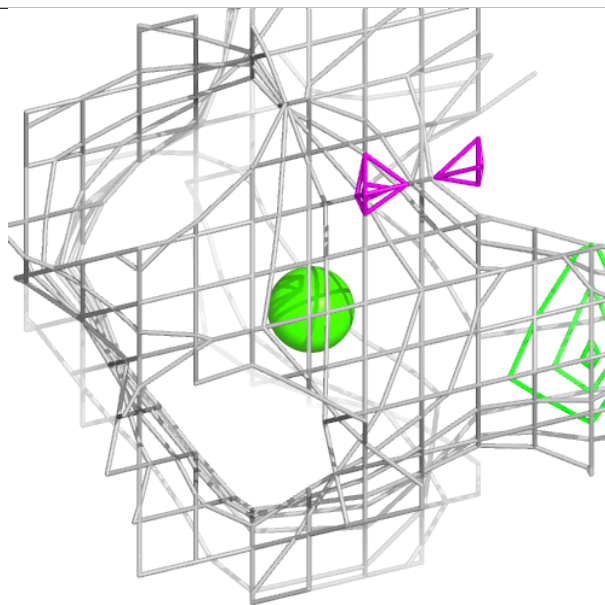
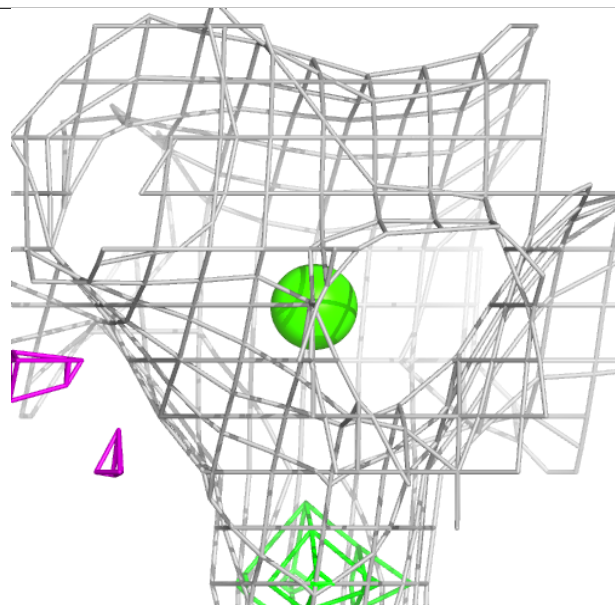
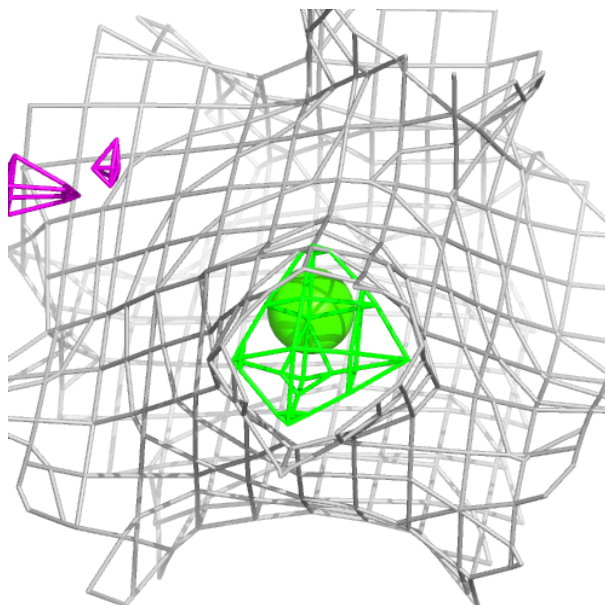
Electron density around CA B 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



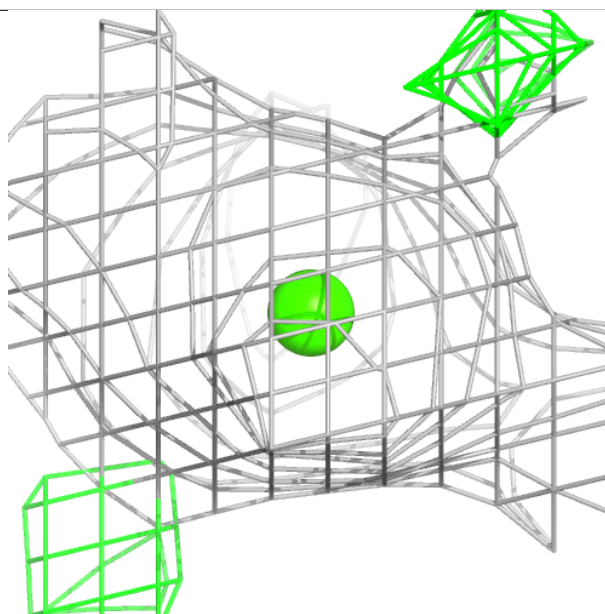
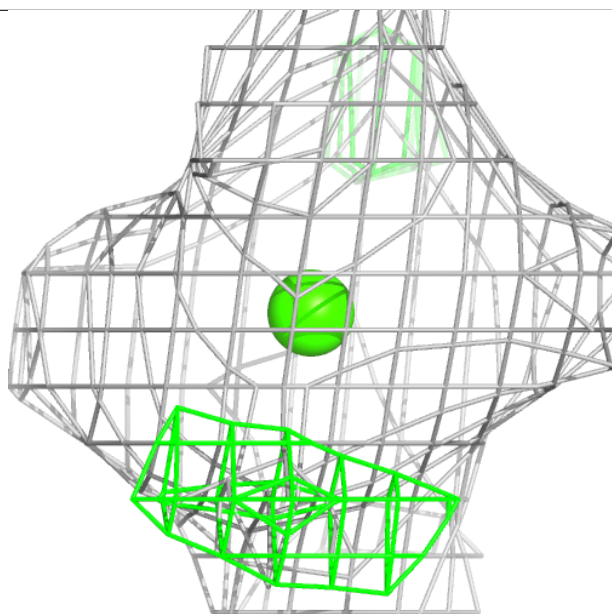
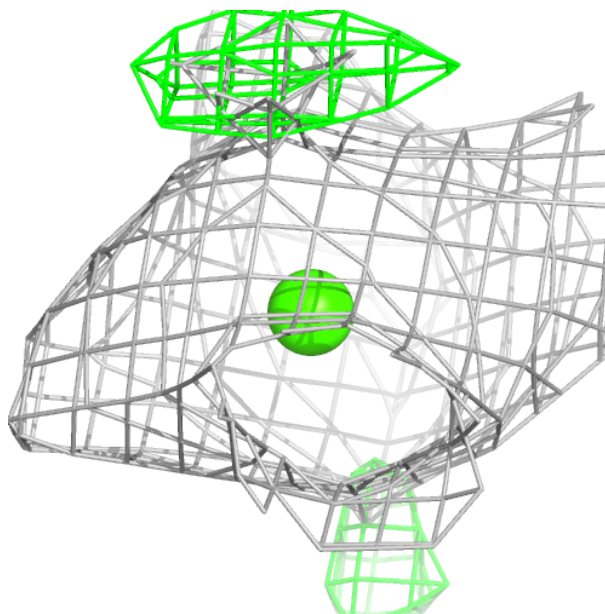
Electron density around CA H 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



