



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2025 – 02:19 PM EST

PDB ID : 9DYR / pdb_00009dyr
Title : Crystal Structure of Rubisco in complex with CABP from *Methanococcoides burtonii*
Authors : Pereira, J.H.; Liu, A.K.; Shih, P.M.; Adams, P.D.
Deposited on : 2024-10-14
Resolution : 2.66 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

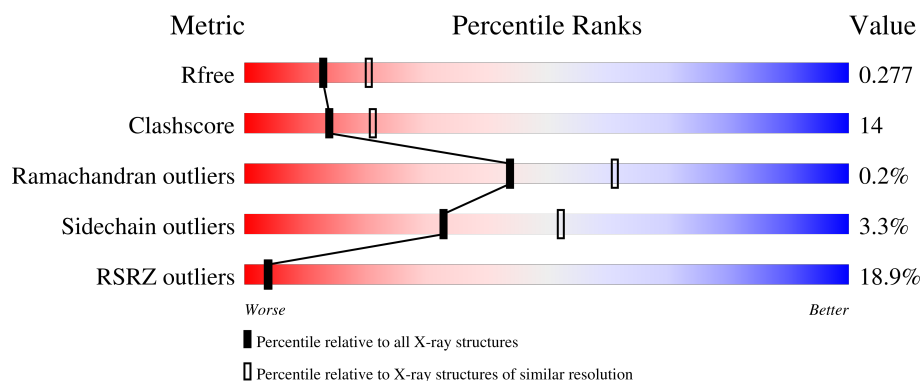
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	

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Mol	Chain	Length	Quality of chain
1	F	468	<div><div></div><div>6%</div><div>65%</div><div>32%</div><div>..</div></div>
1	G	468	<div><div></div><div>36%</div><div>60%</div><div>36%</div><div>..</div></div>
1	H	468	<div><div></div><div>48%</div><div>59%</div><div>38%</div><div>..</div></div>
1	I	468	<div><div></div><div>43%</div><div>63%</div><div>32%</div><div>..</div></div>
1	J	468	<div><div></div><div>39%</div><div>57%</div><div>38%</div><div>..</div></div>

2 Entry composition

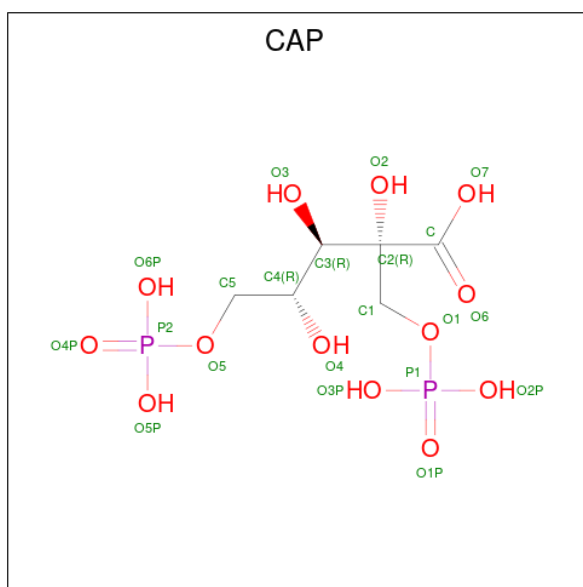
There are 4 unique types of molecules in this entry. The entry contains 36567 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ribulose-1,5-bisphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	B	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	C	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	D	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	E	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	F	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	G	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	H	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	I	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			
1	J	457	Total	C	N	O	S	0	0	0
			3599	2298	597	682	22			

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	6	13	2		
2	B	1	Total	C	O	P	0	0
			21	6	13	2		
2	C	1	Total	C	O	P	0	0
			21	6	13	2		
2	D	1	Total	C	O	P	0	0
			21	6	13	2		
2	E	1	Total	C	O	P	0	0
			21	6	13	2		
2	F	1	Total	C	O	P	0	0
			21	6	13	2		
2	G	1	Total	C	O	P	0	0
			21	6	13	2		
2	H	1	Total	C	O	P	0	0
			21	6	13	2		
2	I	1	Total	C	O	P	0	0
			21	6	13	2		
2	J	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	2	Total 2	Mg 2	0	0
3	E	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0
3	G	2	Total 2	Mg 2	0	0
3	H	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	J	2	Total 2	Mg 2	0	0

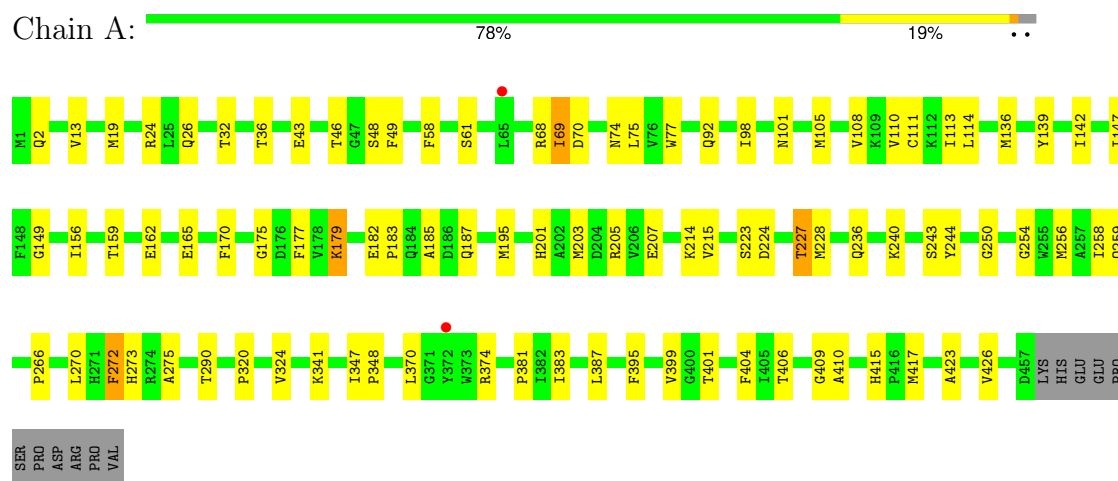
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total 79	O 79	0	0
4	B	72	Total 72	O 72	0	0
4	C	43	Total 43	O 43	0	0
4	D	19	Total 19	O 19	0	0
4	E	54	Total 54	O 54	0	0
4	F	26	Total 26	O 26	0	0
4	G	11	Total 11	O 11	0	0
4	H	18	Total 18	O 18	0	0
4	I	15	Total 15	O 15	0	0
4	J	10	Total 10	O 10	0	0

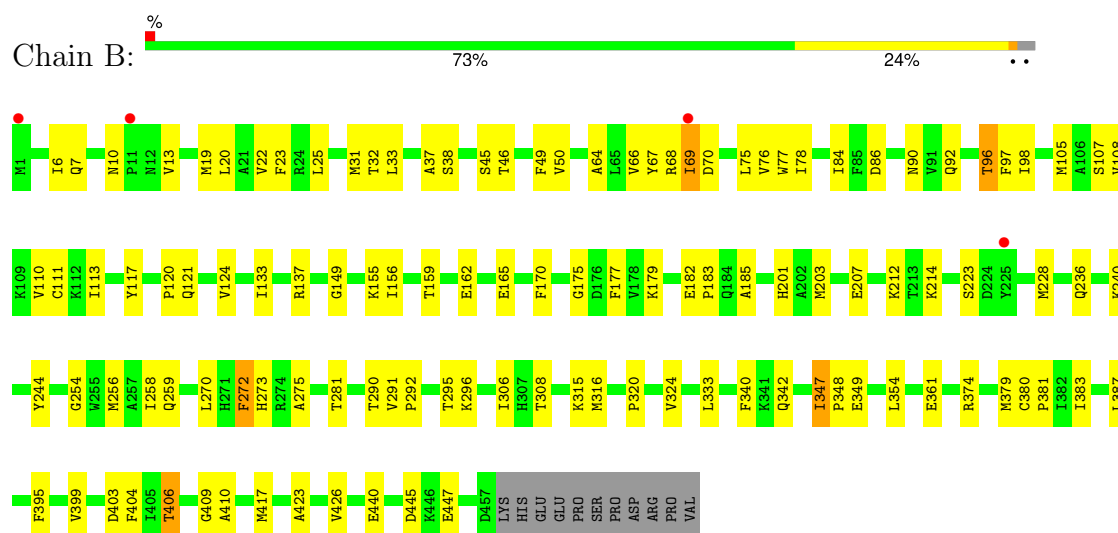
3 Residue-property plots [i](#)

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.

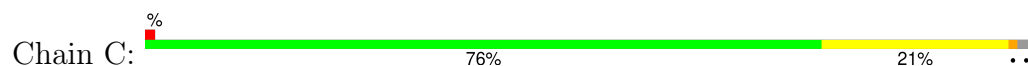
- Molecule 1: ribulose-1,5-bisphosphate carboxylase