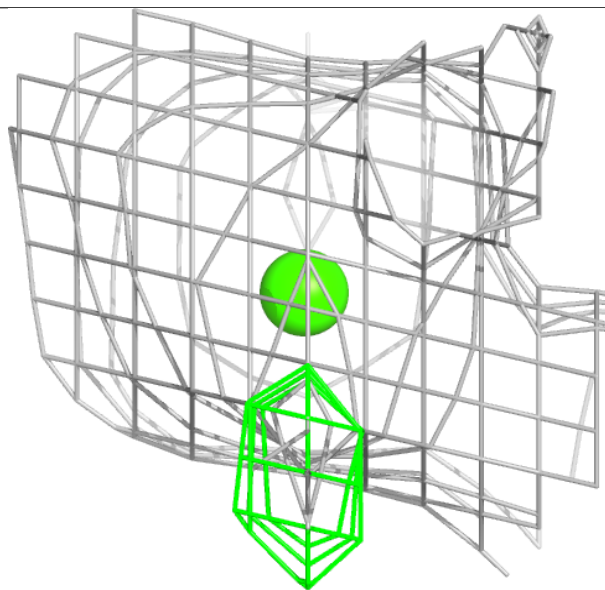
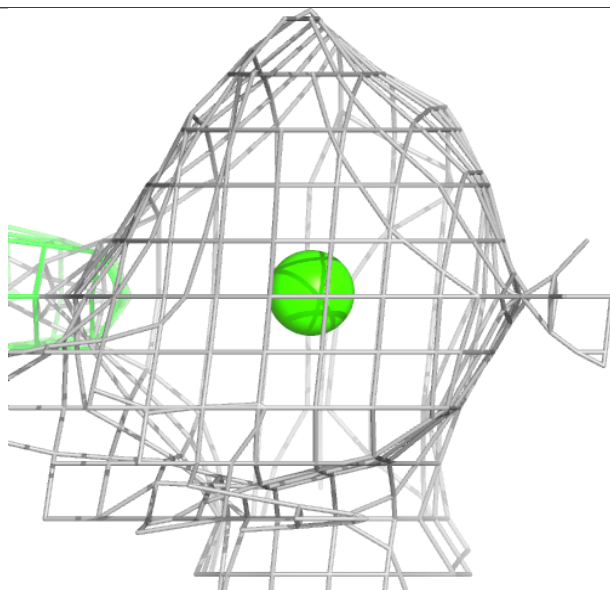
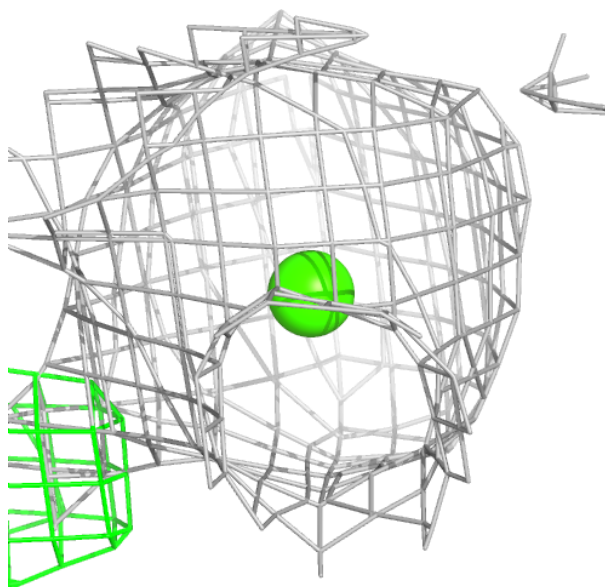
Electron density around CA G 501:

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and green (positive)



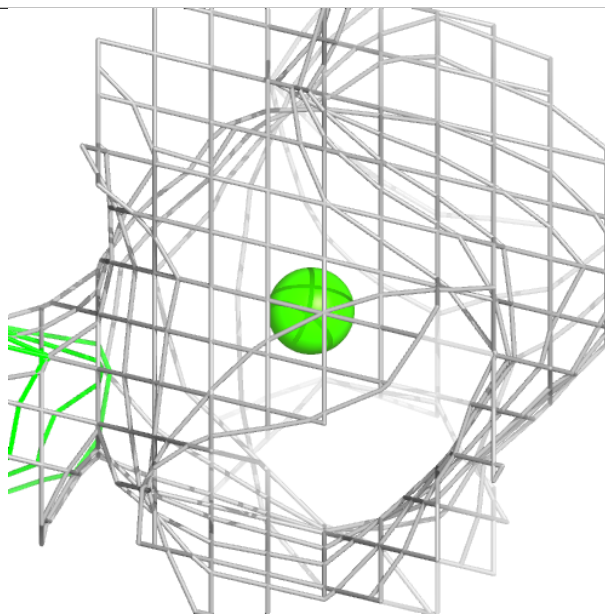
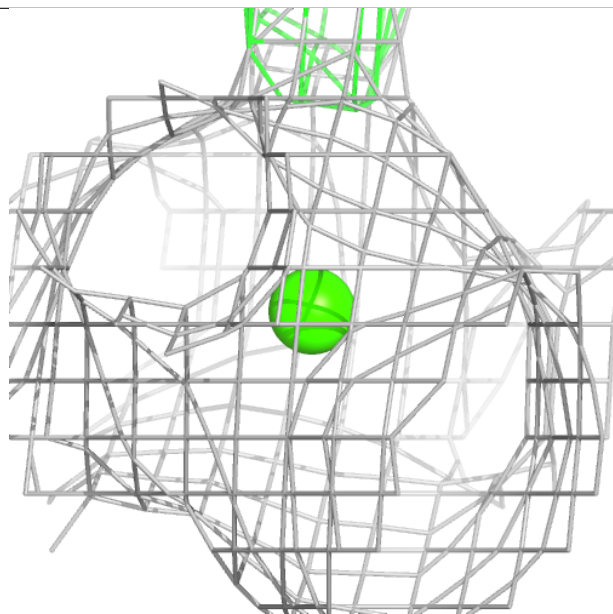
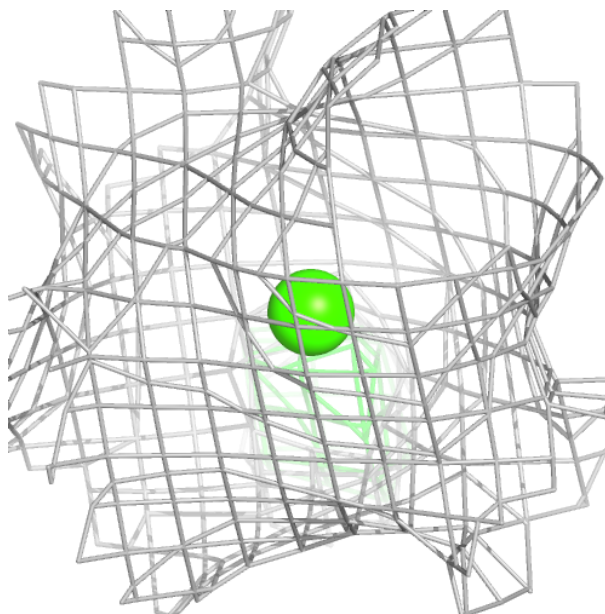
Electron density around CA H 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



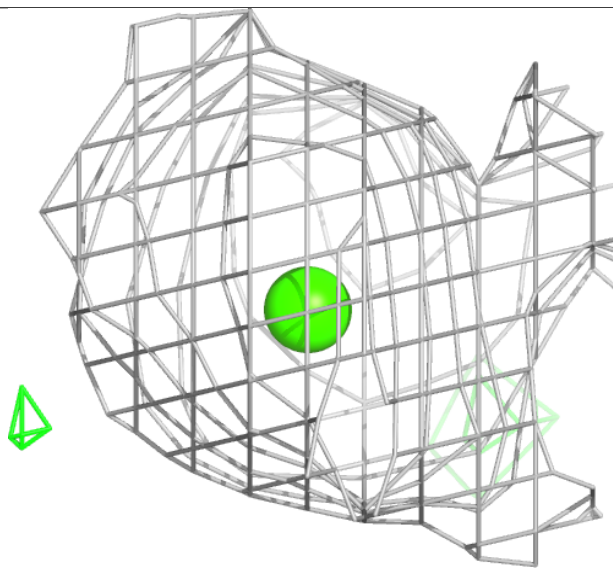
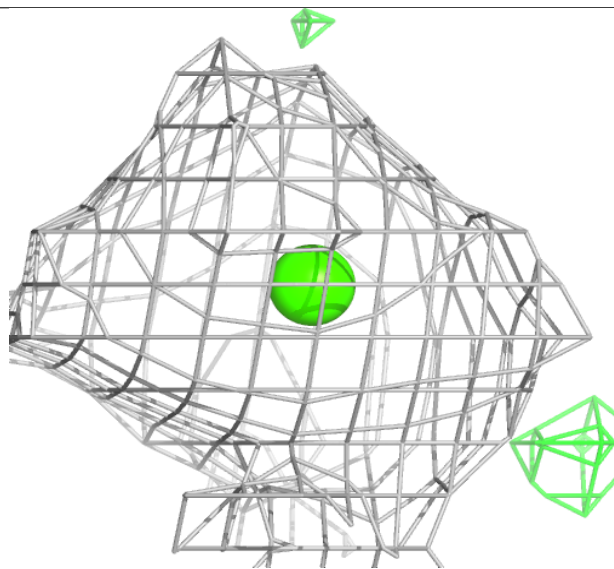
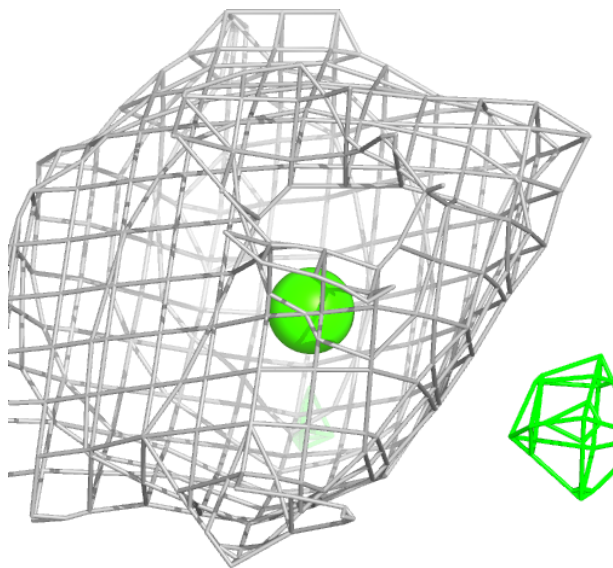
Electron density around CA A 501:

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and green (positive)