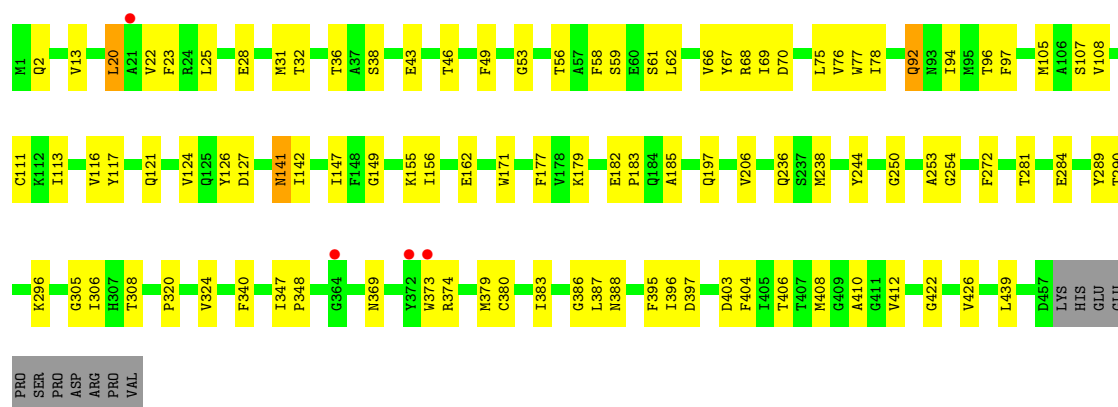


- Molecule 1: ribulose-1,5-bisphosphate carboxylase

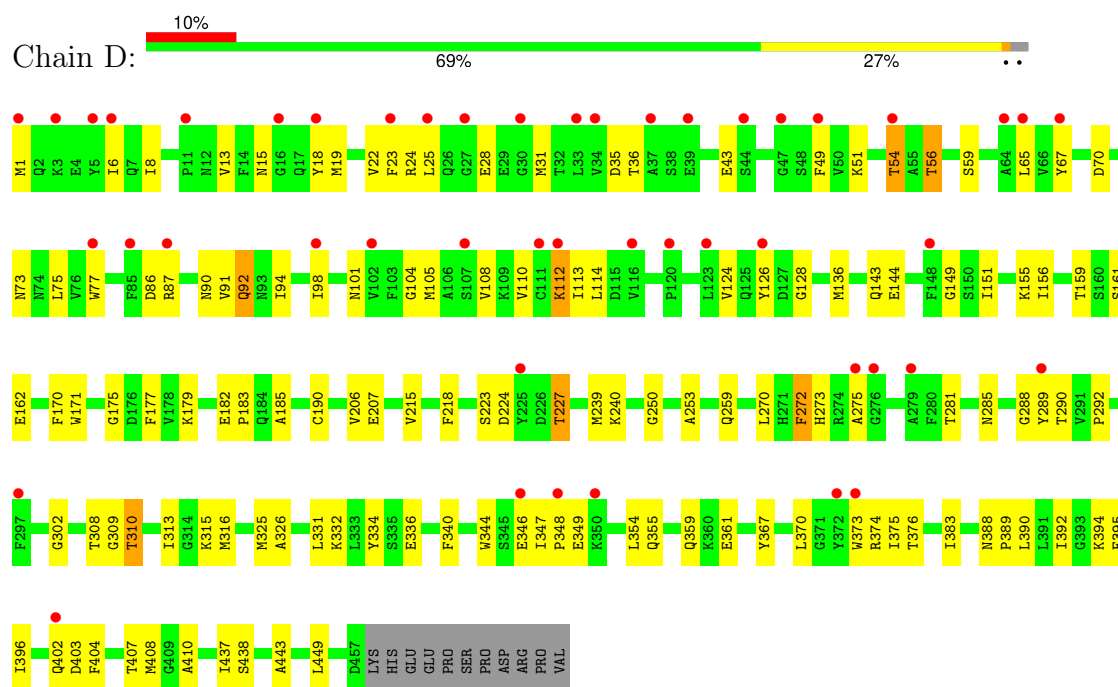


- Molecule 1: ribulose-1,5-bisphosphate carboxylase

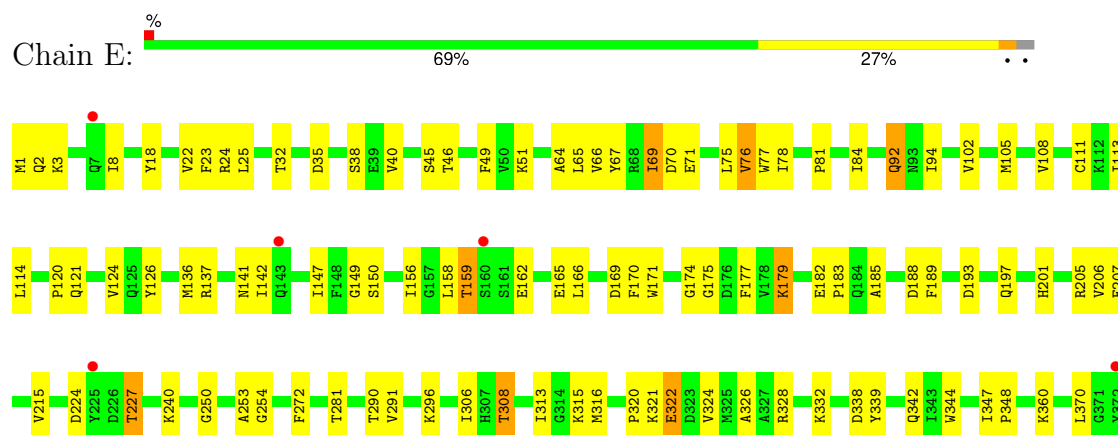


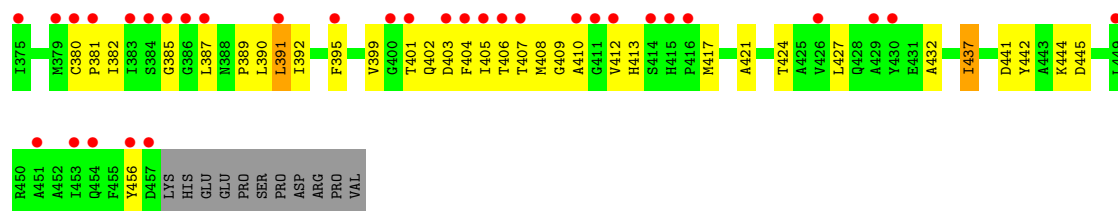


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

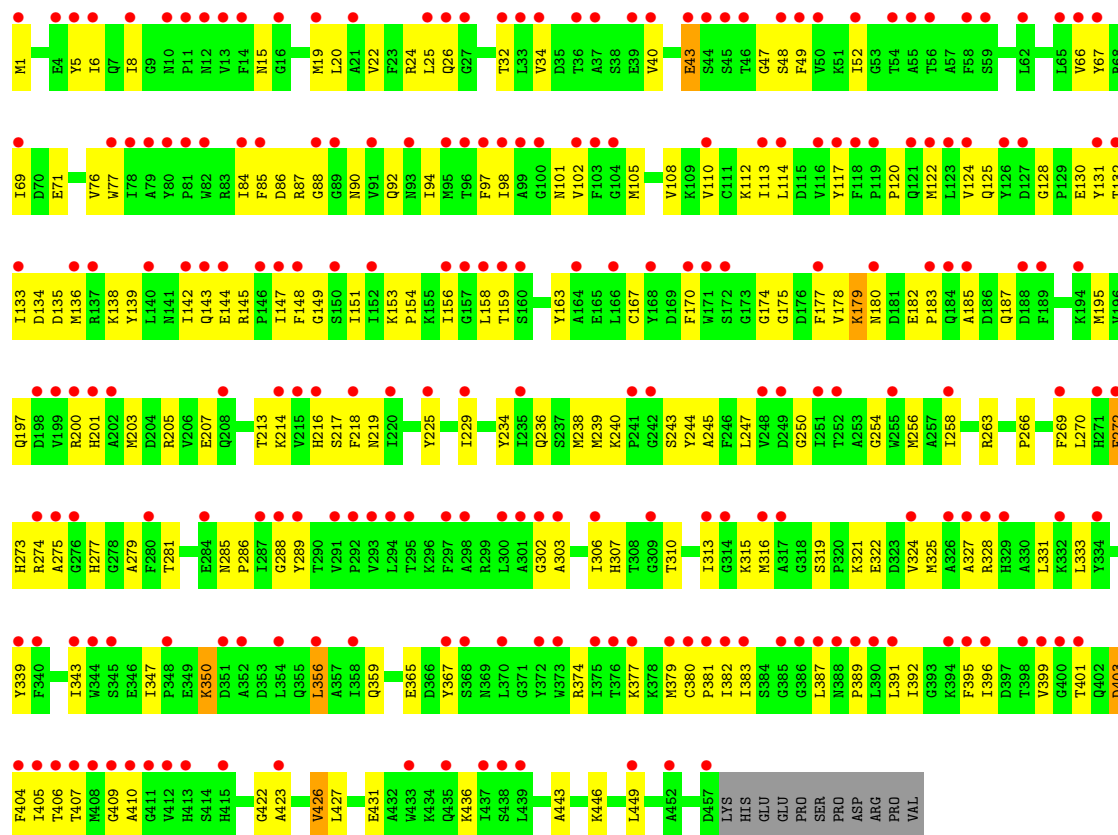


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

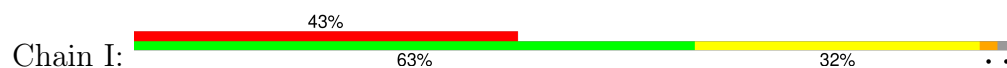


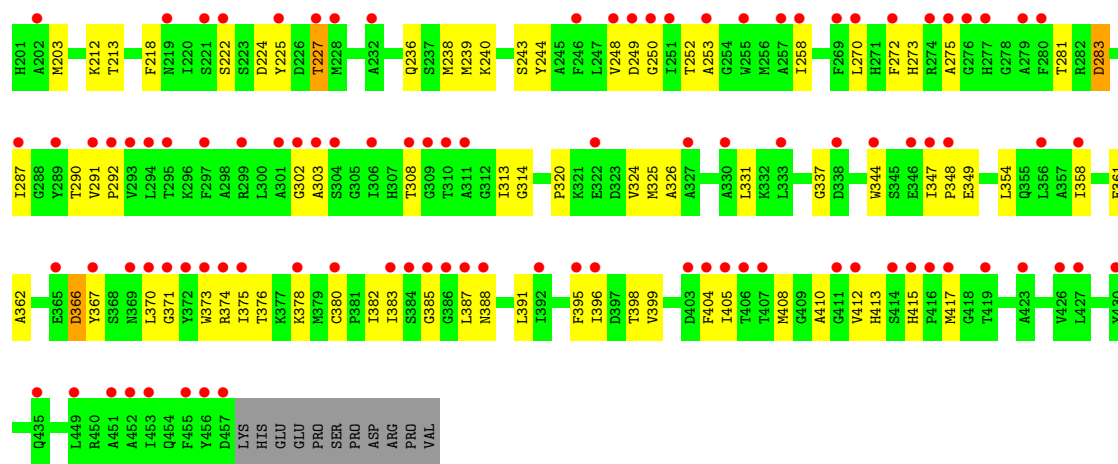


● Molecule 1: ribulose-1,5-bisphosphate carboxylase

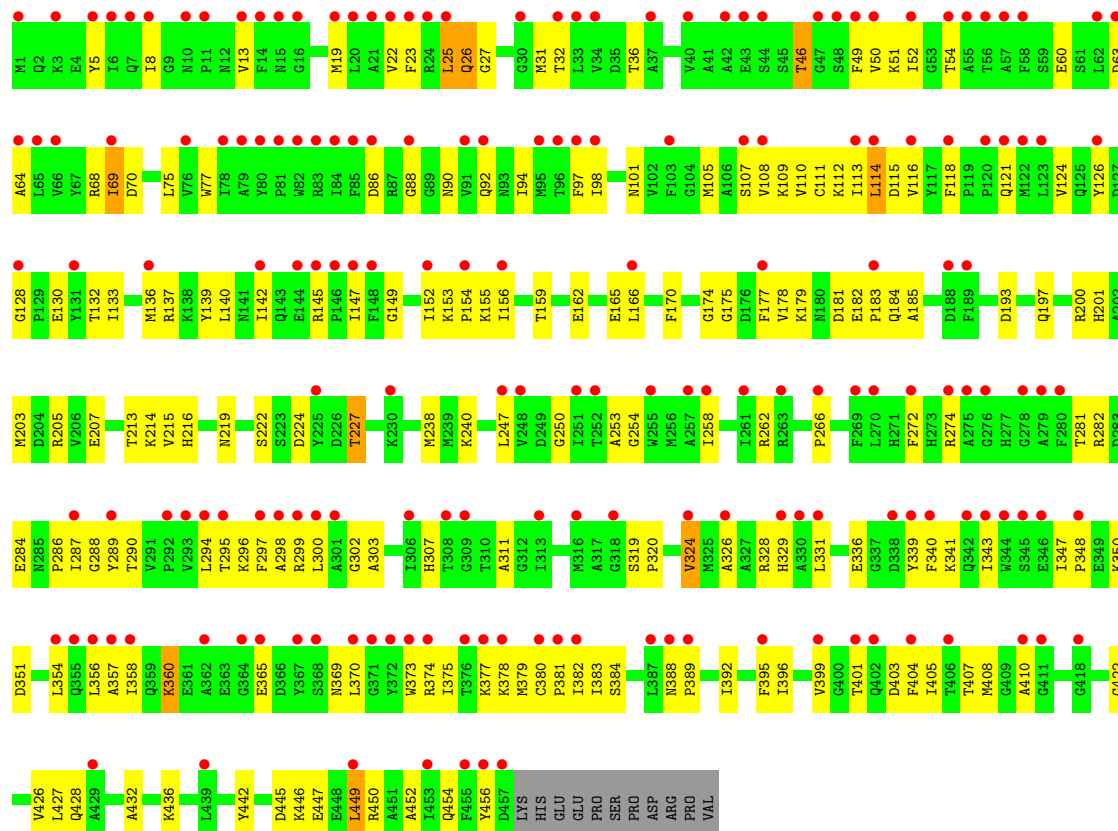
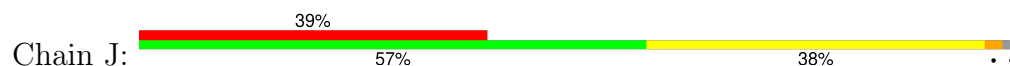


● Molecule 1: ribulose-1,5-bisphosphate carboxylase





• Molecule 1: ribulose-1,5-bisphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.84Å 247.86Å 266.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.66 49.18 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.18-2.66) 92.0 (49.18-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.253 , 0.277 0.253 , 0.277	Depositor DCC
R_{free} test set	1994 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	36567	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, CAP, MG

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	0.23	0/3671	0.46	0/4962
1	B	0.23	0/3671	0.46	0/4962
1	C	0.23	0/3671	0.46	1/4962 (0.0%)
1	D	0.26	0/3671	0.51	0/4962
1	E	0.22	0/3671	0.50	0/4962
1	F	0.27	1/3671 (0.0%)	0.50	0/4962
1	G	0.24	0/3671	0.51	0/4962
1	H	0.27	0/3671	0.54	0/4962
1	I	0.24	0/3671	0.52	0/4962
1	J	0.24	0/3671	0.52	0/4962
All	All	0.24	1/36710 (0.0%)	0.50	1/49620 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	336	GLU	CD-OE1	-5.29	1.15	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	GLN	CA-CB-CG	5.08	124.27	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3599	0	3514	69	0
1	B	3599	0	3514	83	0
1	C	3599	0	3514	70	1
1	D	3599	0	3514	98	0
1	E	3599	0	3514	106	1
1	F	3599	0	3514	124	0
1	G	3599	0	3514	136	0
1	H	3599	0	3514	164	0
1	I	3599	0	3514	127	0
1	J	3599	0	3514	151	0
2	A	21	0	7	2	0
2	B	21	0	7	1	0
2	C	21	0	8	0	0
2	D	21	0	7	1	0
2	E	21	0	7	0	0
2	F	21	0	7	2	0
2	G	21	0	8	0	0
2	H	21	0	8	3	0
2	I	21	0	9	2	0
2	J	21	0	9	2	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
4	A	79	0	0	4	0
4	B	72	0	0	2	0
4	C	43	0	0	4	0
4	D	19	0	0	6	0
4	E	54	0	0	4	0
4	F	26	0	0	10	0
4	G	11	0	0	1	0
4	H	18	0	0	3	0
4	I	15	0	0	6	0
4	J	10	0	0	5	0
All	All	36567	0	35217	1005	1

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 14.