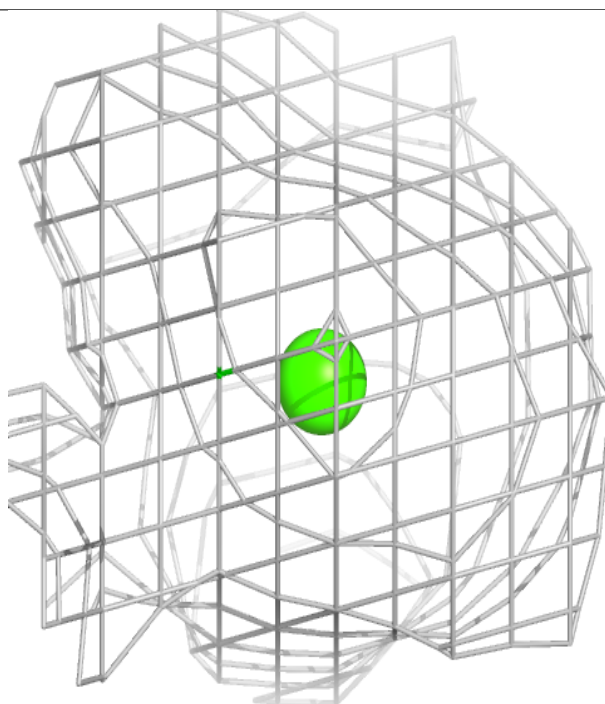
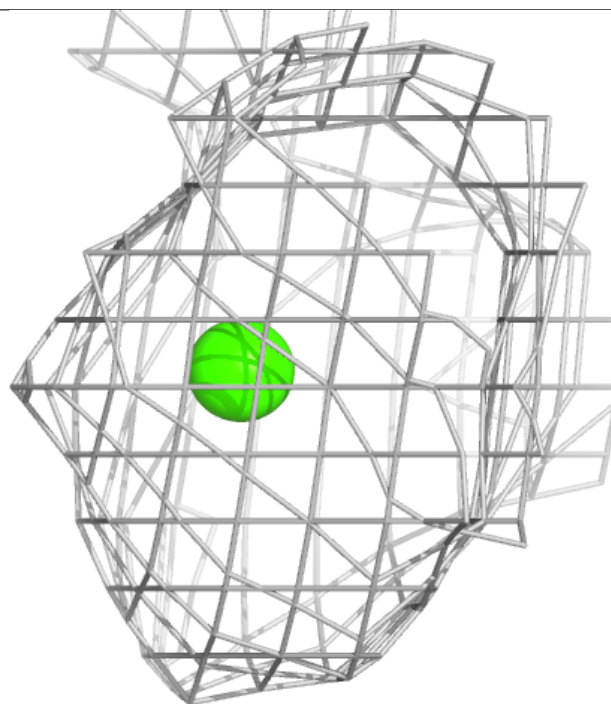
Electron density around CA F 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



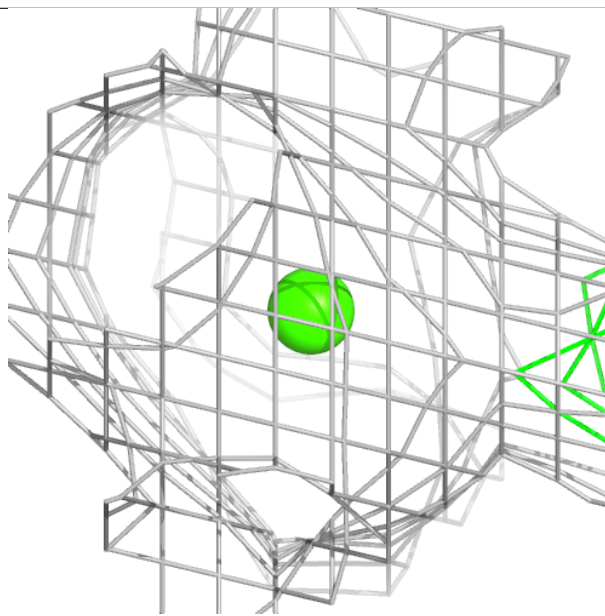
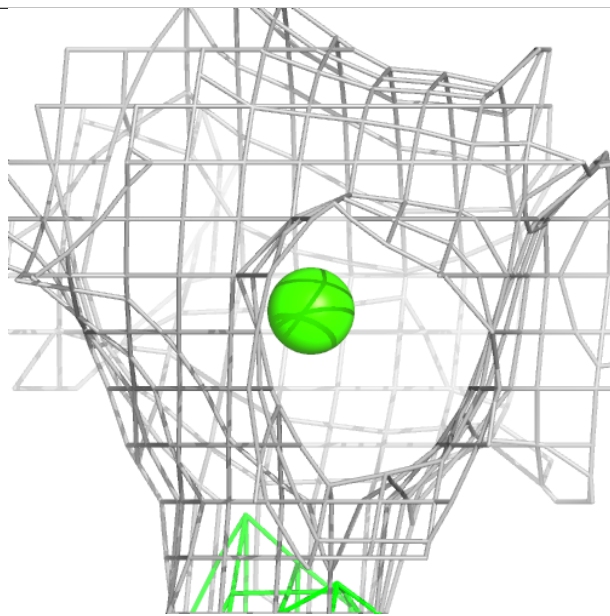
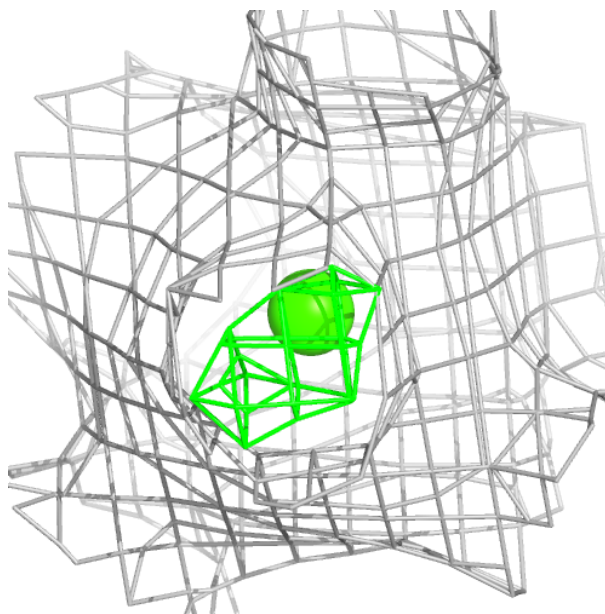
Electron density around CA A 503:

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and green (positive)



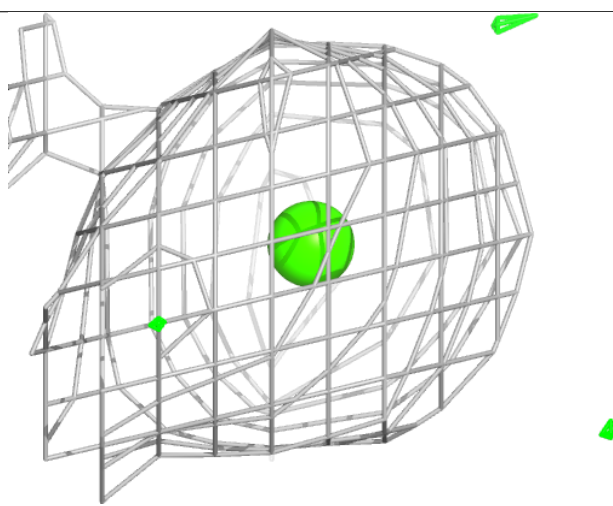
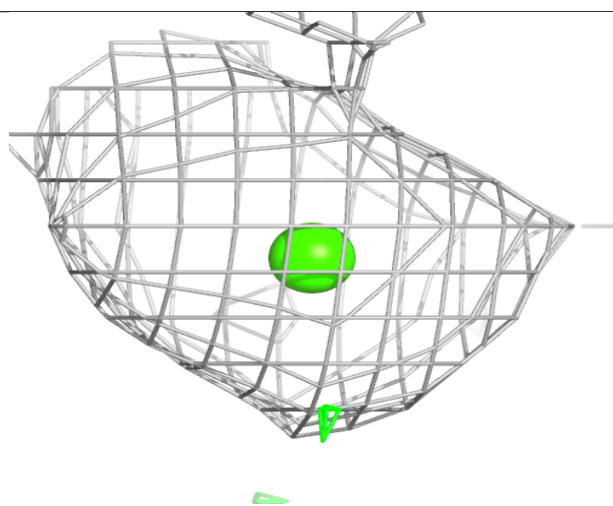
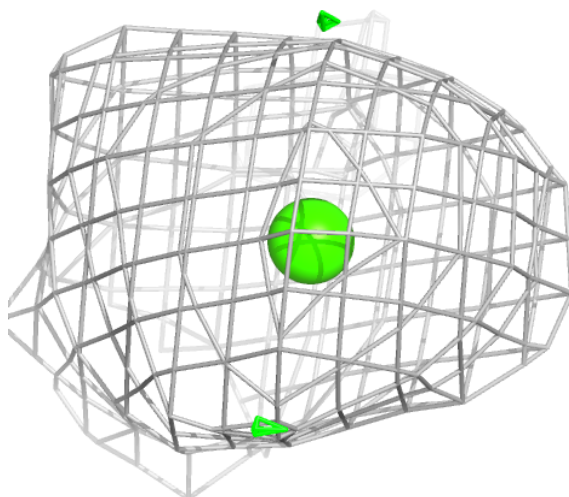
Electron density around CA G 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



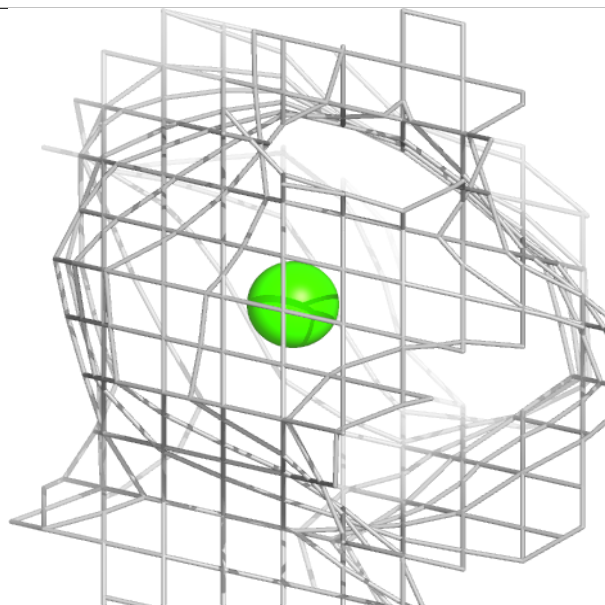
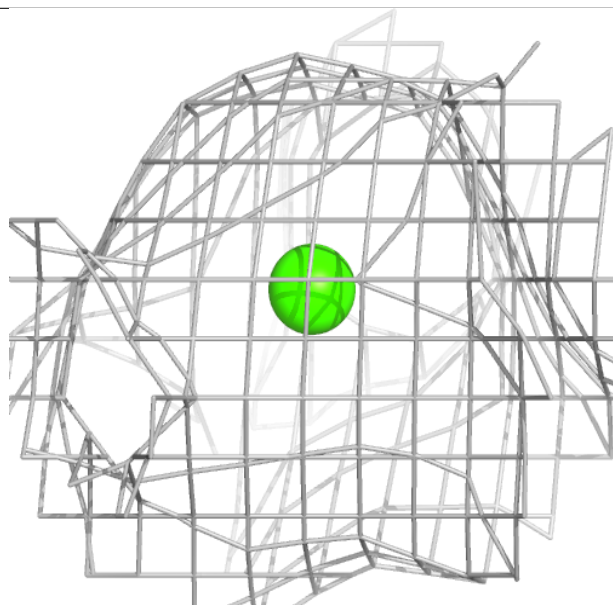
Electron density around CA E 501:

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and green (positive)