All (1005) 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:111:CYS:SG	4:C:639:HOH:O	2.23	0.96
1:H:200:ARG:HH22	1:H:240:LYS:HG3	1.31	0.96
1:J:142:ILE:HD11	1:J:147:ILE:HG12	1.54	0.90
1:G:321:LYS:NZ	1:G:322:GLU:OE2	2.07	0.87
1:F:68:ARG:HB3	1:F:77:TRP:HB2	1.59	0.85
1:I:313:ILE:HG22	1:I:391:LEU:HD23	1.56	0.84
1:H:443:ALA:HB2	1:H:449:LEU:HD22	1.58	0.84
1:E:417:MET:SD	4:E:621:HOH:O	2.36	0.84
1:H:125:GLN:NE2	4:H:601:HOH:O	2.09	0.83
1:H:256:MET:HE2	1:I:253:ALA:HB1	1.60	0.83
1:G:182:GLU:OE2	1:J:101:ASN:ND2	2.13	0.82
1:D:15:ASN:O	4:D:601:HOH:O	1.97	0.81
1:J:147:ILE:HB	1:J:405:ILE:HG13	1.60	0.81
1:G:370:LEU:O	1:G:374:ARG:NE	2.13	0.81
1:G:162:GLU:HG2	1:I:348:PRO:HD3	1.61	0.81
1:H:174:GLY:HA3	1:H:427:LEU:HD11	1.61	0.81
1:C:56:THR:HG23	1:C:59:SER:H	1.44	0.80
1:H:331:LEU:HD21	1:H:381:PRO:HD3	1.65	0.78
1:D:370:LEU:HG	1:D:374:ARG:HD2	1.66	0.78
1:H:201:HIS:HB3	1:J:373:TRP:CE3	2.18	0.78
1:E:142:ILE:HD11	1:E:147:ILE:HG13	1.66	0.77
1:H:389:PRO:HG3	1:H:426:VAL:HG12	1.67	0.77
1:G:200:ARG:NH1	1:G:238:MET:O	2.17	0.77
1:I:200:ARG:HH12	1:I:240:LYS:HG3	1.49	0.77
1:H:132:THR:CG2	1:H:377:LYS:HD3	2.15	0.76
1:I:17:GLN:O	1:I:17:GLN:NE2	2.18	0.76
1:D:155:LYS:NZ	1:D:182:GLU:OE2	2.18	0.76
1:I:136:MET:HE1	1:I:177:PHE:HD2	1.50	0.76
1:J:224:ASP:OD1	1:J:227:THR:OG1	2.04	0.76
1:E:162:GLU:HG2	1:G:348:PRO:HD3	1.69	0.75
1:H:218:PHE:HZ	1:H:239:MET:HE3	1.52	0.75
1:J:23:PHE:HB3	1:J:25:LEU:HD13	1.69	0.75
1:H:313:ILE:HG22	1:H:391:LEU:HD23	1.68	0.75
1:G:349:GLU:O	1:G:355:GLN:NE2	2.16	0.75
1:D:70:ASP:HB3	1:D:75:LEU:HB2	1.67	0.74
1:J:324:VAL:O	1:J:328:ARG:HG3	1.87	0.74
1:C:348:PRO:HD3	1:J:162:GLU:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HG2	1:F:348:PRO:HD3	1.69	0.73
1:J:348:PRO:HB2	1:J:350:LYS:HG2	1.70	0.73
1:F:319:SER:OG	1:F:322:GLU:OE1	2.04	0.73
1:D:51:LYS:H	1:D:51:LYS:HD2	1.54	0.72
2:I:502:CAP:O2P	4:I:601:HOH:O	2.07	0.72
1:H:132:THR:HG23	1:H:377:LYS:HD3	1.72	0.72
1:E:174:GLY:HA3	1:E:427:LEU:HD11	1.73	0.71
1:F:199:VAL:HG11	1:F:216:HIS:HD2	1.55	0.71
1:G:145:ARG:HH22	1:G:176:ASP:CG	1.99	0.71
1:B:348:PRO:HD3	1:D:162:GLU:HG2	1.72	0.70
1:D:124:VAL:HG21	1:I:159:THR:HG21	1.72	0.70
1:E:40:VAL:HG22	1:E:105:MET:HE1	1.72	0.70
1:F:200:ARG:NH1	1:F:240:LYS:HG3	2.07	0.69
1:G:409:GLY:O	1:G:413:HIS:ND1	2.24	0.69
1:H:20:LEU:HD23	1:H:117:TYR:HD2	1.58	0.69
1:F:165:GLU:OE1	4:F:602:HOH:O	2.09	0.69
1:J:197:GLN:HG2	1:J:238:MET:HE2	1.74	0.69
1:J:347:ILE:HG13	1:J:374:ARG:HB2	1.74	0.69
1:F:159:THR:HG21	1:H:124:VAL:HG21	1.75	0.69
1:F:417:MET:HE1	1:F:447:GLU:HG2	1.75	0.69
1:I:36:THR:HG23	1:I:108:VAL:HG22	1.74	0.68
1:B:162:GLU:HG2	1:E:348:PRO:HD3	1.75	0.68
1:E:66:VAL:HG22	1:E:78:ILE:HG12	1.74	0.68
1:H:15:ASN:O	4:H:602:HOH:O	2.11	0.68
1:I:133:ILE:HD11	1:I:147:ILE:HD13	1.74	0.68
1:A:348:PRO:HD3	1:C:162:GLU:HG2	1.76	0.68
1:E:51:LYS:NZ	4:E:603:HOH:O	2.26	0.67
1:G:136:MET:HE1	1:G:177:PHE:CD1	2.29	0.67
1:F:441:ASP:O	1:F:444:LYS:HG2	1.95	0.67
1:I:159:THR:HG22	1:I:161:SER:H	1.59	0.67
1:J:295:THR:HG21	1:J:326:ALA:HB1	1.76	0.67
1:F:387:LEU:HB3	1:F:408:MET:HE2	1.76	0.66
1:I:410:ALA:N	4:I:601:HOH:O	2.27	0.66
1:J:356:LEU:HD23	1:J:360:LYS:HD3	1.77	0.66
1:F:207:GLU:OE1	1:F:240:LYS:NZ	2.26	0.66
1:H:149:GLY:HA2	1:H:177:PHE:O	1.96	0.66
1:H:92:GLN:NE2	1:I:252:THR:OG1	2.29	0.66
1:I:198:ASP:OD1	4:I:602:HOH:O	2.14	0.66
1:J:31:MET:HE2	1:J:36:THR:HG22	1.77	0.66
1:C:369:ASN:O	1:J:205:ARG:NH1	2.29	0.65
1:H:218:PHE:CZ	1:H:239:MET:HE3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:LYS:NZ	1:I:43:GLU:OE2	2.24	0.65
1:D:443:ALA:HB2	1:D:449:LEU:HD22	1.79	0.65
1:D:25:LEU:HD23	1:D:36:THR:HG22	1.79	0.65
1:F:179:KCX:HE2	4:F:601:HOH:O	1.97	0.65
1:I:108:VAL:HG11	1:I:111:CYS:HB2	1.78	0.65
1:D:19:MET:HE1	1:D:98:ILE:HD13	1.77	0.65
1:J:8:ILE:HD11	1:J:69:ILE:HD12	1.77	0.65
1:A:70:ASP:HB3	1:A:75:LEU:HB2	1.78	0.65
1:E:370:LEU:HG	1:E:374:ARG:HD2	1.78	0.65
1:F:147:ILE:HB	1:F:405:ILE:HG13	1.77	0.65
1:G:136:MET:HE1	1:G:177:PHE:HD1	1.60	0.65
1:A:341:LYS:NZ	4:A:605:HOH:O	2.29	0.64
1:B:66:VAL:HG22	1:B:78:ILE:HG12	1.79	0.64
1:J:68:ARG:HB3	1:J:77:TRP:HB2	1.79	0.64
1:H:347:ILE:HG13	1:H:374:ARG:HB2	1.80	0.64
1:G:33:LEU:HD13	1:G:71:GLU:HA	1.80	0.64
1:J:343:ILE:HD13	1:J:358:ILE:HD11	1.79	0.64
1:D:56:THR:HG23	1:D:59:SER:H	1.63	0.63
1:E:25:LEU:HD12	1:E:76:VAL:HG11	1.80	0.63
1:I:37:ALA:HB1	1:I:66:VAL:HG21	1.81	0.63
1:C:142:ILE:HD11	1:C:147:ILE:HG12	1.80	0.63
1:I:136:MET:HE1	1:I:177:PHE:CD2	2.32	0.63
1:D:23:PHE:HB2	1:D:25:LEU:HD11	1.78	0.63
1:E:224:ASP:OD1	1:E:227:THR:OG1	2.14	0.63
1:D:218:PHE:HZ	1:D:239:MET:HE3	1.62	0.63
1:H:149:GLY:O	1:H:407:THR:HA	1.98	0.63
1:H:203:MET:HE1	1:H:243:SER:HB2	1.80	0.63
1:C:155:LYS:NZ	1:C:182:GLU:OE2	2.32	0.63
1:D:224:ASP:OD1	1:D:227:THR:OG1	2.17	0.62
1:G:28:GLU:HG2	1:G:31:MET:HE2	1.81	0.62
1:J:149:GLY:HA2	1:J:177:PHE:O	1.99	0.62
1:I:270:LEU:HD23	1:I:303:ALA:HA	1.80	0.62
1:A:43:GLU:O	1:B:155:LYS:NZ	2.29	0.62
1:D:182:GLU:HG2	1:D:183:PRO:HD3	1.82	0.62
1:E:149:GLY:HA2	1:E:177:PHE:O	2.00	0.62
1:H:324:VAL:O	1:H:328:ARG:HG3	1.99	0.62
1:I:349:GLU:HA	1:I:354:LEU:HD23	1.80	0.62
1:F:22:VAL:HG21	1:F:339:TYR:CD2	2.34	0.62
1:H:383:ILE:HG12	1:H:395:PHE:CZ	2.34	0.62
1:C:20:LEU:HD13	1:C:117:TYR:HD2	1.62	0.62
1:C:347:ILE:HD12	1:J:165:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:MET:HE2	1:J:253:ALA:HB1	1.81	0.62
1:H:130:GLU:HG2	1:H:266:PRO:HB2	1.81	0.62
1:J:182:GLU:HG2	1:J:183:PRO:HD3	1.82	0.62
1:C:23:PHE:HB2	1:C:25:LEU:HD11	1.82	0.62
1:I:224:ASP:OD1	1:I:227:THR:OG1	2.14	0.62
1:A:370:LEU:HG	1:A:374:ARG:HD2	1.80	0.61
1:D:349:GLU:O	1:D:355:GLN:NE2	2.33	0.61
1:H:8:ILE:HA	1:H:67:TYR:HA	1.83	0.61
1:I:383:ILE:HG22	1:I:387:LEU:HD11	1.81	0.61
1:H:92:GLN:NE2	1:I:249:ASP:HB2	2.15	0.61
1:H:403:ASP:OD1	1:H:403:ASP:N	2.32	0.61
1:C:25:LEU:HD23	1:C:36:THR:HG22	1.82	0.61
1:H:380:CYS:SG	1:H:405:ILE:HD12	2.40	0.61
1:F:200:ARG:HH12	1:F:240:LYS:HG3	1.65	0.61
1:H:87:ARG:NH2	4:H:606:HOH:O	2.34	0.61
1:D:54:THR:HG21	1:F:166:LEU:HD21	1.83	0.61
1:E:321:LYS:NZ	1:E:338:ASP:OD1	2.33	0.61
1:I:149:GLY:HA2	1:I:177:PHE:O	2.00	0.61
1:F:399:VAL:O	4:F:603:HOH:O	2.16	0.61
1:H:422:GLY:O	1:H:426:VAL:HG13	2.01	0.61
1:C:53:GLY:N	4:C:602:HOH:O	2.22	0.61
1:G:24:ARG:HB2	1:G:114:LEU:HD11	1.81	0.61
1:H:142:ILE:HD11	1:H:147:ILE:HG12	1.81	0.61
1:C:58:PHE:CD2	1:G:17:GLN:HG2	2.36	0.61
1:I:92:GLN:O	1:I:96:THR:HG23	2.01	0.60
1:I:324:VAL:HG22	1:I:399:VAL:HG23	1.83	0.60
1:H:151:ILE:HB	1:H:153:LYS:NZ	2.16	0.60
1:H:200:ARG:NH2	1:H:240:LYS:HG3	2.11	0.60
1:A:156:ILE:HG21	1:B:84:ILE:HB	1.83	0.60
1:A:254:GLY:HA3	1:B:254:GLY:HA3	1.84	0.60
1:J:447:GLU:OE1	1:J:450:ARG:NH2	2.34	0.60
1:H:92:GLN:HE22	1:I:249:ASP:HB2	1.66	0.60
1:J:286:PRO:HG2	1:J:287:ILE:HD12	1.83	0.60
1:B:133:ILE:HD13	1:B:403:ASP:OD1	2.02	0.59
1:D:24:ARG:HB3	1:D:112:LYS:HB2	1.83	0.59
1:H:97:PHE:HZ	1:I:156:ILE:HG13	1.67	0.59
1:C:69:ILE:HD13	1:C:76:VAL:HG22	1.84	0.59
1:I:290:THR:HB	1:I:292:PRO:HD2	1.84	0.59
1:G:201:HIS:HB3	1:I:373:TRP:CD1	2.37	0.59
1:H:97:PHE:CZ	1:I:156:ILE:HG13	2.38	0.59
1:F:6:ILE:HD11	1:F:38:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLN:NE2	1:A:48:SER:O	2.31	0.59
1:F:70:ASP:HB2	4:F:621:HOH:O	2.01	0.59
1:H:319:SER:OG	1:H:322:GLU:OE1	2.17	0.59
1:I:380:CYS:SG	1:I:405:ILE:HD12	2.43	0.59
1:H:404:PHE:HE1	1:H:406:THR:HB	1.68	0.59
1:J:250:GLY:HA3	1:J:272:PHE:CE1	2.38	0.58
1:C:149:GLY:HA2	1:C:177:PHE:O	2.03	0.58
1:F:142:ILE:HD11	1:F:147:ILE:HG12	1.84	0.58
1:F:324:VAL:O	1:F:328:ARG:HG2	2.02	0.58
1:I:273:HIS:CE1	1:I:275:ALA:HB2	2.38	0.58
1:G:389:PRO:HD2	1:G:456:TYR:CE2	2.38	0.58
1:H:180:ASN:HD21	1:H:195:MET:HE3	1.67	0.58
1:D:218:PHE:CZ	1:D:239:MET:HE3	2.38	0.58
1:F:200:ARG:HH22	1:F:240:LYS:HE3	1.68	0.58
1:G:392:ILE:HD12	1:G:392:ILE:H	1.69	0.58
1:H:197:GLN:NE2	1:H:234:TYR:OH	2.36	0.58
1:A:236:GLN:NE2	4:A:609:HOH:O	2.34	0.58
1:I:218:PHE:HZ	1:I:239:MET:HE3	1.69	0.58
1:H:331:LEU:HD21	1:H:381:PRO:CD	2.33	0.58
1:F:153:LYS:HZ3	1:F:409:GLY:HA3	1.68	0.58
1:F:363:GLU:OE2	4:F:604:HOH:O	2.17	0.58
1:A:410:ALA:HB3	1:B:49:PHE:CE1	2.38	0.58
1:F:184:GLN:O	1:F:219:ASN:ND2	2.34	0.58
1:H:331:LEU:CD2	1:H:381:PRO:HD3	2.34	0.58
1:I:19:MET:HE1	1:I:98:ILE:HD13	1.86	0.57
1:A:207:GLU:OE1	1:A:240:LYS:NZ	2.38	0.57
1:F:450:ARG:O	1:F:453:ILE:HG22	2.05	0.57
1:G:49:PHE:CE1	1:J:410:ALA:HB3	2.39	0.57
1:F:442:TYR:CD1	1:F:446:LYS:HD3	2.38	0.57
1:G:153:LYS:HE2	1:G:409:GLY:HA3	1.86	0.57
1:H:273:HIS:HE1	2:H:501:CAP:H51	1.69	0.57
1:H:383:ILE:HG12	1:H:395:PHE:CE2	2.39	0.57
1:C:68:ARG:HB3	1:C:77:TRP:HB2	1.87	0.57
1:G:149:GLY:HA2	1:G:177:PHE:O	2.04	0.57
1:H:40:VAL:HG13	1:H:102:VAL:HG11	1.85	0.57
1:J:105:MET:HB2	1:J:108:VAL:HG22	1.87	0.57
1:B:159:THR:HG21	1:E:121:GLN:HA	1.87	0.57
1:F:149:GLY:O	1:F:407:THR:HA	2.04	0.57
1:H:203:MET:HE3	1:H:214:LYS:H	1.69	0.57
1:A:149:GLY:HA2	1:A:177:PHE:O	2.05	0.57
1:G:313:ILE:HG23	1:G:391:LEU:HG	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:GLN:HB3	1:H:110:VAL:HB	1.87	0.57
1:A:68:ARG:HB3	1:A:77:TRP:HB2	1.87	0.57
1:B:236:GLN:NE2	4:B:601:HOH:O	2.17	0.57
1:G:46:THR:HG22	1:J:156:ILE:O	2.05	0.56
1:H:25:LEU:HD12	1:H:76:VAL:HG21	1.86	0.56
1:H:85:PHE:CZ	1:H:94:ILE:HG23	2.41	0.56
1:F:182:GLU:HG2	1:F:183:PRO:HD3	1.88	0.56
1:F:370:LEU:O	1:F:374:ARG:HD3	2.06	0.56
1:F:392:ILE:HD13	1:F:406:THR:HG21	1.87	0.56
1:E:320:PRO:O	1:E:324:VAL:HB	2.06	0.56
1:F:394:LYS:O	1:F:398:THR:HG23	2.05	0.56
1:H:52:ILE:HD12	1:H:52:ILE:N	2.19	0.56
1:A:423:ALA:O	1:A:426:VAL:HG12	2.05	0.56
1:I:37:ALA:HB2	1:I:76:VAL:HG21	1.87	0.56
1:I:94:ILE:HD11	1:I:126:TYR:OH	2.06	0.56
1:J:174:GLY:HA3	1:J:427:LEU:HD21	1.88	0.56
1:J:250:GLY:HA2	1:J:258:ILE:HD11	1.88	0.56
1:G:149:GLY:O	1:G:407:THR:HA	2.06	0.56
1:H:149:GLY:CA	1:H:177:PHE:O	2.54	0.56
1:E:442:TYR:CE2	1:E:446:LYS:HE3	2.41	0.56
1:A:399:VAL:HG22	1:A:401:THR:HG22	1.87	0.56
1:C:182:GLU:HG2	1:C:183:PRO:HD3	1.88	0.56
1:G:101:ASN:ND2	1:J:182:GLU:OE2	2.39	0.56
1:G:193:ASP:O	1:G:197:GLN:HG3	2.05	0.56
1:J:25:LEU:HD12	1:J:111:CYS:HA	1.88	0.56
1:C:121:GLN:HA	1:J:159:THR:HG21	1.87	0.56
1:D:347:ILE:HG13	4:I:609:HOH:O	2.06	0.56
1:B:212:LYS:NZ	4:B:606:HOH:O	2.32	0.55
1:D:388:ASN:HB2	1:D:389:PRO:HD2	1.87	0.55
1:J:383:ILE:HG12	1:J:395:PHE:CE2	2.41	0.55
1:J:388:ASN:HB2	1:J:389:PRO:HD2	1.87	0.55
1:A:136:MET:HE2	1:A:215:VAL:HG11	1.88	0.55
1:E:344:TRP:HB3	1:E:376:THR:HB	1.88	0.55
1:D:22:VAL:HG23	1:D:340:PHE:HE1	1.71	0.55
1:E:182:GLU:HG2	1:E:183:PRO:HD3	1.88	0.55
1:F:307:HIS:NE2	4:F:601:HOH:O	2.04	0.55
1:G:94:ILE:HD11	1:G:126:TYR:OH	2.06	0.55
1:B:320:PRO:O	1:B:324:VAL:HB	2.07	0.55
1:G:151:ILE:O	1:G:413:HIS:CE1	2.59	0.55
1:J:26:GLN:HB2	1:J:110:VAL:HB	1.88	0.55
1:E:159:THR:HG21	1:G:124:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:ILE:HG12	1:E:404:PHE:HZ	1.71	0.55
1:H:153:LYS:NZ	1:H:409:GLY:HA3	2.21	0.55
1:I:24:ARG:HB2	1:I:114:LEU:HD11	1.88	0.55
1:J:70:ASP:HB3	1:J:75:LEU:HB2	1.88	0.55
1:F:380:CYS:SG	1:F:405:ILE:HD12	2.47	0.55
1:H:256:MET:HE3	1:I:225:TYR:HE1	1.70	0.55
1:C:61:SER:OG	1:G:17:GLN:NE2	2.38	0.55
1:I:281:THR:HB	1:I:291:VAL:HG23	1.89	0.55
1:J:357:ALA:HA	1:J:360:LYS:HE2	1.87	0.55
1:G:142:ILE:HG21	1:G:145:ARG:NH2	2.22	0.55
1:A:320:PRO:O	1:A:324:VAL:HB	2.07	0.54
1:H:5:TYR:O	1:H:66:VAL:HG12	2.06	0.54
1:H:84:ILE:HB	1:I:156:ILE:HG21	1.88	0.54
1:J:351:ASP:OD2	1:J:354:LEU:N	2.37	0.54
1:D:22:VAL:HG23	1:D:340:PHE:CE1	2.42	0.54
1:D:410:ALA:HB3	1:F:49:PHE:CE1	2.42	0.54
1:J:200:ARG:NH1	1:J:238:MET:O	2.37	0.54
1:A:49:PHE:CE2	1:B:410:ALA:HB3	2.42	0.54
1:C:23:PHE:CE2	1:C:113:ILE:HG12	2.42	0.54
1:D:332:LYS:HB3	1:D:361:GLU:OE2	2.08	0.54
1:J:392:ILE:HD11	1:J:408:MET:HE1	1.90	0.54
1:B:149:GLY:HA2	1:B:177:PHE:O	2.07	0.54
1:B:423:ALA:O	1:B:426:VAL:HG12	2.07	0.54
1:C:141:ASN:O	1:C:141:ASN:ND2	2.34	0.54
1:E:383:ILE:HB	1:E:406:THR:HG22	1.88	0.54
1:G:97:PHE:CZ	1:J:156:ILE:HG13	2.43	0.54
1:G:152:ILE:HG21	1:G:163:TYR:CD1	2.43	0.54
1:G:156:ILE:O	1:J:46:THR:HG22	2.06	0.54
1:J:22:VAL:HG13	1:J:340:PHE:CZ	2.43	0.54
1:D:331:LEU:O	1:D:367:TYR:OH	2.24	0.54
1:E:1:MET:HG3	1:E:35:ASP:HA	1.90	0.54
1:H:19:MET:HE1	1:H:98:ILE:HD13	1.90	0.54
1:H:43:GLU:CD	1:H:101:ASN:HB2	2.32	0.54
1:G:380:CYS:SG	1:G:405:ILE:HD12	2.48	0.54
1:J:442:TYR:O	1:J:446:LYS:HD3	2.08	0.54
1:G:395:PHE:O	1:G:399:VAL:HG12	2.08	0.54
1:B:182:GLU:HG2	1:B:183:PRO:HD3	1.89	0.53
1:H:156:ILE:O	1:I:46:THR:HG22	2.09	0.53
1:E:136:MET:HE2	1:E:215:VAL:HG11	1.90	0.53
1:F:313:ILE:HG22	1:F:391:LEU:HD23	1.90	0.53
1:D:49:PHE:CE1	1:F:410:ALA:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ASN:OD1	1:F:92:GLN:HG3	2.08	0.53
1:G:56:THR:HG22	1:G:58:PHE:H	1.74	0.53
1:H:383:ILE:HD13	1:H:404:PHE:CD1	2.44	0.53
1:F:396:ILE:HG12	1:F:404:PHE:HZ	1.73	0.53
1:D:347:ILE:HG12	1:D:348:PRO:HD2	1.90	0.53
1:E:332:LYS:NZ	4:E:606:HOH:O	2.29	0.53
1:H:128:GLY:C	1:H:302:GLY:HA2	2.34	0.53
1:J:307:HIS:ND1	2:J:502:CAP:O4P	2.37	0.53
1:D:308:THR:HG23	1:D:326:ALA:HB3	1.91	0.53
1:D:388:ASN:HA	1:D:408:MET:HE3	1.89	0.53
1:E:250:GLY:HA3	1:E:272:PHE:CE1	2.44	0.53
1:A:395:PHE:O	1:A:399:VAL:HG12	2.09	0.53
1:C:46:THR:HG22	1:E:156:ILE:O	2.08	0.53
1:H:147:ILE:HB	1:H:405:ILE:HG13	1.90	0.53
1:J:422:GLY:O	1:J:426:VAL:HG23	2.09	0.53
1:B:349:GLU:HA	1:B:354:LEU:HD23	1.90	0.52
1:H:43:GLU:OE2	1:H:101:ASN:HB2	2.09	0.52
1:H:153:LYS:HZ3	1:H:409:GLY:HA3	1.75	0.52
1:J:395:PHE:O	1:J:399:VAL:HG22	2.08	0.52
1:D:149:GLY:HA2	1:D:177:PHE:O	2.09	0.52
1:I:218:PHE:CZ	1:I:239:MET:HE3	2.44	0.52
1:J:94:ILE:HD11	1:J:126:TYR:OH	2.09	0.52
1:J:383:ILE:HG12	1:J:395:PHE:CZ	2.44	0.52
1:J:401:THR:OG1	4:J:601:HOH:O	2.16	0.52
1:A:182:GLU:HG2	1:A:183:PRO:HD3	1.91	0.52
1:F:250:GLY:HA3	1:F:272:PHE:CE1	2.45	0.52
1:G:334:TYR:HB3	1:G:361:GLU:OE2	2.09	0.52
1:H:153:LYS:HZ3	1:H:409:GLY:CA	2.23	0.52
1:J:207:GLU:OE1	1:J:240:LYS:NZ	2.41	0.52
1:A:383:ILE:HG22	1:A:387:LEU:HD11	1.91	0.52
1:E:149:GLY:CA	1:E:177:PHE:O	2.58	0.52
1:G:162:GLU:HG2	1:I:348:PRO:CD	2.36	0.52
1:G:432:ALA:HB2	1:G:442:TYR:CD1	2.44	0.52
1:I:396:ILE:HG12	1:I:404:PHE:HZ	1.75	0.52
1:C:67:TYR:CE1	1:C:77:TRP:HB3	2.44	0.52
1:C:197:GLN:HG2	1:C:238:MET:CE	2.40	0.52
1:F:455:PHE:HD1	1:F:455:PHE:O	1.93	0.52
1:H:24:ARG:HH12	1:H:114:LEU:HD21	1.73	0.52
1:H:47:GLY:HA2	1:H:52:ILE:HD11	1.91	0.52
1:H:258:ILE:HG23	1:H:270:LEU:HD21	1.91	0.52
1:H:324:VAL:HG13	1:H:399:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:ILE:CG1	1:H:374:ARG:HB2	2.39	0.52
1:B:92:GLN:O	1:B:96:THR:OG1	2.22	0.52
1:B:347:ILE:HD13	1:B:374:ARG:HA	1.91	0.52
1:F:94:ILE:HD11	1:F:126:TYR:OH	2.09	0.52
1:I:388:ASN:HA	1:I:408:MET:HE3	1.91	0.52
1:C:66:VAL:HG22	1:C:78:ILE:HG12	1.92	0.52
1:H:154:PRO:HD2	1:H:158:LEU:HD11	1.91	0.52
1:B:90:ASN:OD1	1:B:92:GLN:HG3	2.10	0.52
1:C:23:PHE:HD2	4:C:639:HOH:O	1.92	0.52