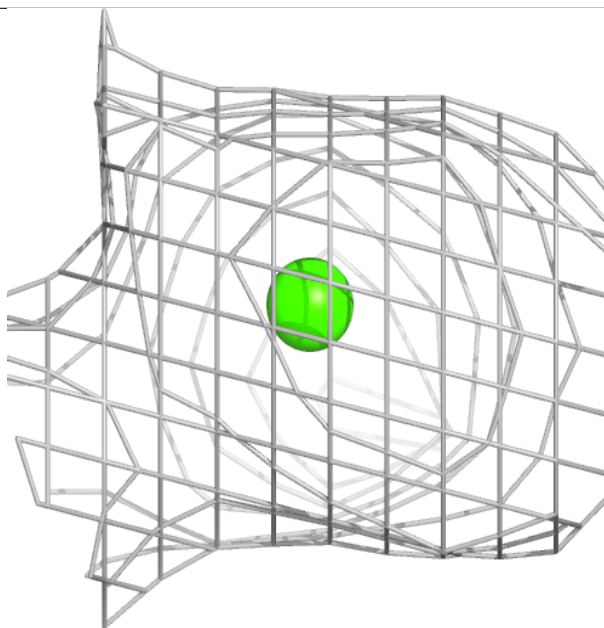
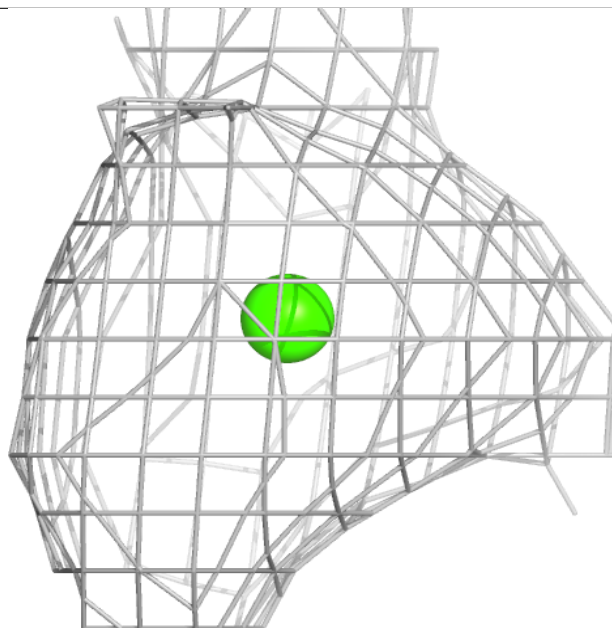
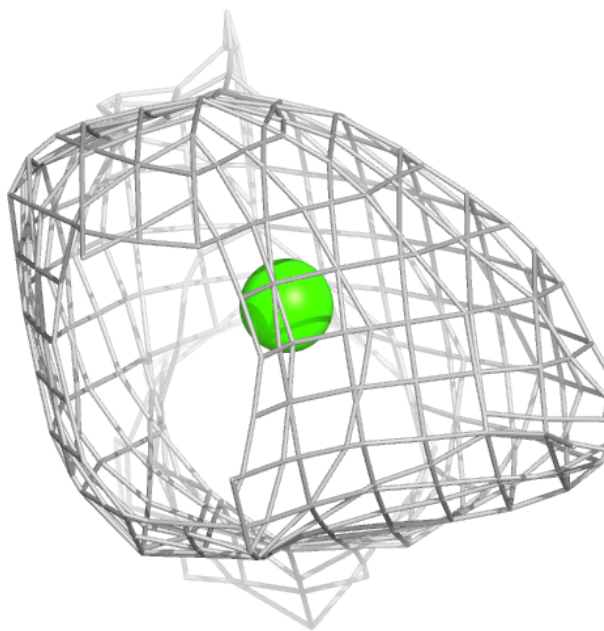
Electron density around CA E 502:

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and green (positive)



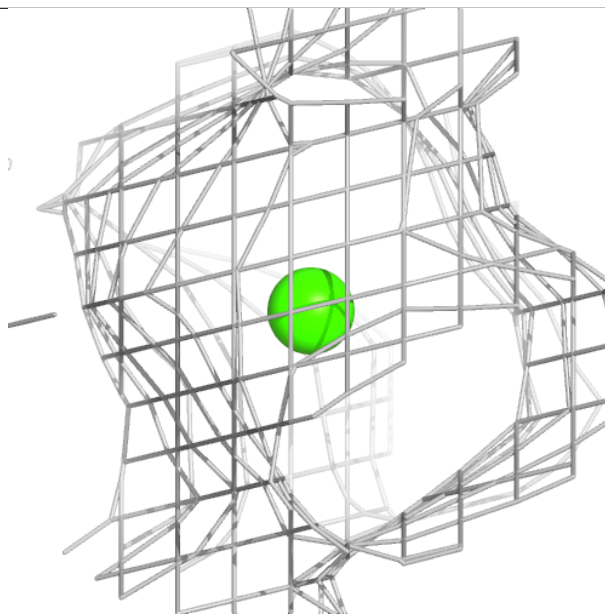
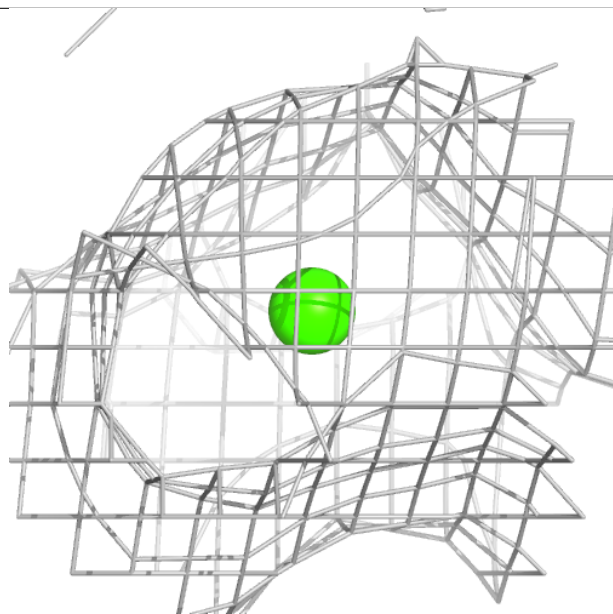
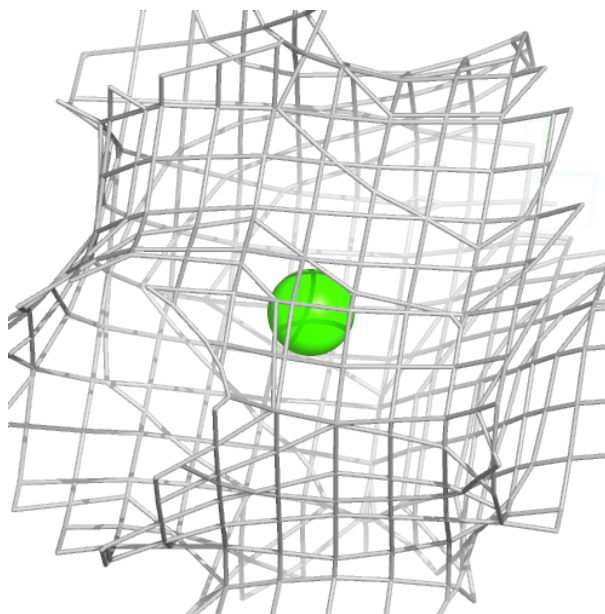
Electron density around CA B 501:

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and green (positive)



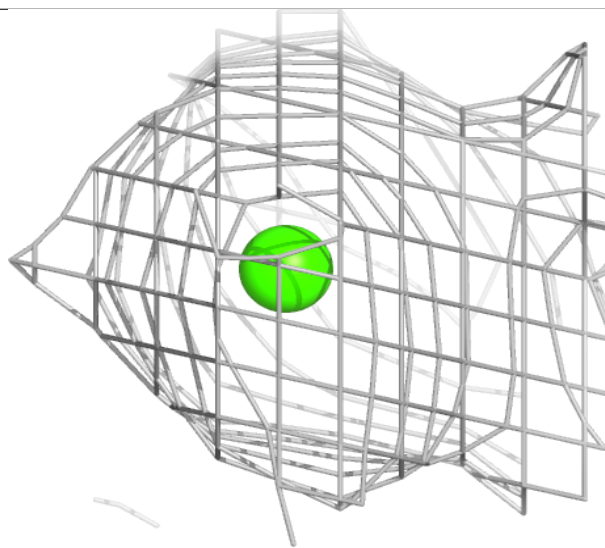
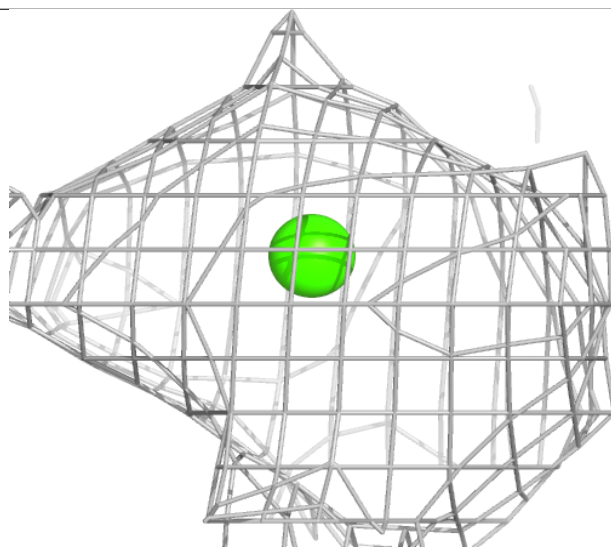
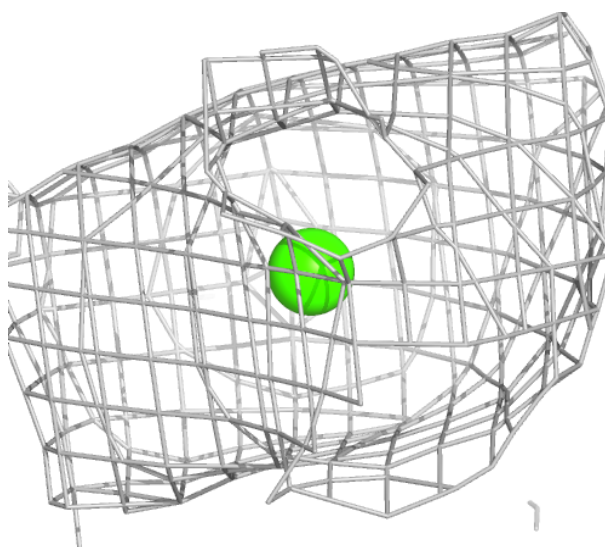
Electron density around CA C 502:

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and green (positive)



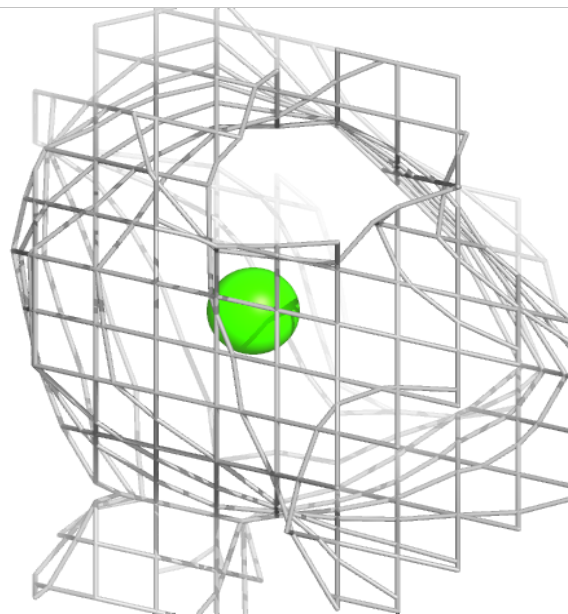
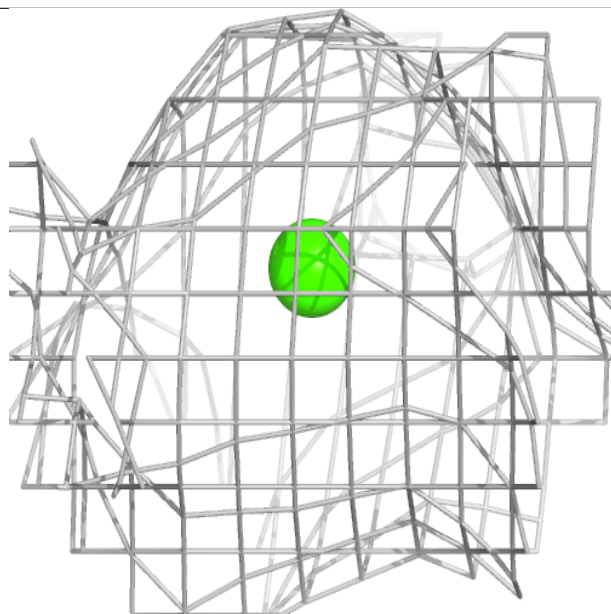
Electron density around CA D 501:

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and green (positive)