1:D:250:GLY:HA3	1:D:272:PHE:CE1	2.45	0.52
1:G:5:TYR:O	1:G:66:VAL:HG12	2.10	0.52
1:G:37:ALA:HB2	1:G:76:VAL:HG21	1.91	0.52
1:G:182:GLU:HG2	1:G:183:PRO:HD3	1.90	0.52
1:J:281:THR:HG21	1:J:294:LEU:HD22	1.92	0.52
1:E:387:LEU:HB3	1:E:408:MET:HE2	1.92	0.51
1:F:383:ILE:HG13	1:F:395:PHE:HE2	1.75	0.51
1:J:219:ASN:HA	1:J:247:LEU:HB3	1.91	0.51
1:B:68:ARG:HB3	1:B:77:TRP:HB2	1.92	0.51
1:E:201:HIS:HB3	1:G:373:TRP:CD1	2.45	0.51
1:E:383:ILE:HG22	1:E:387:LEU:HD11	1.93	0.51
1:G:163:TYR:OH	1:G:216:HIS:NE2	2.32	0.51
1:H:274:ARG:NH2	2:H:501:CAP:O5P	2.38	0.51
1:B:67:TYR:CZ	1:B:77:TRP:HB3	2.46	0.51
1:D:136:MET:HE2	1:D:215:VAL:HG11	1.93	0.51
1:G:25:LEU:HD23	1:G:111:CYS:HA	1.92	0.51
1:H:178:VAL:O	1:H:216:HIS:HA	2.11	0.51
1:I:415:HIS:HE1	1:I:417:MET:HE3	1.75	0.51
1:D:51:LYS:H	1:D:51:LYS:CD	2.23	0.51
1:G:174:GLY:HA3	1:G:427:LEU:HD11	1.92	0.51
1:I:28:GLU:HA	1:I:109:LYS:HE2	1.93	0.51
1:E:399:VAL:HG22	1:E:401:THR:HG22	1.93	0.51
1:E:423:ALA:O	1:E:427:LEU:HG	2.10	0.51
1:J:137:ARG:HH21	1:J:403:ASP:HA	1.74	0.51
1:J:282:ARG:NH2	1:J:284:GLU:OE2	2.44	0.51
1:B:7:GLN:OE1	1:B:10:ASN:ND2	2.42	0.51
1:D:86:ASP:HB3	1:D:90:ASN:HB3	1.92	0.51
1:E:389:PRO:HG3	1:E:426:VAL:HG12	1.92	0.51
1:G:93:ASN:ND2	1:J:183:PRO:O	2.43	0.51
1:H:151:ILE:HG13	1:H:407:THR:OG1	2.10	0.51
1:H:201:HIS:HB3	1:J:373:TRP:CD2	2.45	0.51
1:I:203:MET:SD	1:I:243:SER:OG	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:ARG:HG3	1:D:375:ILE:HG23	1.93	0.51
1:G:331:LEU:O	1:G:367:TYR:OH	2.17	0.51
1:H:134:ASP:O	1:H:138:LYS:HG2	2.10	0.51
1:H:273:HIS:CD2	1:H:275:ALA:HB2	2.46	0.51
1:H:307:HIS:HA	1:H:382:ILE:O	2.11	0.51
1:J:378:LYS:NZ	1:J:403:ASP:OD2	2.43	0.51
1:B:90:ASN:HD21	1:B:92:GLN:HE21	1.58	0.50
1:I:222:SER:HB3	1:I:227:THR:HB	1.93	0.50
1:J:299:ARG:NH1	1:J:329:HIS:O	2.39	0.50
1:C:254:GLY:HA3	1:E:254:GLY:HA3	1.94	0.50
1:E:158:LEU:HD12	1:E:158:LEU:H	1.76	0.50
1:H:86:ASP:HB3	1:H:90:ASN:HB3	1.92	0.50
1:I:142:ILE:HD11	1:I:147:ILE:HG13	1.93	0.50
1:C:149:GLY:CA	1:C:177:PHE:O	2.59	0.50
1:E:113:ILE:O	1:E:290:THR:HG23	2.11	0.50
1:H:133:ILE:HD13	1:H:380:CYS:SG	2.51	0.50
1:H:306:ILE:HG22	1:H:379:MET:HE3	1.92	0.50
1:J:347:ILE:CG1	1:J:374:ARG:HB2	2.39	0.50
1:D:309:GLY:O	4:D:602:HOH:O	2.19	0.50
1:F:5:TYR:O	1:F:66:VAL:HG12	2.10	0.50
1:F:273:HIS:CE1	1:F:275:ALA:HB2	2.47	0.50
1:I:155:LYS:HZ3	1:I:181:ASP:CG	2.18	0.50
1:J:450:ARG:O	1:J:454:GLN:HG2	2.11	0.50
1:F:137:ARG:HH21	1:F:403:ASP:HA	1.76	0.50
1:I:145:ARG:NH2	1:I:176:ASP:OD2	2.44	0.50
1:D:18:TYR:HE2	1:D:65:LEU:HD13	1.75	0.50
1:E:392:ILE:HG12	1:E:408:MET:HE1	1.93	0.50
1:G:1:MET:HE3	1:G:3:LYS:HB2	1.93	0.50
1:G:324:VAL:HG23	1:G:399:VAL:HA	1.94	0.50
1:H:71:GLU:CD	1:H:71:GLU:H	2.20	0.50
1:H:219:ASN:HA	1:H:247:LEU:HB3	1.94	0.50
1:H:272:PHE:O	1:H:306:ILE:HG13	2.10	0.50
1:I:66:VAL:HG22	1:I:78:ILE:HG12	1.94	0.50
1:J:311:ALA:HB1	1:J:320:PRO:HA	1.94	0.50
1:B:383:ILE:HB	1:B:406:THR:HG22	1.94	0.50
1:I:153:LYS:NZ	1:I:181:ASP:OD2	2.41	0.50
1:I:344:TRP:HB3	1:I:376:THR:HB	1.94	0.50
1:J:389:PRO:HA	1:J:392:ILE:HD13	1.92	0.50
1:I:57:ALA:O	1:I:61:SER:OG	2.28	0.50
1:B:20:LEU:HD13	1:B:117:TYR:HD2	1.76	0.50
1:B:201:HIS:HB3	1:E:373:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:THR:HG23	1:D:108:VAL:HG12	1.93	0.50
1:F:432:ALA:HB2	1:F:442:TYR:CD1	2.47	0.50
1:H:105:MET:HB2	1:H:108:VAL:HG22	1.93	0.50
1:J:19:MET:HE1	1:J:98:ILE:HD13	1.93	0.50
1:J:116:VAL:O	1:J:296:LYS:HE2	2.12	0.50
1:J:139:TYR:CE2	1:J:213:THR:HB	2.47	0.50
1:J:370:LEU:HD23	1:J:375:ILE:HG21	1.93	0.50
1:C:383:ILE:HG13	1:C:395:PHE:CE2	2.46	0.49
1:D:113:ILE:O	1:D:290:THR:HG23	2.11	0.49
1:C:58:PHE:CE2	1:G:17:GLN:HG2	2.48	0.49
1:C:422:GLY:O	1:C:426:VAL:HG23	2.12	0.49
1:D:113:ILE:HD12	1:D:288:GLY:O	2.11	0.49
1:G:133:ILE:HD12	1:G:380:CYS:SG	2.51	0.49
1:H:110:VAL:HG22	1:H:286:PRO:HB2	1.93	0.49
1:J:320:PRO:O	1:J:324:VAL:HB	2.12	0.49
1:C:94:ILE:HD11	1:C:126:TYR:OH	2.13	0.49
1:C:254:GLY:HA3	1:E:253:ALA:O	2.11	0.49
1:D:207:GLU:OE1	1:D:240:LYS:NZ	2.42	0.49
1:E:423:ALA:O	1:E:426:VAL:HG22	2.13	0.49
1:F:70:ASP:HB3	1:F:75:LEU:HB2	1.95	0.49
1:G:410:ALA:HB1	1:J:50:VAL:HG12	1.93	0.49
1:I:408:MET:HE2	1:I:412:VAL:HG23	1.94	0.49
1:F:168:TYR:HE2	1:F:205:ARG:HG2	1.76	0.49
1:H:49:PHE:CE1	1:I:410:ALA:HB3	2.47	0.49
1:I:152:ILE:HD11	1:I:178:VAL:HG13	1.94	0.49
1:H:88:GLY:O	1:H:263:ARG:NH2	2.38	0.49
1:C:156:ILE:O	1:E:46:THR:HG22	2.13	0.49
1:D:190:CYS:SG	4:D:619:HOH:O	2.60	0.49
1:E:23:PHE:HB2	1:E:76:VAL:HG13	1.94	0.49
1:E:162:GLU:O	1:E:166:LEU:HD13	2.12	0.49
1:B:383:ILE:HG22	1:B:387:LEU:HD11	1.95	0.49
1:E:315:LYS:HE3	1:E:316:MET:HE2	1.95	0.49
1:G:239:MET:HB2	1:G:244:TYR:CD2	2.47	0.49
1:H:112:LYS:HA	1:H:288:GLY:O	2.13	0.49
1:J:130:GLU:O	1:J:377:LYS:NZ	2.34	0.49
1:E:67:TYR:CZ	1:E:77:TRP:HB3	2.47	0.49
1:G:291:VAL:O	1:G:295:THR:OG1	2.26	0.49
1:I:366:ASP:OD1	1:I:378:LYS:NZ	2.45	0.49
1:J:130:GLU:HB2	1:J:262:ARG:CZ	2.42	0.49
1:A:26:GLN:HB3	1:A:110:VAL:HB	1.94	0.49
1:A:201:HIS:HB3	1:F:373:TRP:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:HB3	1:B:75:LEU:HB2	1.95	0.49
1:D:313:ILE:HD12	1:D:394:LYS:HE2	1.94	0.49
1:I:128:GLY:C	1:I:302:GLY:HA2	2.38	0.49
1:C:121:GLN:NE2	1:G:56:THR:HG21	2.27	0.49
1:D:325:MET:SD	4:D:603:HOH:O	2.60	0.49
1:F:25:LEU:HA	1:F:110:VAL:O	2.13	0.49
1:H:47:GLY:HA2	1:H:52:ILE:CD1	2.43	0.49
1:H:313:ILE:HD12	1:H:395:PHE:HD1	1.76	0.49
1:F:307:HIS:HA	1:F:382:ILE:O	2.13	0.48
1:H:343:ILE:O	1:H:343:ILE:HG13	2.11	0.48
1:A:381:PRO:HG2	1:A:404:PHE:HB3	1.94	0.48
1:D:87:ARG:NH1	1:F:188:ASP:HB3	2.27	0.48
1:E:70:ASP:HB3	1:E:75:LEU:HB2	1.95	0.48
1:F:22:VAL:HG23	1:F:114:LEU:HB2	1.94	0.48
1:F:315:LYS:HE3	1:F:316:MET:HE2	1.94	0.48
1:F:328:ARG:NH1	4:F:603:HOH:O	2.45	0.48
1:H:182:GLU:HG2	1:H:183:PRO:HD3	1.95	0.48
1:J:356:LEU:O	4:J:602:HOH:O	2.20	0.48
1:D:24:ARG:NH2	4:D:609:HOH:O	2.45	0.48
1:A:256:MET:HE1	1:B:228:MET:HE2	1.95	0.48
1:C:28:GLU:HG2	1:C:31:MET:SD	2.53	0.48
1:F:105:MET:HB2	1:F:108:VAL:HG22	1.96	0.48
1:J:303:ALA:HB3	1:J:379:MET:HE3	1.95	0.48
1:F:168:TYR:CD1	1:F:168:TYR:C	2.91	0.48
1:F:328:ARG:HD2	1:F:332:LYS:HD2	1.96	0.48
1:F:383:ILE:HG13	1:F:395:PHE:CE2	2.48	0.48
1:G:142:ILE:HG21	1:G:145:ARG:HH21	1.79	0.48
1:H:6:ILE:HA	1:H:66:VAL:CG1	2.43	0.48
1:I:150:SER:OG	1:I:413:HIS:HE1	1.96	0.48
1:A:149:GLY:CA	1:A:177:PHE:O	2.62	0.48
1:B:258:ILE:HG23	1:B:270:LEU:HD21	1.95	0.48
1:G:292:PRO:HB3	1:G:329:HIS:HD2	1.79	0.48
1:G:387:LEU:HD13	1:G:391:LEU:HB3	1.95	0.48
1:J:149:GLY:O	1:J:407:THR:HA	2.13	0.48
1:C:36:THR:HG23	1:C:108:VAL:HG22	1.95	0.48
1:C:388:ASN:HA	1:C:408:MET:HE3	1.95	0.48
1:G:437:ILE:HG22	1:G:442:TYR:HB2	1.96	0.48
1:C:410:ALA:HB3	1:E:49:PHE:CE2	2.47	0.48
1:D:171:TRP:HB3	1:D:206:VAL:HG11	1.95	0.48
1:D:437:ILE:HG22	1:D:438:SER:O	2.12	0.48
1:H:203:MET:O	1:H:207:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:GLY:CA	1:J:177:PHE:O	2.61	0.48
1:A:409:GLY:N	2:A:501:CAP:O1P	2.40	0.48
1:G:273:HIS:CD2	1:G:275:ALA:HB2	2.48	0.48
1:I:182:GLU:HG2	1:I:183:PRO:HD3	1.95	0.48
1:B:347:ILE:HD12	1:D:161:SER:HB3	1.96	0.48
1:H:151:ILE:HB	1:H:153:LYS:HZ2	1.76	0.48
1:H:156:ILE:HG21	1:I:84:ILE:HB	1.96	0.48
1:I:58:PHE:HB2	1:J:121:GLN:HG3	1.96	0.48
1:J:22:VAL:HG21	1:J:339:TYR:CD1	2.49	0.48
1:J:90:ASN:OD1	1:J:92:GLN:HG3	2.14	0.47
1:J:445:ASP:OD1	1:J:445:ASP:N	2.44	0.47
1:D:94:ILE:HD11	1:D:126:TYR:OH	2.14	0.47
1:G:66:VAL:HG23	1:G:76:VAL:HG13	1.95	0.47
1:H:183:PRO:HB2	1:I:97:PHE:CZ	2.49	0.47
1:I:150:SER:HB2	1:I:170:PHE:CE1	2.47	0.47
1:E:281:THR:HB	1:E:291:VAL:HG23	1.96	0.47
1:G:97:PHE:CE1	1:J:156:ILE:HG13	2.49	0.47
1:G:113:ILE:H	1:G:113:ILE:HD12	1.78	0.47
1:H:183:PRO:HB2	1:I:97:PHE:CE1	2.48	0.47
1:A:139:TYR:OH	1:A:243:SER:HB3	2.14	0.47
1:B:409:GLY:N	2:B:501:CAP:O1P	2.40	0.47
1:G:399:VAL:HG22	1:G:401:THR:HG22	1.95	0.47
1:H:203:MET:HE2	1:H:207:GLU:OE2	2.13	0.47
1:A:165:GLU:HB2	1:F:347:ILE:HD12	1.97	0.47
1:H:236:GLN:HG2	1:H:244:TYR:CE2	2.49	0.47
1:H:410:ALA:HB3	1:I:49:PHE:HE1	1.79	0.47
1:J:336:GLU:CD	1:J:341:LYS:HZ2	2.21	0.47
1:G:250:GLY:HA3	1:G:272:PHE:CE1	2.50	0.47
1:G:445:ASP:OD1	1:G:445:ASP:N	2.48	0.47
1:J:298:ALA:HB1	1:J:379:MET:HE1	1.96	0.47
1:B:25:LEU:HA	1:B:110:VAL:O	2.14	0.47
1:B:201:HIS:HB3	1:E:373:TRP:HD1	1.79	0.47
1:D:170:PHE:CE2	1:D:175:GLY:HA3	2.49	0.47
1:E:306:ILE:HG22	1:E:379:MET:HE3	1.95	0.47
1:F:199:VAL:HG11	1:F:216:HIS:CD2	2.44	0.47
1:G:258:ILE:HG23	1:G:270:LEU:HD21	1.97	0.47
1:G:349:GLU:HA	1:G:354:LEU:HD23	1.96	0.47
1:G:408:MET:HE2	1:G:412:VAL:HG23	1.95	0.47
1:J:184:GLN:O	1:J:219:ASN:ND2	2.28	0.47
1:C:124:VAL:HG21	1:J:159:THR:HB	1.97	0.47
1:C:171:TRP:HB3	1:C:206:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:VAL:O	1:E:328:ARG:HG2	2.14	0.47
1:H:170:PHE:CE2	1:H:175:GLY:HA3	2.50	0.47
1:J:132:THR:CG2	1:J:377:LYS:HD3	2.45	0.47
1:A:273:HIS:CE1	1:A:275:ALA:HB2	2.49	0.47
1:A:383:ILE:HG13	1:A:395:PHE:CE2	2.50	0.47
1:B:315:LYS:HE3	1:B:316:MET:HE2	1.96	0.47
1:D:67:TYR:CZ	1:D:77:TRP:HB3	2.50	0.47
1:E:395:PHE:O	1:E:399:VAL:HG12	2.15	0.47
1:F:148:PHE:HB2	4:F:610:HOH:O	2.14	0.47
1:F:442:TYR:CE1	1:F:446:LYS:HD3	2.50	0.47
1:G:29:GLU:OE1	1:G:29:GLU:N	2.44	0.47
1:H:22:VAL:HG11	1:H:339:TYR:CE2	2.50	0.47
1:G:137:ARG:NH1	1:G:145:ARG:O	2.29	0.47
1:H:321:LYS:NZ	1:H:325:MET:HE2	2.30	0.47
1:I:31:MET:HE3	1:I:35:ASP:OD2	2.14	0.47
1:A:223:SER:HB2	1:B:259:GLN:HE22	1.80	0.46
1:A:244:TYR:O	4:A:601:HOH:O	2.20	0.46
1:D:101:ASN:ND2	1:F:182:GLU:OE2	2.49	0.46
1:H:120:PRO:O	1:H:124:VAL:HG23	2.15	0.46
1:H:423:ALA:O	1:H:426:VAL:HG22	2.15	0.46
1:A:156:ILE:O	1:B:46:THR:HG22	2.14	0.46
1:B:417:MET:HE1	1:B:447:GLU:HG2	1.97	0.46
1:D:18:TYR:CE2	1:D:65:LEU:HD13	2.50	0.46
1:E:308:THR:HG22	1:E:326:ALA:HB1	1.97	0.46
1:G:18:TYR:CE1	1:G:81:PRO:HG3	2.51	0.46
1:H:350:LYS:HD2	1:H:350:LYS:O	2.16	0.46
1:F:158:LEU:HD23	1:F:162:GLU:HB3	1.97	0.46
1:H:43:GLU:HG3	1:H:102:VAL:HG13	1.97	0.46
1:I:371:GLY:O	1:I:375:ILE:HG12	2.15	0.46
1:J:27:GLY:HA2	1:J:108:VAL:HA	1.97	0.46
1:D:373:TRP:HZ3	1:I:161:SER:O	1.98	0.46
1:G:159:THR:HG22	1:G:189:PHE:O	2.14	0.46
1:G:183:PRO:HB2	1:J:97:PHE:CZ	2.50	0.46
1:C:22:VAL:HG23	1:C:340:PHE:CE1	2.51	0.46
1:F:145:ARG:HH22	1:F:176:ASP:CG	2.22	0.46
1:I:141:ASN:O	1:I:141:ASN:ND2	2.41	0.46
1:J:193:ASP:O	1:J:197:GLN:HG3	2.15	0.46
1:D:334:TYR:OH	1:D:336:GLU:OE2	2.33	0.46
1:G:171:TRP:HB3	1:G:206:VAL:HG11	1.97	0.46
1:D:290:THR:OG1	1:D:292:PRO:HD2	2.16	0.46
1:E:171:TRP:HB3	1:E:206:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:TYR:CZ	1:E:446:LYS:HE3	2.51	0.46
1:F:26:GLN:O	1:F:109:LYS:N	2.38	0.46
1:F:178:VAL:O	1:F:216:HIS:ND1	2.46	0.46
1:A:113:ILE:O	1:A:290:THR:HG23	2.16	0.46
1:B:133:ILE:HD12	1:B:380:CYS:SG	2.56	0.46
1:E:449:LEU:O	1:E:453:ILE:HG13	2.16	0.46
1:F:344:TRP:HB3	1:F:376:THR:HB	1.97	0.46
1:H:187:GLN:OE1	1:H:187:GLN:N	2.45	0.46
1:I:142:ILE:HG21	1:I:145:ARG:HH21	1.80	0.46
1:J:152:ILE:HD12	1:J:166:LEU:HB2	1.97	0.46
1:A:250:GLY:HA3	1:A:272:PHE:CE1	2.51	0.46
1:D:43:GLU:O	1:F:155:LYS:NZ	2.44	0.46
1:D:70:ASP:OD2	1:D:73:ASN:HB2	2.15	0.46
1:F:153:LYS:NZ	1:F:409:GLY:HA3	2.31	0.46
1:H:67:TYR:CZ	1:H:77:TRP:HB3	2.51	0.46
1:H:163:TYR:OH	1:H:216:HIS:NE2	2.47	0.46
1:J:118:PHE:HZ	1:J:297:PHE:CE1	2.34	0.46
1:B:121:GLN:HA	1:D:159:THR:HG21	1.98	0.46
1:G:67:TYR:CZ	1:G:77:TRP:HB3	2.51	0.46
1:H:48:SER:OG	2:I:502:CAP:O2P	2.31	0.46
1:E:165:GLU:HA	1:G:373:TRP:HH2	1.81	0.45
1:E:445:ASP:OD1	1:E:445:ASP:N	2.49	0.45
1:F:49:PHE:CD2	1:F:50:VAL:HG23	2.51	0.45
1:F:168:TYR:HB2	1:F:202:ALA:HB1	1.98	0.45
1:G:28:GLU:N	1:G:107:SER:O	2.49	0.45
1:H:205:ARG:NH1	1:J:369:ASN:O	2.49	0.45
1:I:325:MET:SD	1:I:337:GLY:HA2	2.56	0.45
1:J:113:ILE:O	1:J:290:THR:HG23	2.17	0.45
1:J:222:SER:HB3	1:J:227:THR:HB	1.97	0.45
1:J:274:ARG:NH1	4:J:606:HOH:O	2.48	0.45
1:A:108:VAL:HG11	1:A:111:CYS:HB2	1.98	0.45
1:B:19:MET:HE1	1:B:98:ILE:HD13	1.97	0.45
1:B:306:ILE:HG22	1:B:379:MET:HE3	1.96	0.45
1:E:443:ALA:HA	1:E:446:LYS:HB2	1.97	0.45
1:G:25:LEU:HA	1:G:110:VAL:O	2.16	0.45
1:G:146:PRO:HD3	1:G:402:GLN:OE1	2.16	0.45
1:H:272:PHE:CD1	1:H:272:PHE:C	2.94	0.45
1:J:250:GLY:CA	1:J:258:ILE:HD11	2.45	0.45
1:A:223:SER:HB2	1:B:259:GLN:NE2	2.31	0.45
1:A:224:ASP:OD1	1:A:227:THR:OG1	2.21	0.45
1:E:71:GLU:OE1	4:E:601:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:TYR:HB2	1:I:225:TYR:CD2	2.51	0.45
1:F:133:ILE:HD12	1:F:380:CYS:SG	2.57	0.45
1:H:245:ALA:HB1	1:H:269:PHE:HD2	1.81	0.45
1:I:19:MET:HE3	1:I:116:VAL:HG21	1.98	0.45
1:I:308:THR:HG23	1:I:326:ALA:HB3	1.98	0.45
1:A:36:THR:HG23	1:A:108:VAL:HG22	1.98	0.45
1:D:104:GLY:HA2	1:F:282:ARG:HD3	1.98	0.45
1:D:285:ASN:HD21	1:F:287:ILE:HB	1.81	0.45
1:G:315:LYS:HE3	1:G:316:MET:HE2	1.99	0.45
1:I:171:TRP:CZ2	1:I:178:VAL:HB	2.51	0.45
1:J:128:GLY:C	1:J:302:GLY:HA2	2.42	0.45
1:J:178:VAL:O	1:J:216:HIS:HA	2.17	0.45
1:A:159:THR:HG21	1:F:121:GLN:HA	1.97	0.45
1:D:28:GLU:HG2	1:D:31:MET:SD	2.57	0.45
1:F:94:ILE:O	1:F:98:ILE:HG13	2.16	0.45
1:G:239:MET:HB2	1:G:244:TYR:HD2	1.81	0.45
1:H:274:ARG:HB2	1:H:277:HIS:HB3	1.99	0.45
1:I:395:PHE:HA	1:I:398:THR:HG22	1.97	0.45
1:B:22:VAL:HG23	1:B:340:PHE:CE2	2.51	0.45
1:H:97:PHE:CZ	1:I:183:PRO:HB2	2.52	0.45
1:I:320:PRO:O	1:I:324:VAL:HB	2.17	0.45
1:I:347:ILE:HG13	1:I:374:ARG:HB2	1.98	0.45
1:A:195:MET:HE3	1:A:195:MET:HB3	1.86	0.45
1:B:37:ALA:HB2	1:B:76:VAL:HG11	1.99	0.45
1:C:2:GLN:O	1:C:38:SER:HB2	2.16	0.45
1:D:24:ARG:HB2	1:D:114:LEU:HD11	1.99	0.45
1:E:193:ASP:O	1:E:197:GLN:HG3	2.17	0.45
1:H:327:ALA:O	1:H:331:LEU:HD23	2.17	0.45
1:D:112:LYS:HA	1:D:112:LYS:HD2	1.56	0.45
1:E:108:VAL:HG11	1:E:111:CYS:HB2	1.99	0.45
1:E:322:GLU:H	1:E:322:GLU:HG2	1.39	0.45
1:G:392:ILE:N	4:G:605:HOH:O	2.50	0.45
1:I:361:GLU:HG3	1:I:362:ALA:N	2.31	0.45
1:B:296:LYS:HZ1	1:B:342:GLN:HB2	1.80	0.45
1:C:49:PHE:CE1	1:E:410:ALA:HB3	2.52	0.45
1:E:165:GLU:HB2	1:G:347:ILE:HD12	1.99	0.45
1:F:176:ASP:N	4:F:610:HOH:O	2.36	0.45
1:F:193:ASP:O	1:F:197:GLN:HG3	2.17	0.45
1:G:19:MET:HE3	1:G:116:VAL:HG21	1.99	0.45
1:G:149:GLY:CA	1:G:177:PHE:O	2.65	0.45
1:G:274:ARG:HB2	1:G:277:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:GLU:HG2	1:G:355:GLN:HE22	1.82	0.45
1:H:20:LEU:HD23	1:H:117:TYR:CD2	2.46	0.45
1:H:217:SER:HA	1:H:245:ALA:HB3	1.99	0.45
1:H:310:THR:HB	1:H:387:LEU:HD11	1.99	0.45
1:I:152:ILE:N	1:I:152:ILE:HD12	2.32	0.45
1:I:153:LYS:HA	1:I:154:PRO:C	2.42	0.45
1:J:51:LYS:HD3	1:J:52:ILE:N	2.32	0.45
1:I:34:VAL:HG22	1:I:69:ILE:HD13	1.98	0.44
1:I:156:ILE:HD11	1:I:184:GLN:HA	1.98	0.44
1:A:203:MET:HE2	1:A:214:LYS:C	2.42	0.44
1:B:383:ILE:HG13	1:B:395:PHE:CE2	2.53	0.44
1:F:68:ARG:HD2	1:F:77:TRP:CD2	2.53	0.44
1:J:90:ASN:HD21	1:J:92:GLN:HE21	1.64	0.44
1:A:236:GLN:HG2	1:A:244:TYR:OH	2.17	0.44
1:A:258:ILE:HG23	1:A:270:LEU:HD21	2.00	0.44
1:B:149:GLY:CA	1:B:177:PHE:O	2.66	0.44