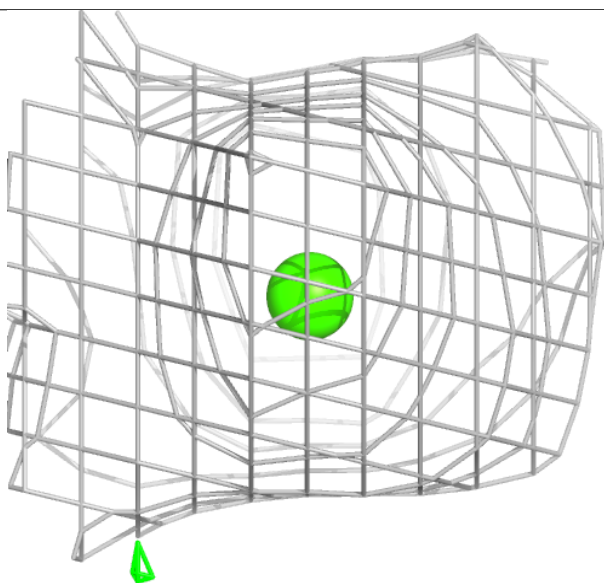
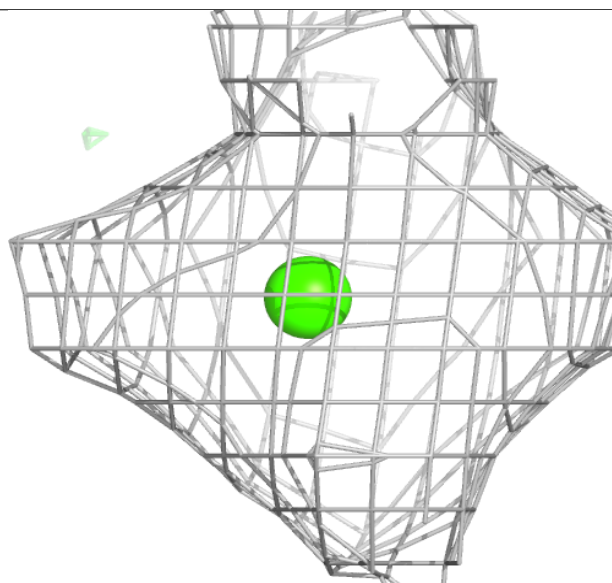
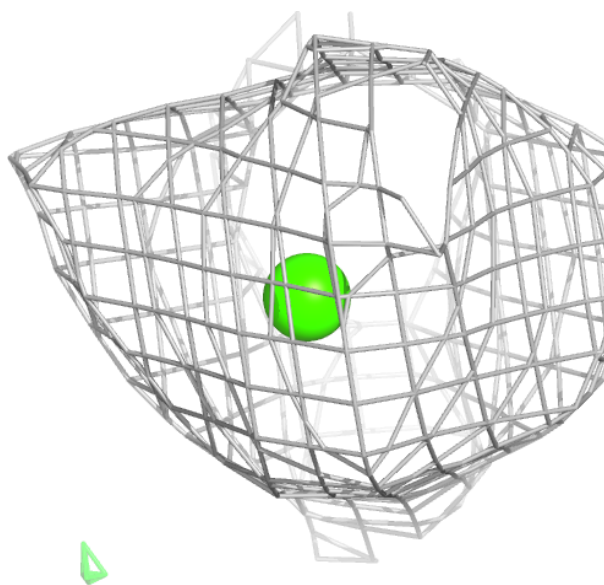
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and green (positive)



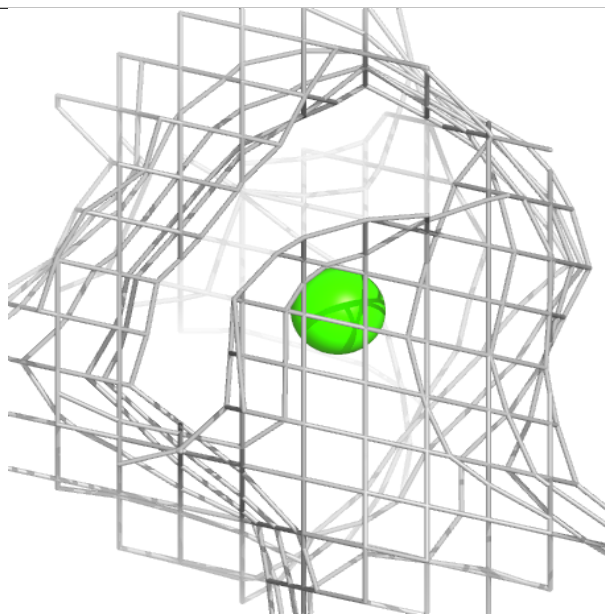
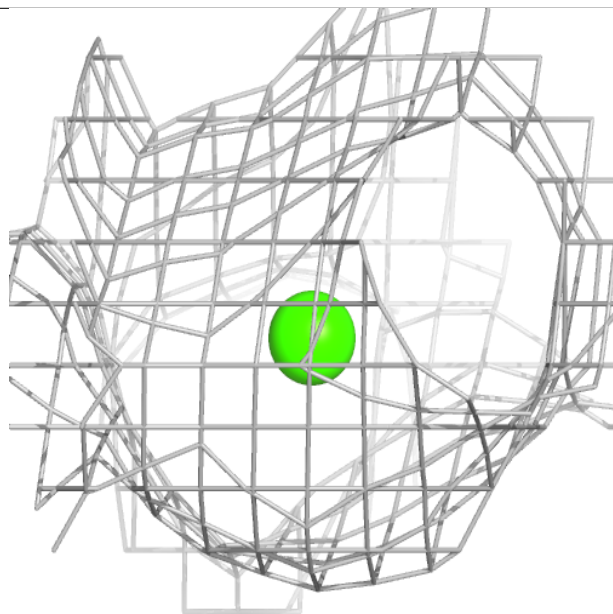
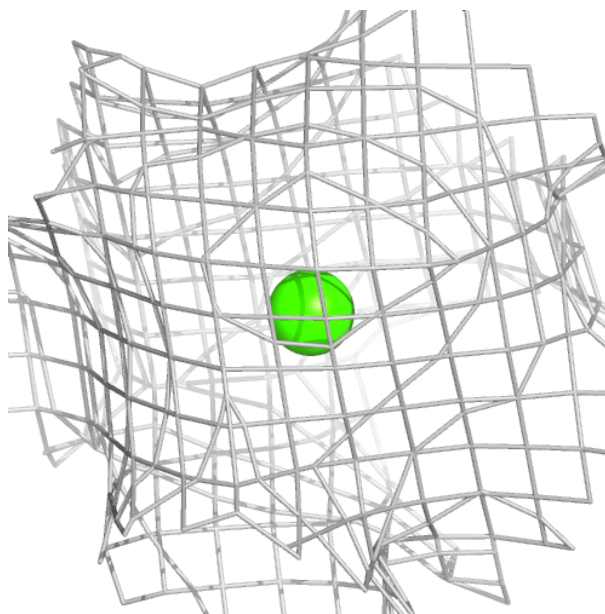
Electron density around CA C 501:

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



Electron density around CA F 502:

$2mF_o-DF_c$ (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.