1:E:22:VAL:HG11	1:E:339:TYR:CE2	2.53	0.44
1:E:169:ASP:HB3	1:E:419:THR:HB	1.99	0.44
1:F:22:VAL:HG12	1:F:77:TRP:CD1	2.53	0.44
1:H:143:GLN:O	1:H:144:GLU:HB3	2.18	0.44
1:I:93:ASN:OD1	1:I:97:PHE:HE1	2.01	0.44
1:I:139:TYR:OH	1:I:243:SER:HB2	2.18	0.44
1:J:381:PRO:HG2	1:J:404:PHE:HB3	1.98	0.44
1:J:396:ILE:HG12	1:J:404:PHE:HZ	1.82	0.44
1:B:170:PHE:CE2	1:B:175:GLY:HA3	2.52	0.44
1:C:373:TRP:CE3	1:J:201:HIS:HB3	2.51	0.44
1:E:170:PHE:CE2	1:E:175:GLY:HA3	2.52	0.44
1:F:152:ILE:HD12	1:F:166:LEU:HB3	1.99	0.44
1:G:170:PHE:CE2	1:G:175:GLY:HA3	2.52	0.44
1:H:105:MET:O	1:H:108:VAL:HG22	2.18	0.44
1:H:254:GLY:HA3	1:I:253:ALA:O	2.15	0.44
1:J:360:LYS:HB3	1:J:365:GLU:HB2	1.99	0.44
1:E:24:ARG:HB2	1:E:114:LEU:HD11	1.99	0.44
1:F:272:PHE:CD1	1:F:272:PHE:C	2.96	0.44
1:J:170:PHE:CE2	1:J:175:GLY:HA3	2.53	0.44
1:A:43:GLU:HG3	1:A:105:MET:SD	2.58	0.44
1:A:179:KCX:OQ1	2:A:501:CAP:O3	2.36	0.44
1:E:328:ARG:HD2	1:E:332:LYS:HD2	2.00	0.44
1:G:90:ASN:OD1	1:G:92:GLN:HG3	2.17	0.44
1:G:314:GLY:HA3	1:G:385:GLY:O	2.18	0.44
1:H:197:GLN:HG2	1:H:238:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:356:LEU:HA	1:H:359:GLN:OE1	2.18	0.44
1:E:102:VAL:HA	1:E:105:MET:HE2	2.00	0.44
1:F:153:LYS:NZ	2:F:501:CAP:O1	2.50	0.44
1:H:281:THR:HA	1:H:289:TYR:O	2.17	0.44
1:H:383:ILE:N	1:H:383:ILE:HD12	2.33	0.44
1:C:116:VAL:O	1:C:296:LYS:NZ	2.39	0.44
1:H:151:ILE:HD13	2:H:501:CAP:O2	2.18	0.44
1:J:133:ILE:HD12	1:J:380:CYS:SG	2.58	0.44
1:J:307:HIS:HA	1:J:382:ILE:O	2.18	0.44
1:A:58:PHE:O	1:A:61:SER:OG	2.28	0.44
1:B:203:MET:HE2	1:B:214:LYS:C	2.42	0.44
1:D:392:ILE:O	1:D:396:ILE:HG13	2.18	0.44
1:E:205:ARG:NH2	1:G:369:ASN:O	2.50	0.44
1:E:296:LYS:HZ1	1:E:342:GLN:HB2	1.82	0.44
1:H:256:MET:HE3	1:I:225:TYR:CE1	2.51	0.44
1:H:272:PHE:C	1:H:272:PHE:HD1	2.25	0.44
1:J:140:LEU:HB3	1:J:142:ILE:HG23	2.00	0.44
1:B:381:PRO:HG2	1:B:404:PHE:HB3	2.00	0.43
1:E:177:PHE:HE1	1:E:179:KCX:HB2	1.83	0.43
1:F:281:THR:HB	1:F:291:VAL:HG23	2.00	0.43
1:G:310:THR:O	1:G:313:ILE:HB	2.18	0.43
1:I:26:GLN:HB3	1:I:110:VAL:HB	1.99	0.43
1:C:49:PHE:HD1	1:C:49:PHE:H	1.66	0.43
1:C:69:ILE:CD1	1:C:76:VAL:HG22	2.48	0.43
1:E:373:TRP:HH2	1:E:374:ARG:HH21	1.62	0.43
1:G:167:CYS:SG	1:G:178:VAL:HG11	2.58	0.43
1:C:31:MET:SD	1:C:107:SER:HB2	2.58	0.43
1:G:307:HIS:HA	1:G:382:ILE:O	2.18	0.43
1:H:85:PHE:CD2	1:H:94:ILE:HG12	2.53	0.43
1:H:167:CYS:SG	1:H:178:VAL:HG11	2.59	0.43
1:I:86:ASP:HB3	1:I:90:ASN:HB3	1.99	0.43
1:J:281:THR:HA	1:J:289:TYR:O	2.19	0.43
1:A:68:ARG:O	1:A:69:ILE:HD12	2.18	0.43
1:C:43:GLU:HG3	1:C:105:MET:SD	2.59	0.43
1:C:156:ILE:HG21	1:E:84:ILE:HB	2.01	0.43
1:D:156:ILE:O	1:F:46:THR:HG22	2.19	0.43
1:D:272:PHE:CD1	1:D:272:PHE:C	2.96	0.43
1:E:120:PRO:O	1:E:124:VAL:HG23	2.18	0.43
1:E:207:GLU:OE1	1:E:240:LYS:NZ	2.36	0.43
1:F:113:ILE:O	1:F:290:THR:HG23	2.19	0.43
1:H:392:ILE:O	1:H:396:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:MET:HE3	1:I:116:VAL:CG2	2.48	0.43
1:I:93:ASN:O	1:I:97:PHE:HD1	2.00	0.43
1:J:432:ALA:HB2	1:J:442:TYR:CD2	2.53	0.43
1:A:19:MET:HE1	1:A:98:ILE:HD13	2.00	0.43
1:D:91:VAL:H	1:D:259:GLN:NE2	2.16	0.43
1:E:373:TRP:CD1	1:E:373:TRP:H	2.35	0.43
1:F:170:PHE:CE2	1:F:175:GLY:HA3	2.54	0.43
1:F:272:PHE:C	1:F:272:PHE:HD1	2.26	0.43
1:G:113:ILE:O	1:G:290:THR:HG23	2.19	0.43
1:G:149:GLY:HA3	1:G:177:PHE:HB3	2.00	0.43
1:B:33:LEU:HD23	1:B:69:ILE:HG23	2.01	0.43
1:C:320:PRO:O	1:C:324:VAL:HB	2.19	0.43
1:F:177:PHE:HE1	1:F:217:SER:HB2	1.84	0.43
1:F:203:MET:HE2	1:F:214:LYS:HB2	2.01	0.43
1:H:250:GLY:HA3	1:H:272:PHE:CE1	2.54	0.43
1:H:427:LEU:O	1:H:431:GLU:HG2	2.18	0.43
1:J:203:MET:HE2	1:J:214:LYS:C	2.44	0.43
1:B:108:VAL:HG11	1:B:111:CYS:HB2	2.01	0.43
1:C:396:ILE:HG12	1:C:404:PHE:HZ	1.83	0.43
1:E:347:ILE:HG23	1:E:348:PRO:HD2	2.01	0.43
1:G:8:ILE:HA	1:G:67:TYR:HA	2.01	0.43
1:G:350:LYS:H	1:G:350:LYS:HD2	1.84	0.43
1:G:402:GLN:HA	1:G:404:PHE:CE2	2.54	0.43
1:H:113:ILE:HB	1:H:289:TYR:HB3	2.01	0.43
1:I:149:GLY:CA	1:I:177:PHE:O	2.64	0.43
1:J:130:GLU:HG2	1:J:266:PRO:HB2	2.00	0.43
1:C:383:ILE:HG22	1:C:387:LEU:HD11	2.00	0.43
1:D:383:ILE:HG13	1:D:395:PHE:CE2	2.54	0.43
1:E:188:ASP:OD2	1:G:87:ARG:NH2	2.50	0.43
1:F:168:TYR:HE2	1:F:205:ARG:CG	2.30	0.43
1:F:182:GLU:OE1	1:F:273:HIS:NE2	2.50	0.43
1:G:205:ARG:HA	1:G:205:ARG:NE	2.33	0.43
1:H:279:ALA:O	1:H:285:ASN:ND2	2.38	0.43
1:I:35:ASP:O	1:I:39:GLU:HG2	2.19	0.43
1:I:45:SER:HB3	1:I:64:ALA:HB2	2.00	0.43
1:I:139:TYR:CE2	1:I:213:THR:HB	2.54	0.43
1:I:258:ILE:HG23	1:I:270:LEU:HD21	2.01	0.43
1:J:60:GLU:HA	1:J:63:ASP:OD1	2.19	0.43
1:B:165:GLU:HB2	1:E:347:ILE:HD12	2.01	0.43
1:C:97:PHE:CZ	1:E:183:PRO:HB2	2.54	0.43
1:D:155:LYS:NZ	2:D:502:CAP:O7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LYS:HG3	1:D:316:MET:HE2	2.00	0.43
1:F:331:LEU:HD11	1:F:403:ASP:O	2.18	0.43
1:I:73:ASN:O	1:I:75:LEU:HD13	2.18	0.43
1:I:150:SER:OG	1:I:413:HIS:CE1	2.72	0.43
1:I:382:ILE:HG13	1:I:405:ILE:HD13	2.00	0.43
1:C:250:GLY:HA3	1:C:272:PHE:CE1	2.53	0.43
1:C:281:THR:HA	1:C:289:TYR:O	2.19	0.43
1:G:142:ILE:HD11	1:G:147:ILE:HD12	2.00	0.43
1:G:183:PRO:HB2	1:J:97:PHE:CE1	2.54	0.43
1:H:177:PHE:CE1	1:H:179:KCX:HB2	2.53	0.43
1:H:446:LYS:HD2	1:H:446:LYS:N	2.34	0.43
1:J:113:ILE:HB	1:J:289:TYR:HB3	2.01	0.43
1:A:101:ASN:ND2	1:B:182:GLU:OE2	2.52	0.42
1:B:86:ASP:HB3	1:B:90:ASN:HB3	2.01	0.42
1:B:113:ILE:O	1:B:290:THR:HG23	2.19	0.42
1:D:273:HIS:CE1	1:D:275:ALA:HB2	2.53	0.42
1:E:389:PRO:HA	1:E:392:ILE:HD11	1.99	0.42
1:F:152:ILE:HG21	1:F:163:TYR:CD2	2.54	0.42
1:H:34:VAL:HG22	1:H:69:ILE:HD12	2.00	0.42
1:I:236:GLN:HG2	1:I:244:TYR:OH	2.18	0.42
1:I:331:LEU:O	1:I:367:TYR:OH	2.26	0.42
1:J:19:MET:SD	1:J:118:PHE:HE1	2.41	0.42
1:J:428:GLN:HB3	1:J:449:LEU:HD12	2.01	0.42
1:A:24:ARG:HA	1:A:74:ASN:O	2.19	0.42
1:B:281:THR:HB	1:B:291:VAL:HG23	2.01	0.42
1:D:402:GLN:HA	1:D:404:PHE:CE1	2.54	0.42
1:F:177:PHE:CE1	1:F:217:SER:HB2	2.54	0.42
1:G:441:ASP:O	1:G:444:LYS:HG2	2.19	0.42
1:H:178:VAL:O	1:H:216:HIS:ND1	2.52	0.42
1:A:170:PHE:CE2	1:A:175:GLY:HA3	2.53	0.42
1:B:31:MET:SD	1:B:107:SER:HB2	2.59	0.42
1:D:25:LEU:HA	1:D:110:VAL:O	2.20	0.42
1:D:67:TYR:CE1	1:D:77:TRP:HB3	2.54	0.42
1:G:154:PRO:HD2	1:G:158:LEU:HD11	2.01	0.42
1:H:410:ALA:HB3	1:I:49:PHE:CE1	2.53	0.42
1:I:91:VAL:O	1:I:95:MET:HG2	2.18	0.42
1:J:31:MET:SD	1:J:107:SER:HB2	2.60	0.42
1:A:205:ARG:NH2	1:F:369:ASN:O	2.49	0.42
1:A:370:LEU:O	1:A:374:ARG:HD2	2.18	0.42
1:D:344:TRP:HB3	1:D:376:THR:HB	2.01	0.42
1:H:182:GLU:HB3	1:H:273:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:LYS:HG3	1:H:316:MET:HE2	2.01	0.42
1:J:26:GLN:O	1:J:109:LYS:N	2.50	0.42
1:C:236:GLN:HG2	1:C:244:TYR:OH	2.19	0.42
1:D:143:GLN:O	1:D:144:GLU:HB3	2.19	0.42
1:E:1:MET:HE3	1:E:3:LYS:HB2	2.00	0.42
1:E:150:SER:HB2	1:E:170:PHE:CE1	2.55	0.42
1:E:165:GLU:HA	1:G:373:TRP:CH2	2.55	0.42
1:G:159:THR:HB	1:I:124:VAL:HG21	2.00	0.42
1:I:141:ASN:HD22	1:I:141:ASN:C	2.25	0.42
1:I:212:LYS:HB3	4:I:604:HOH:O	2.19	0.42
1:B:273:HIS:CE1	1:B:275:ALA:HB2	2.55	0.42
1:B:324:VAL:HG22	1:B:399:VAL:HA	2.02	0.42
1:C:347:ILE:HG13	1:C:374:ARG:HB2	2.02	0.42
1:D:281:THR:HA	1:D:289:TYR:O	2.19	0.42
1:E:149:GLY:O	1:E:407:THR:HA	2.20	0.42
1:I:283:ASP:OD1	1:I:283:ASP:N	2.44	0.42
1:B:137:ARG:HH21	1:B:403:ASP:HA	1.85	0.42
1:D:272:PHE:C	1:D:272:PHE:HD1	2.27	0.42
1:F:25:LEU:HD12	1:F:76:VAL:HG21	2.01	0.42
1:F:145:ARG:NH1	1:F:146:PRO:O	2.53	0.42
1:G:18:TYR:HE1	1:G:81:PRO:HG3	1.84	0.42
1:G:417:MET:HB3	1:G:421:ALA:CB	2.49	0.42
1:H:395:PHE:CZ	1:H:399:VAL:HG21	2.55	0.42
1:J:392:ILE:O	1:J:396:ILE:HG13	2.19	0.42
1:A:415:HIS:HE1	1:A:417:MET:HE3	1.84	0.42
1:B:236:GLN:HG2	1:B:244:TYR:OH	2.20	0.42
1:D:315:LYS:HE3	1:D:316:MET:HE3	2.00	0.42
1:E:45:SER:HB3	1:E:64:ALA:HB2	2.02	0.42
1:F:133:ILE:HB	1:F:380:CYS:HB2	2.01	0.42
1:F:166:LEU:HA	1:F:166:LEU:HD23	1.81	0.42
1:F:333:LEU:HB2	1:F:367:TYR:CD2	2.55	0.42
1:I:192:TYR:O	1:I:196:VAL:HG23	2.20	0.42
1:J:113:ILE:HD13	1:J:289:TYR:HB3	2.01	0.42
1:J:384:SER:OG	2:J:502:CAP:H11	2.19	0.42
1:J:388:ASN:ND2	1:J:456:TYR:HB3	2.35	0.42
1:A:347:ILE:HG23	1:A:348:PRO:HD2	2.02	0.42
1:B:25:LEU:HD23	1:B:111:CYS:HA	2.01	0.42
1:G:76:VAL:HG12	1:G:78:ILE:HG13	2.02	0.42
1:H:139:TYR:CE2	1:H:213:THR:HB	2.55	0.42
1:H:333:LEU:HD12	1:H:367:TYR:CD1	2.55	0.42
1:J:118:PHE:CE2	1:J:300:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:MET:HE2	1:J:215:VAL:HG11	2.02	0.42
1:J:155:LYS:HE2	1:J:181:ASP:OD1	2.20	0.42
1:D:285:ASN:ND2	1:F:287:ILE:HB	2.34	0.42
1:E:159:THR:HG23	1:E:189:PHE:O	2.19	0.42
1:F:128:GLY:C	1:F:302:GLY:HA2	2.45	0.42
1:F:416:PRO:HD3	1:F:455:PHE:HD2	1.85	0.42
1:G:91:VAL:O	1:G:95:MET:HG2	2.20	0.42
1:I:105:MET:HE2	1:I:108:VAL:HG23	2.02	0.42
1:J:347:ILE:CG2	1:J:348:PRO:HD2	2.50	0.42
1:J:392:ILE:HD11	1:J:408:MET:CE	2.49	0.42
1:A:256:MET:HE2	1:A:256:MET:HB3	1.84	0.41
1:B:347:ILE:CD1	1:D:161:SER:HB3	2.50	0.41
1:C:113:ILE:O	1:C:290:THR:HG23	2.19	0.41
1:E:2:GLN:O	1:E:38:SER:HB2	2.20	0.41
1:F:151:ILE:HD13	2:F:501:CAP:O2	2.19	0.41
1:G:315:LYS:CD	1:J:49:PHE:HB3	2.50	0.41
1:J:88:GLY:N	4:J:610:HOH:O	2.53	0.41
1:J:142:ILE:HG22	1:J:145:ARG:NH2	2.35	0.41
1:C:284:GLU:OE1	1:C:284:GLU:N	2.46	0.41
1:C:408:MET:HE2	1:C:412:VAL:HG23	2.01	0.41
1:D:223:SER:HB2	1:F:259:GLN:HE22	1.84	0.41
1:G:8:ILE:HD12	1:G:66:VAL:O	2.20	0.41
1:G:155:LYS:HG3	1:G:181:ASP:CG	2.44	0.41
1:G:166:LEU:HD21	1:J:54:THR:HG21	2.01	0.41
1:G:187:GLN:OE1	1:G:187:GLN:N	2.52	0.41
1:G:281:THR:HB	1:G:291:VAL:HG23	2.01	0.41
1:H:19:MET:HB2	1:H:122:MET:SD	2.60	0.41
1:H:148:PHE:HE1	1:H:392:ILE:HG12	1.85	0.41
1:I:373:TRP:HZ2	1:I:374:ARG:HH21	1.67	0.41
1:B:105:MET:HE2	1:B:108:VAL:HG23	2.01	0.41
1:E:92:GLN:CD	1:E:92:GLN:C	2.88	0.41
1:G:331:LEU:HG	1:G:381:PRO:HD3	2.01	0.41
1:H:205:ARG:HH12	1:J:370:LEU:C	2.28	0.41
1:J:113:ILE:HD12	1:J:113:ILE:H	1.85	0.41
1:J:401:THR:O	1:J:404:PHE:HE2	2.03	0.41
1:A:142:ILE:HD11	1:A:147:ILE:HG12	2.03	0.41
1:A:228:MET:HE2	1:B:256:MET:HE1	2.02	0.41
1:B:207:GLU:OE1	1:B:240:LYS:NZ	2.45	0.41
1:D:43:GLU:HG3	1:D:105:MET:SD	2.61	0.41
1:E:383:ILE:HG13	1:E:395:PHE:CE2	2.56	0.41
1:F:290:THR:OG1	1:F:292:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:THR:CB	1:J:124:VAL:HG21	2.51	0.41
1:H:399:VAL:HG12	1:H:401:THR:HG22	2.02	0.41
1:J:86:ASP:OD2	1:J:90:ASN:ND2	2.42	0.41
1:D:128:GLY:C	1:D:302:GLY:HA2	2.45	0.41
1:D:308:THR:HG22	4:D:602:HOH:O	2.20	0.41
1:F:179:KCX:NZ	1:F:180:ASN:O	2.51	0.41
1:G:24:ARG:HA	1:G:74:ASN:O	2.21	0.41
1:I:200:ARG:NH2	4:I:611:HOH:O	2.53	0.41
1:I:250:GLY:HA3	1:I:272:PHE:CE1	2.55	0.41
1:J:436:LYS:HD3	1:J:436:LYS:N	2.35	0.41
1:A:46:THR:HG22	1:B:156:ILE:O	2.20	0.41
1:C:70:ASP:HB3	1:C:75:LEU:HB2	2.01	0.41
1:D:24:ARG:O	1:D:110:VAL:HG12	2.21	0.41
1:E:8:ILE:HD11	1:E:69:ILE:HD11	2.02	0.41
1:F:137:ARG:NH2	1:F:403:ASP:HA	2.36	0.41
1:I:358:ILE:HA	1:I:361:GLU:HG2	2.03	0.41
1:A:24:ARG:HB2	1:A:114:LEU:HD11	2.02	0.41
1:A:272:PHE:C	1:A:272:PHE:CD1	2.98	0.41
1:C:386:GLY:HA2	1:E:49:PHE:CE2	2.56	0.41
1:E:360:LYS:HA	1:E:360:LYS:HD3	1.84	0.41
1:F:146:PRO:HD3	1:F:402:GLN:OE1	2.19	0.41
1:G:311:ALA:HB1	1:G:320:PRO:HA	2.02	0.41
1:B:67:TYR:CE2	1:B:77:TRP:HB3	2.56	0.41
1:C:253:ALA:O	1:E:254:GLY:HA3	2.20	0.41
1:D:6:ILE:HG23	1:D:8:ILE:HG13	2.02	0.41
1:J:63:ASP:O	4:J:603:HOH:O	2.22	0.41
1:A:183:PRO:HB2	1:B:97:PHE:CE2	2.56	0.41
1:B:159:THR:HB	1:E:124:VAL:HG21	2.03	0.41
1:C:305:GLY:HA2	1:C:380:CYS:O	2.21	0.41
1:D:1:MET:SD	1:D:35:ASP:HB2	2.61	0.41
1:D:156:ILE:HG21	1:F:84:ILE:HB	2.02	0.41
1:D:373:TRP:HH2	1:I:165:GLU:HA	1.84	0.41
1:E:66:VAL:HG13	1:E:76:VAL:HG23	2.03	0.41
1:E:396:ILE:HG12	1:E:404:PHE:CZ	2.55	0.41
1:F:18:TYR:CE2	1:F:81:PRO:HG3	2.55	0.41
1:F:105:MET:O	1:F:108:VAL:HG22	2.21	0.41
1:F:149:GLY:C	1:F:407:THR:HA	2.46	0.41
1:G:32:THR:OG1	1:G:33:LEU:N	2.53	0.41
1:G:137:ARG:HH21	1:G:403:ASP:HA	1.86	0.41
1:G:361:GLU:HG3	1:G:362:ALA:N	2.34	0.41
1:H:225:TYR:CD1	1:I:225:TYR:HD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:392:ILE:HD12	1:H:392:ILE:HA	1.97	0.41
1:I:36:THR:CG2	1:I:108:VAL:HG22	2.48	0.41
1:J:112:LYS:HA	1:J:288:GLY:O	2.21	0.41
1:J:360:LYS:HE2	1:J:360:LYS:HB2	1.60	0.41
1:J:389:PRO:HG2	1:J:452:ALA:HB1	2.03	0.41
1:A:259:GLN:HE22	1:B:223:SER:HB2	1.86	0.41
1:B:6:ILE:HD11	1:B:38:SER:HB3	2.03	0.41
1:B:120:PRO:O	1:B:124:VAL:HG23	2.20	0.41
1:C:306:ILE:HG22	1:C:379:MET:HE3	2.02	0.41
1:D:310:THR:O	1:D:310:THR:OG1	2.31	0.41
1:E:18:TYR:CE2	1:E:81:PRO:HG3	2.56	0.41
1:F:179:KCX:HE3	1:F:179:KCX:HB3	1.86	0.41
1:G:86:ASP:HB3	1:G:90:ASN:HB3	2.03	0.41
1:G:254:GLY:HA3	1:J:253:ALA:O	2.21	0.41
1:E:137:ARG:NH2	1:E:403:ASP:HA	2.36	0.40
1:G:253:ALA:O	1:J:254:GLY:HA3	2.20	0.40
1:H:1:MET:HE3	1:H:1:MET:HB2	1.96	0.40
1:I:111:CYS:H	1:I:287:ILE:HD13	1.86	0.40
1:A:187:GLN:OE1	1:A:187:GLN:N	2.49	0.40
1:B:290:THR:OG1	1:B:292:PRO:HD2	2.21	0.40
1:C:20:LEU:HD23	1:C:67:TYR:OH	2.21	0.40
1:F:120:PRO:O	1:F:124:VAL:HG23	2.20	0.40
1:G:150:SER:OG	1:G:413:HIS:CE1	2.74	0.40
1:H:347:ILE:HD13	1:H:347:ILE:HA	1.91	0.40
1:J:112:LYS:O	1:J:114:LEU:HD23	2.20	0.40
1:A:266:PRO:HA	4:A:647:HOH:O	2.21	0.40
1:D:124:VAL:HG22	1:D:346:GLU:HB3	2.03	0.40
1:F:281:THR:HA	1:F:289:TYR:O	2.21	0.40
1:G:349:GLU:HG2	1:G:355:GLN:NE2	2.36	0.40
1:H:321:LYS:HZ2	1:H:325:MET:HE2	1.86	0.40
1:J:155:LYS:HE2	1:J:181:ASP:CG	2.46	0.40
1:J:445:ASP:C	1:J:446:LYS:HD2	2.47	0.40
1:A:410:ALA:HB1	1:B:50:VAL:HG12	2.02	0.40
1:B:23:PHE:HB2	1:B:76:VAL:CG2	2.51	0.40
1:B:45:SER:HB3	1:B:64:ALA:HB2	2.04	0.40
1:B:333:LEU:N	1:B:361:GLU:OE2	2.38	0.40
1:D:92:GLN:NE2	1:F:221:SER:HB3	2.36	0.40
1:D:151:ILE:HD11	1:D:407:THR:HB	2.03	0.40
1:G:19:MET:HE3	1:G:116:VAL:CG2	2.51	0.40
1:G:23:PHE:CE1	1:G:78:ILE:HD12	2.57	0.40
1:G:272:PHE:C	1:G:272:PHE:CD1	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ILE:HA	1:H:66:VAL:HG12	2.03	0.40
1:H:131:TYR:CE1	1:H:135:ASP:HB2	2.56	0.40
1:H:270:LEU:HD23	1:H:303:ALA:HA	2.04	0.40
1:I:23:PHE:CD1	1:I:78:ILE:HD12	2.56	0.40
1:I:314:GLY:HA3	1:I:385:GLY:O	2.21	0.40
1:I:370:LEU:HD23	1:I:375:ILE:CG2	2.51	0.40
1:J:153:LYS:HA	1:J:154:PRO:C	2.47	0.40
1:J:380:CYS:SG	1:J:405:ILE:HD12	2.62	0.40
1:B:25:LEU:HD12	1:B:76:VAL:HG21	2.03	0.40
1:B:272:PHE:C	1:B:272:PHE:CD1	3.00	0.40
1:C:127:ASP:OD2	4:C:603:HOH:O	2.22	0.40
1:C:272:PHE:CD1	1:C:272:PHE:C	3.00	0.40
1:D:253:ALA:O	1:F:254:GLY:HA3	2.22	0.40
1:E:65:LEU:O	1:E:78:ILE:HA	2.21	0.40
1:E:94:ILE:HD11	1:E:126:TYR:OH	2.21	0.40
1:E:137:ARG:O	1:E:141:ASN:N	2.54	0.40
1:E:272:PHE:CD1	1:E:272:PHE:C	2.99	0.40
1:F:175:GLY:HA2	4:F:610:HOH:O	2.20	0.40
1:F:395:PHE:O	1:F:399:VAL:HG22	2.22	0.40
1:G:356:LEU:O	1:G:360:LYS:HG2	2.21	0.40
1:H:151:ILE:HD11	1:H:407:THR:HG23	2.02	0.40
1:I:120:PRO:O	1:I:124:VAL:HG23	2.22	0.40
1:I:272:PHE:C	1:I:272:PHE:CD1	3.00	0.40
1:J:5:TYR:HD1	1:J:64:ALA:O	2.04	0.40
1:J:115:ASP:C	1:J:340:PHE:HE2	2.29	0.40

All (1) 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:C:397:ASP:OD1	1:E:436:LYS:NZ[1_655]	1.98	0.22

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	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	44	61
1	B	454/468 (97%)	441 (97%)	12 (3%)	1 (0%)	44	61
1	C	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	44	61
1	D	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	44	61
1	E	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	44	61
1	F	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	44	61
1	G	454/468 (97%)	441 (97%)	12 (3%)	1 (0%)	44	61
1	H	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	44	61
1	I	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	44	61
1	J	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	44	61
All	All	4540/4680 (97%)	4398 (97%)	132 (3%)	10 (0%)	44	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	185	ALA
1	G	185	ALA
1	A	185	ALA
1	C	185	ALA
1	E	185	ALA
1	F	185	ALA
1	H	185	ALA
1	I	185	ALA
1	J	185	ALA
1	B	185	ALA

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	377/388 (97%)	370 (98%)	7 (2%)	52	72
1	B	377/388 (97%)	366 (97%)	11 (3%)	37	58
1	C	377/388 (97%)	366 (97%)	11 (3%)	37	58
1	D	377/388 (97%)	364 (97%)	13 (3%)	32	51
1	E	377/388 (97%)	366 (97%)	11 (3%)	37	58
1	F	377/388 (97%)	364 (97%)	13 (3%)	32	51
1	G	377/388 (97%)	359 (95%)	18 (5%)	21	36
1	H	377/388 (97%)	365 (97%)	12 (3%)	34	54
1	I	377/388 (97%)	363 (96%)	14 (4%)	29	48
1	J	377/388 (97%)	364 (97%)	13 (3%)	32	51
All	All	3770/3880 (97%)	3647 (97%)	123 (3%)	33	52

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	32	THR
1	A	69	ILE
1	A	92	GLN
1	A	227	THR
1	A	272	PHE
1	A	406	THR
1	B	13	VAL
1	B	32	THR
1	B	69	ILE
1	B	96	THR
1	B	272	PHE
1	B	295	THR
1	B	308	THR
1	B	347	ILE
1	B	406	THR
1	B	440	GLU
1	B	445	ASP
1	C	13	VAL
1	C	20	LEU
1	C	32	THR
1	C	62	LEU
1	C	92	GLN
1	C	96	THR

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Mol	Chain	Res	Type
1	C	141	ASN
1	C	308	THR
1	C	403	ASP
1	C	406	THR
1	C	439	LEU
1	D	13	VAL
1	D	54	THR
1	D	56	THR
1	D	92	GLN
1	D	112	LYS
1	D	227	THR
1	D	270	LEU
1	D	272	PHE
1	D	310	THR
1	D	354	LEU
1	D	359	GLN
1	D	390	LEU
1	D	403	ASP
1	E	32	THR
1	E	69	ILE
1	E	76	VAL
1	E	92	GLN
1	E	159	THR
1	E	227	THR
1	E	308	THR
1	E	313	ILE
1	E	322	GLU
1	E	392	ILE
1	E	406	THR
1	F	1	MET
1	F	32	THR
1	F	65	LEU
1	F	92	GLN
1	F	168	TYR
1	F	264	LYS
1	F	324	VAL
1	F	356	LEU
1	F	360	LYS
1	F	391	LEU
1	F	426	VAL
1	F	427	LEU
1	F	446	LYS

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Mol	Chain	Res	Type
1	G	8	ILE
1	G	13	VAL
1	G	20	LEU
1	G	32	THR
1	G	38	SER
1	G	46	THR
1	G	159	THR
1	G	166	LEU
1	G	236	GLN
1	G	294	LEU
1	G	308	THR
1	G	313	ILE
1	G	324	VAL
1	G	390	LEU
1	G	391	LEU
1	G	406	THR
1	G	424	THR
1	G	437	ILE
1	H	32	THR
1	H	43	GLU
1	H	136	MET
1	H	145	ARG
1	H	229	ILE
1	H	272	PHE
1	H	350	LYS
1	H	356	LEU
1	H	365	GLU
1	H	403	ASP
1	H	426	VAL
1	H	436	LYS
1	I	13	VAL
1	I	17	GLN
1	I	61	SER
1	I	66	VAL
1	I	75	LEU
1	I	92	GLN
1	I	141	ASN
1	I	188	ASP
1	I	194	LYS
1	I	227	THR
1	I	238	MET
1	I	248	VAL

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Mol	Chain	Res	Type
1	I	283	ASP
1	I	366	ASP
1	J	13	VAL
1	J	25	LEU
1	J	26	GLN
1	J	32	THR
1	J	46	THR
1	J	69	ILE
1	J	114	LEU
1	J	227	THR
1	J	319	SER
1	J	324	VAL
1	J	331	LEU
1	J	360	LYS
1	J	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	B	92	GLN
1	B	208	GLN
1	C	143	GLN
1	D	2	GLN
1	D	7	GLN
1	D	259	GLN
1	E	197	GLN
1	E	236	GLN
1	E	355	GLN
1	E	359	GLN
1	F	197	GLN
1	G	143	GLN
1	G	435	GLN
1	H	92	GLN
1	H	273	HIS
1	I	413	HIS
1	J	92	GLN
1	J	369	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	KCX	E	179	3,1	10,11,12	2.02	2 (20%)	6,12,14	1.94	2 (33%)
1	KCX	G	179	3,1	10,11,12	2.10	2 (20%)	6,12,14	1.62	1 (16%)
1	KCX	I	179	3,1	10,11,12	2.15	2 (20%)	6,12,14	1.58	1 (16%)
1	KCX	D	179	3,1	10,11,12	2.10	2 (20%)	6,12,14	1.41	1 (16%)
1	KCX	J	179	1	10,11,12	2.10	2 (20%)	6,12,14	1.27	1 (16%)
1	KCX	A	179	3,1	10,11,12	2.01	2 (20%)	6,12,14	1.65	1 (16%)
1	KCX	B	179	3,1	10,11,12	1.98	2 (20%)	6,12,14	1.75	1 (16%)
1	KCX	F	179	3,1	10,11,12	2.17	2 (20%)	6,12,14	2.33	3 (50%)
1	KCX	H	179	3,1	10,11,12	2.09	2 (20%)	6,12,14	1.34	1 (16%)
1	KCX	C	179	3,1	10,11,12	2.08	2 (20%)	6,12,14	1.33	1 (16%)

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
1	KCX	E	179	3,1	-	0/9/10/12	-
1	KCX	G	179	3,1	-	1/9/10/12	-
1	KCX	I	179	3,1	-	0/9/10/12	-
1	KCX	D	179	3,1	-	0/9/10/12	-
1	KCX	J	179	1	-	0/9/10/12	-
1	KCX	A	179	3,1	-	0/9/10/12	-
1	KCX	B	179	3,1	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	179	3,1	-	0/9/10/12	-
1	KCX	H	179	3,1	-	0/9/10/12	-
1	KCX	C	179	3,1	-	1/9/10/12	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	KCX	CX-NZ	5.96	1.45	1.35
1	I	179	KCX	CX-NZ	5.87	1.45	1.35
1	J	179	KCX	CX-NZ	5.74	1.45	1.35
1	G	179	KCX	CX-NZ	5.73	1.45	1.35
1	D	179	KCX	CX-NZ	5.71	1.45	1.35
1	H	179	KCX	CX-NZ	5.70	1.45	1.35
1	E	179	KCX	CX-NZ	5.50	1.45	1.35
1	C	179	KCX	CX-NZ	5.46	1.44	1.35
1	A	179	KCX	CX-NZ	5.38	1.44	1.35
1	B	179	KCX	CX-NZ	5.30	1.44	1.35
1	C	179	KCX	OQ1-CX	2.77	1.26	1.21
1	I	179	KCX	OQ1-CX	2.61	1.26	1.21
1	F	179	KCX	OQ1-CX	2.60	1.26	1.21
1	D	179	KCX	OQ1-CX	2.58	1.26	1.21
1	H	179	KCX	OQ1-CX	2.49	1.26	1.21
1	B	179	KCX	OQ1-CX	2.47	1.26	1.21
1	E	179	KCX	OQ1-CX	2.47	1.26	1.21
1	A	179	KCX	OQ1-CX	2.44	1.26	1.21
1	G	179	KCX	OQ1-CX	2.42	1.26	1.21
1	J	179	KCX	OQ1-CX	2.39	1.26	1.21

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	KCX	OQ1-CX-NZ	-3.77	119.19	124.92
1	A	179	KCX	OQ1-CX-NZ	-3.65	119.37	124.92
1	F	179	KCX	OQ1-CX-NZ	-3.64	119.39	124.92
1	F	179	KCX	CE-NZ-CX	-3.55	115.96	121.98
1	B	179	KCX	OQ1-CX-NZ	-3.40	119.76	124.92
1	D	179	KCX	OQ1-CX-NZ	-3.25	119.99	124.92
1	G	179	KCX	OQ1-CX-NZ	-3.23	120.01	124.92
1	I	179	KCX	OQ1-CX-NZ	-2.96	120.43	124.92
1	C	179	KCX	OQ1-CX-NZ	-2.95	120.44	124.92
1	H	179	KCX	OQ1-CX-NZ	-2.86	120.57	124.92
1	J	179	KCX	OQ1-CX-NZ	-2.62	120.94	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	KCX	CE-NZ-CX	-2.44	117.85	121.98
1	F	179	KCX	CD-CG-CB	-2.24	105.18	113.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	179	KCX	O-C-CA-CB
1	G	179	KCX	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	179	KCX	1	0
1	A	179	KCX	1	0
1	F	179	KCX	3	0
1	H	179	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CAP	D	502	3	18,20,20	1.05	0	23,31,31	1.12	1 (4%)
2	CAP	C	501	3	18,20,20	1.04	0	23,31,31	1.06	1 (4%)
2	CAP	A	501	3	18,20,20	1.06	0	23,31,31	1.13	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAP	E	501	3	18,20,20	1.06	0	23,31,31	1.04	1 (4%)
2	CAP	F	501	3	18,20,20	1.07	0	23,31,31	1.15	1 (4%)
2	CAP	J	502	3	18,20,20	1.07	0	23,31,31	1.08	1 (4%)
2	CAP	I	502	3	18,20,20	1.07	0	23,31,31	1.05	1 (4%)
2	CAP	H	501	3	18,20,20	1.07	0	23,31,31	1.09	2 (8%)
2	CAP	B	501	3	18,20,20	1.03	0	23,31,31	1.23	1 (4%)
2	CAP	G	501	3	18,20,20	1.06	0	23,31,31	1.07	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	D	502	3	-	11/29/29/29	-
2	CAP	C	501	3	-	13/29/29/29	-
2	CAP	A	501	3	-	10/29/29/29	-
2	CAP	E	501	3	-	7/29/29/29	-
2	CAP	F	501	3	-	7/29/29/29	-
2	CAP	J	502	3	-	11/29/29/29	-
2	CAP	I	502	3	-	5/29/29/29	-
2	CAP	H	501	3	-	14/29/29/29	-
2	CAP	B	501	3	-	9/29/29/29	-
2	CAP	G	501	3	-	3/29/29/29	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	CAP	O7-C-C2	3.71	120.27	114.06
2	D	502	CAP	O7-C-C2	3.62	120.12	114.06
2	A	501	CAP	O7-C-C2	3.47	119.86	114.06
2	C	501	CAP	O7-C-C2	3.40	119.75	114.06
2	E	501	CAP	O7-C-C2	3.11	119.27	114.06
2	I	502	CAP	O7-C-C2	3.03	119.14	114.06
2	J	502	CAP	O7-C-C2	3.02	119.11	114.06
2	F	501	CAP	O7-C-C2	2.99	119.07	114.06
2	G	501	CAP	O7-C-C2	2.96	119.02	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	CAP	O7-C-C2	2.87	118.86	114.06
2	A	501	CAP	O3P-P1-O1	2.37	112.85	106.67
2	H	501	CAP	C2-C3-C4	-2.37	109.30	114.03

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CAP	O2-C2-C3-C4
2	A	501	CAP	O6-C-C2-C3
2	A	501	CAP	O6-C-C2-O2
2	A	501	CAP	O7-C-C2-O2
2	A	501	CAP	O3-C3-C4-O4
2	B	501	CAP	O6-C-C2-C1
2	B	501	CAP	O7-C-C2-C1
2	B	501	CAP	O7-C-C2-C3
2	B	501	CAP	O6-C-C2-O2
2	B	501	CAP	O7-C-C2-O2
2	B	501	CAP	C2-C3-C4-O4
2	B	501	CAP	O3-C3-C4-O4
2	C	501	CAP	C2-C3-C4-O4
2	C	501	CAP	O3-C3-C4-O4
2	D	502	CAP	C2-C3-C4-O4
2	D	502	CAP	O3-C3-C4-O4
2	D	502	CAP	O4-C4-C5-O5
2	E	501	CAP	C2-C3-C4-O4
2	E	501	CAP	O3-C3-C4-O4
2	F	501	CAP	O3-C3-C4-O4
2	G	501	CAP	O3-C3-C4-O4
2	H	501	CAP	O6-C-C2-C3
2	H	501	CAP	O6-C-C2-O2
2	H	501	CAP	C2-C3-C4-O4
2	H	501	CAP	O3-C3-C4-O4
2	H	501	CAP	O4-C4-C5-O5
2	I	502	CAP	C1-C2-C3-C4
2	I	502	CAP	O2-C2-C3-C4
2	I	502	CAP	O3-C3-C4-O4
2	I	502	CAP	O4-C4-C5-O5
2	J	502	CAP	O6-C-C2-O2
2	J	502	CAP	C2-C3-C4-O4
2	J	502	CAP	O3-C3-C4-O4
2	J	502	CAP	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	A	501	CAP	O6-C-C2-C1
2	A	501	CAP	O7-C-C2-C1
2	H	501	CAP	O6-C-C2-C1
2	H	501	CAP	O7-C-C2-C1
2	H	501	CAP	O7-C-C2-O2
2	C	501	CAP	O6-C-C2-O2
2	B	501	CAP	O6-C-C2-C3
2	C	501	CAP	O6-C-C2-C3
2	J	502	CAP	O6-C-C2-C3
2	C	501	CAP	O6-C-C2-C1
2	C	501	CAP	O7-C-C2-C1
2	D	502	CAP	O6-C-C2-C1
2	J	502	CAP	O6-C-C2-C1
2	H	501	CAP	O1-C1-C2-O2
2	H	501	CAP	O3-C3-C4-C5
2	C	501	CAP	O7-C-C2-O2
2	B	501	CAP	O2-C2-C3-C4
2	C	501	CAP	O2-C2-C3-C4
2	D	502	CAP	O2-C2-C3-C4
2	E	501	CAP	O2-C2-C3-C4
2	F	501	CAP	O2-C2-C3-C4
2	G	501	CAP	O2-C2-C3-C4
2	H	501	CAP	O2-C2-C3-C4
2	I	502	CAP	C1-C2-C3-O3
2	J	502	CAP	O2-C2-C3-C4
2	H	501	CAP	C4-C5-O5-P2
2	J	502	CAP	O7-C-C2-C1
2	A	501	CAP	O7-C-C2-C3
2	C	501	CAP	O7-C-C2-C3
2	D	502	CAP	O7-C-C2-C3
2	E	501	CAP	O7-C-C2-C3
2	H	501	CAP	O7-C-C2-C3
2	J	502	CAP	O7-C-C2-C3
2	C	501	CAP	C4-C5-O5-P2
2	D	502	CAP	O7-C-C2-C1
2	E	501	CAP	O6-C-C2-C1
2	F	501	CAP	O6-C-C2-C1
2	J	502	CAP	O7-C-C2-O2
2	A	501	CAP	C2-C3-C4-O4
2	F	501	CAP	C2-C3-C4-O4
2	D	502	CAP	O6-C-C2-O2
2	C	501	CAP	O4-C4-C5-O5

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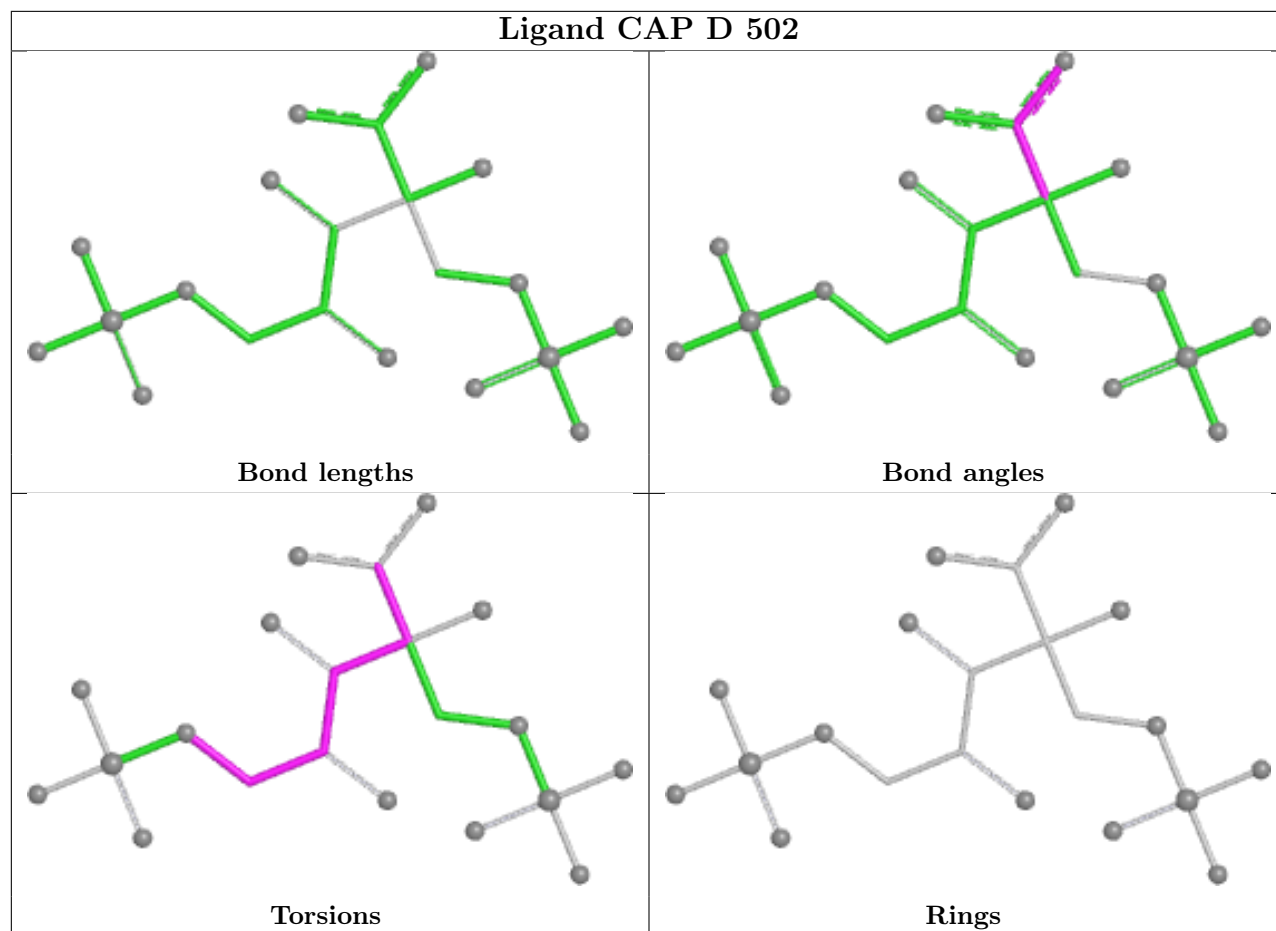
Mol	Chain	Res	Type	Atoms
2	D	502	CAP	O6-C-C2-C3
2	E	501	CAP	O6-C-C2-C3
2	F	501	CAP	O6-C-C2-C3
2	E	501	CAP	O7-C-C2-C1
2	F	501	CAP	O7-C-C2-C1
2	D	502	CAP	C3-C4-C5-O5
2	J	502	CAP	C3-C4-C5-O5
2	D	502	CAP	C4-C5-O5-P2
2	C	501	CAP	O3-C3-C4-C5
2	F	501	CAP	C4-C5-O5-P2
2	C	501	CAP	C2-C3-C4-C5
2	H	501	CAP	C2-C3-C4-C5
2	A	501	CAP	C1-C2-C3-O3
2	G	501	CAP	C2-C3-C4-O4

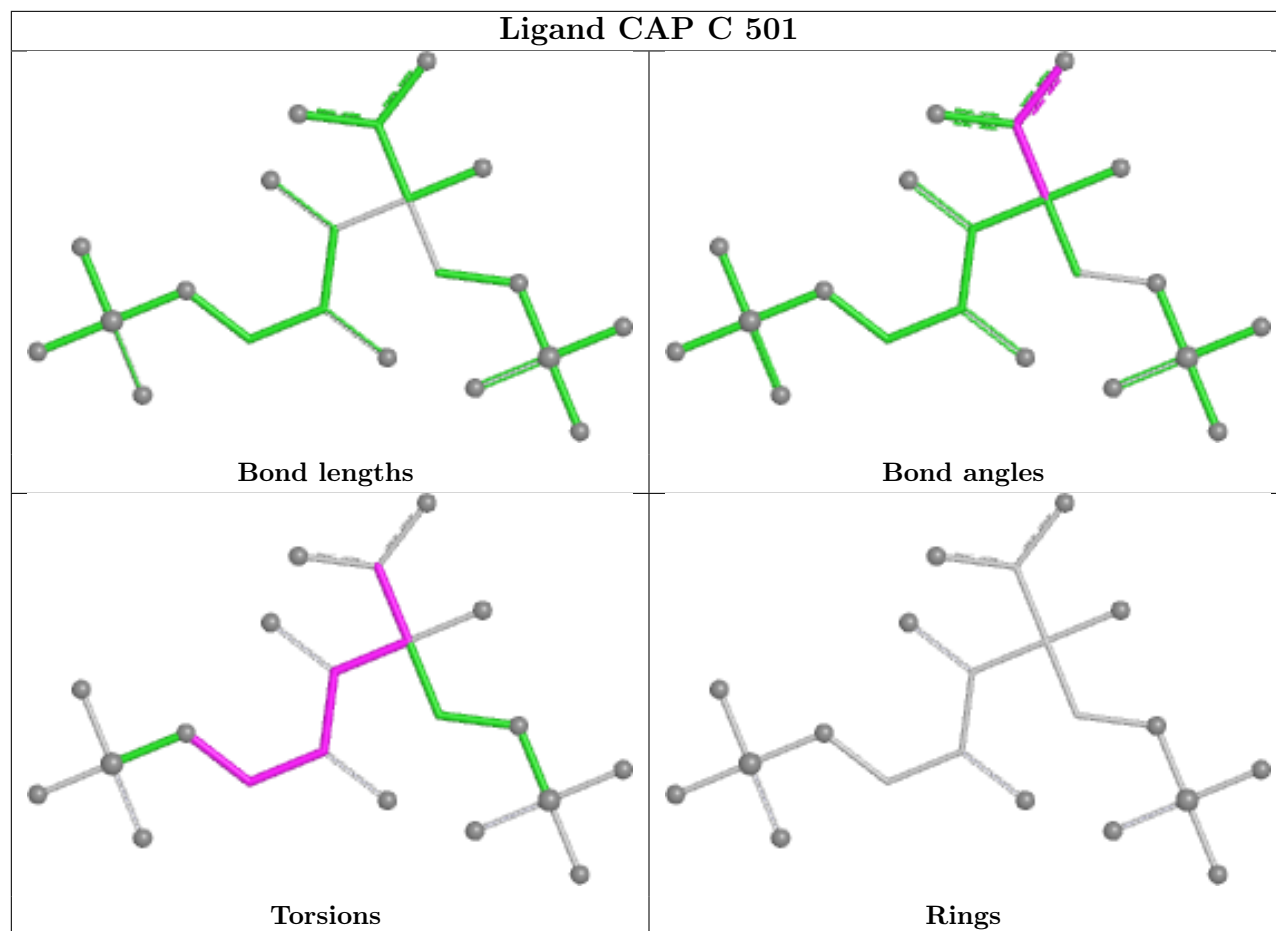
There are no ring outliers.

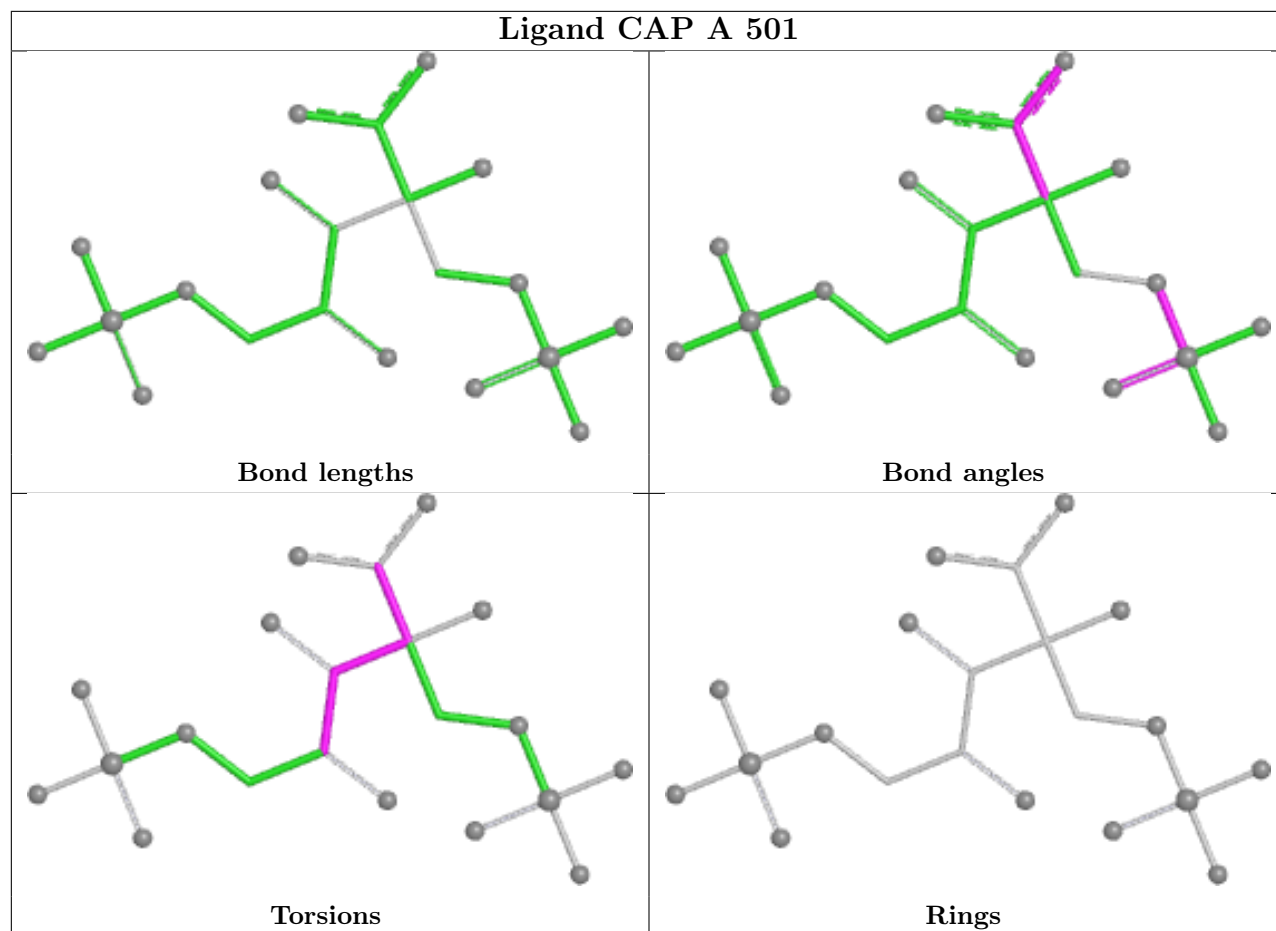
7 monomers are involved in 13 short contacts:

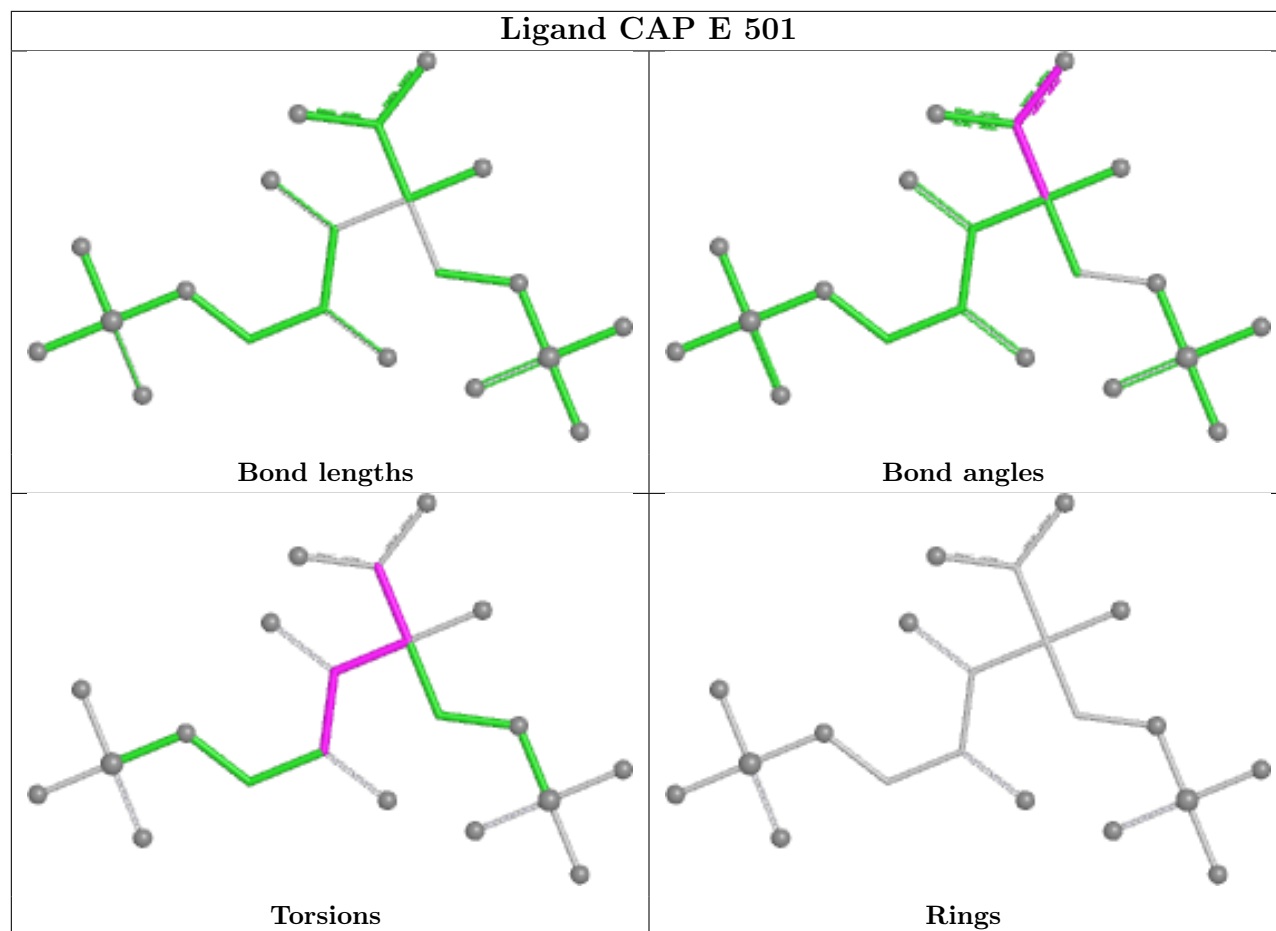
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	CAP	1	0
2	A	501	CAP	2	0
2	F	501	CAP	2	0
2	J	502	CAP	2	0
2	I	502	CAP	2	0
2	H	501	CAP	3	0
2	B	501	CAP	1	0

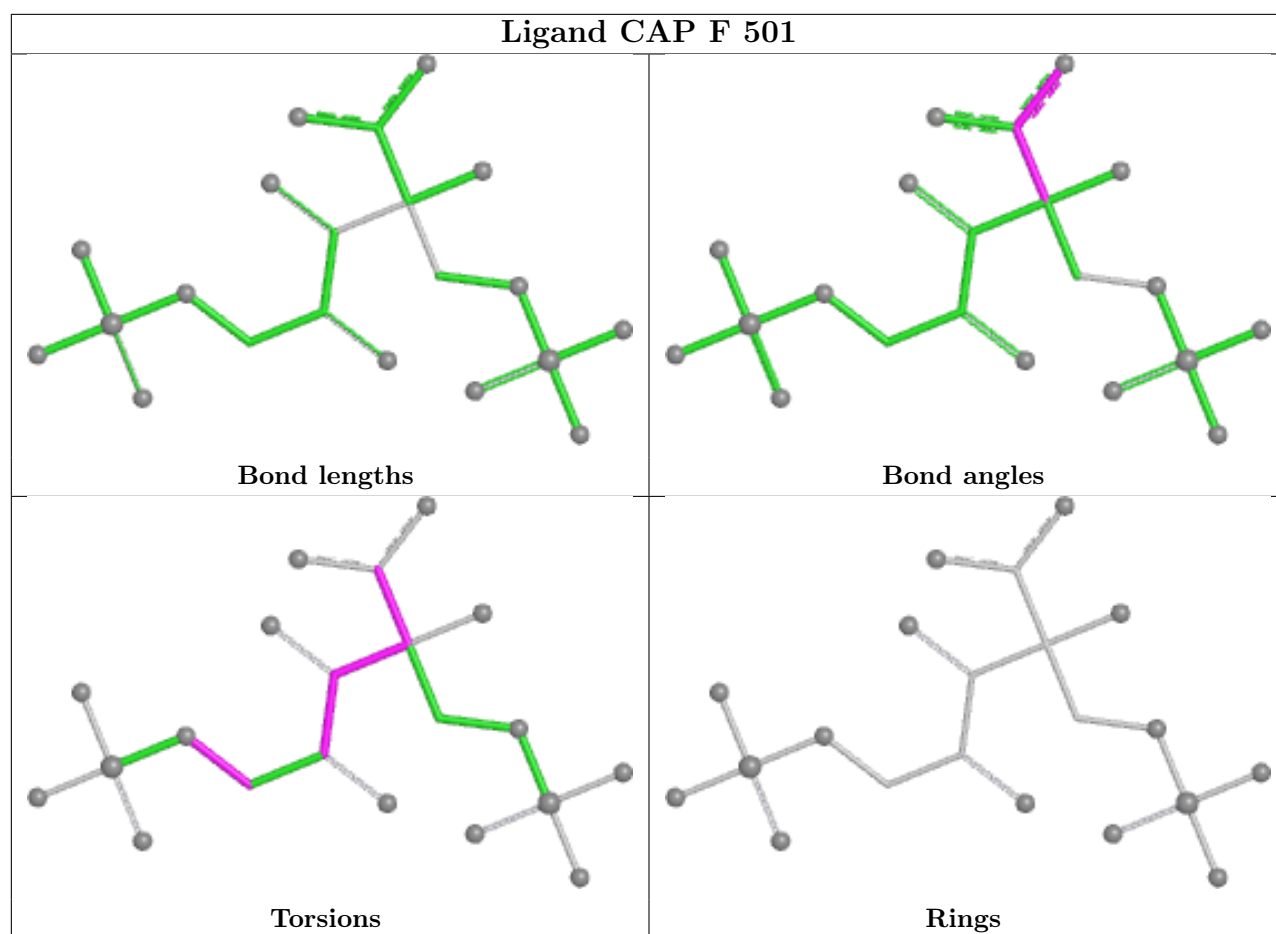
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



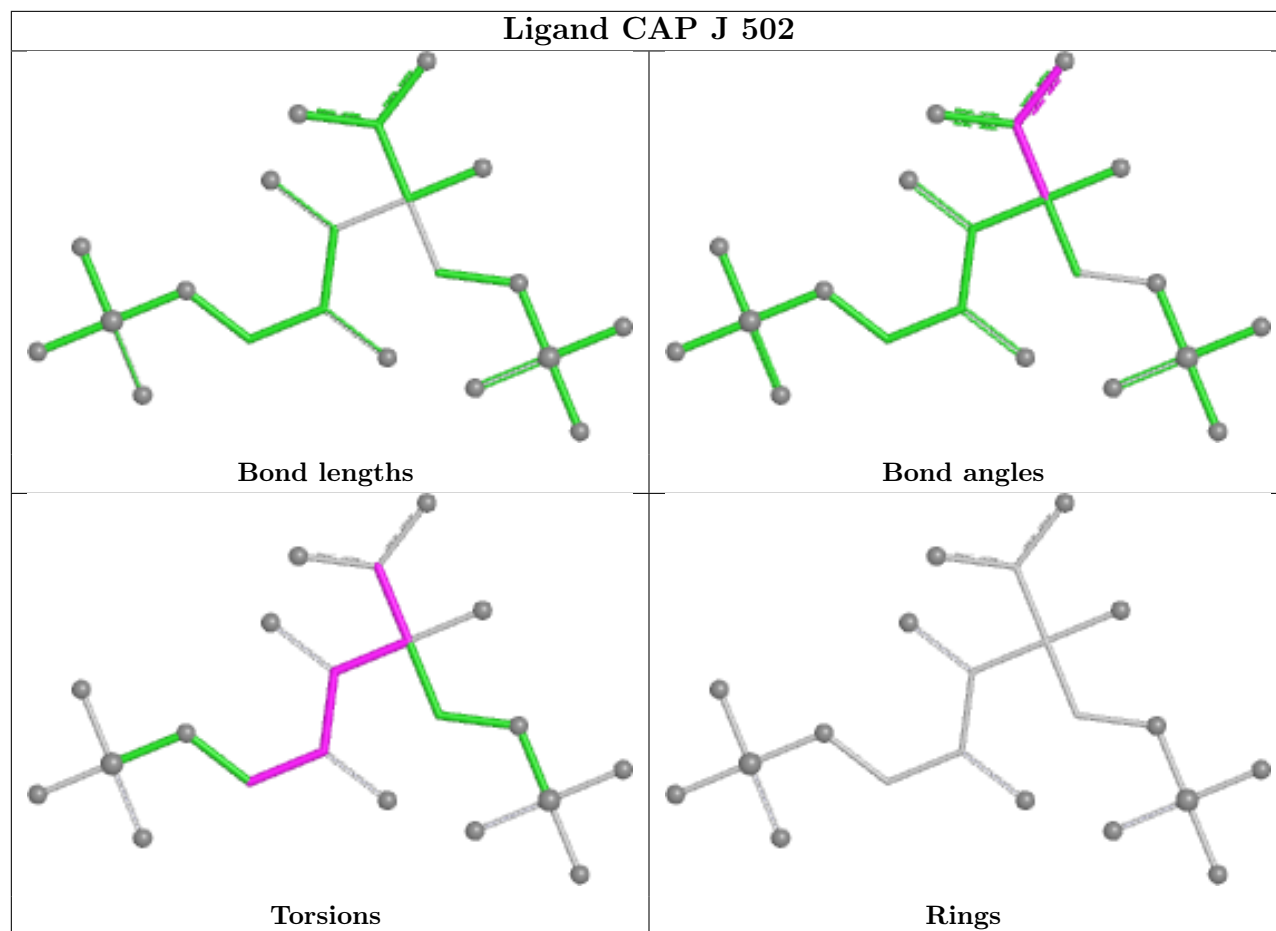




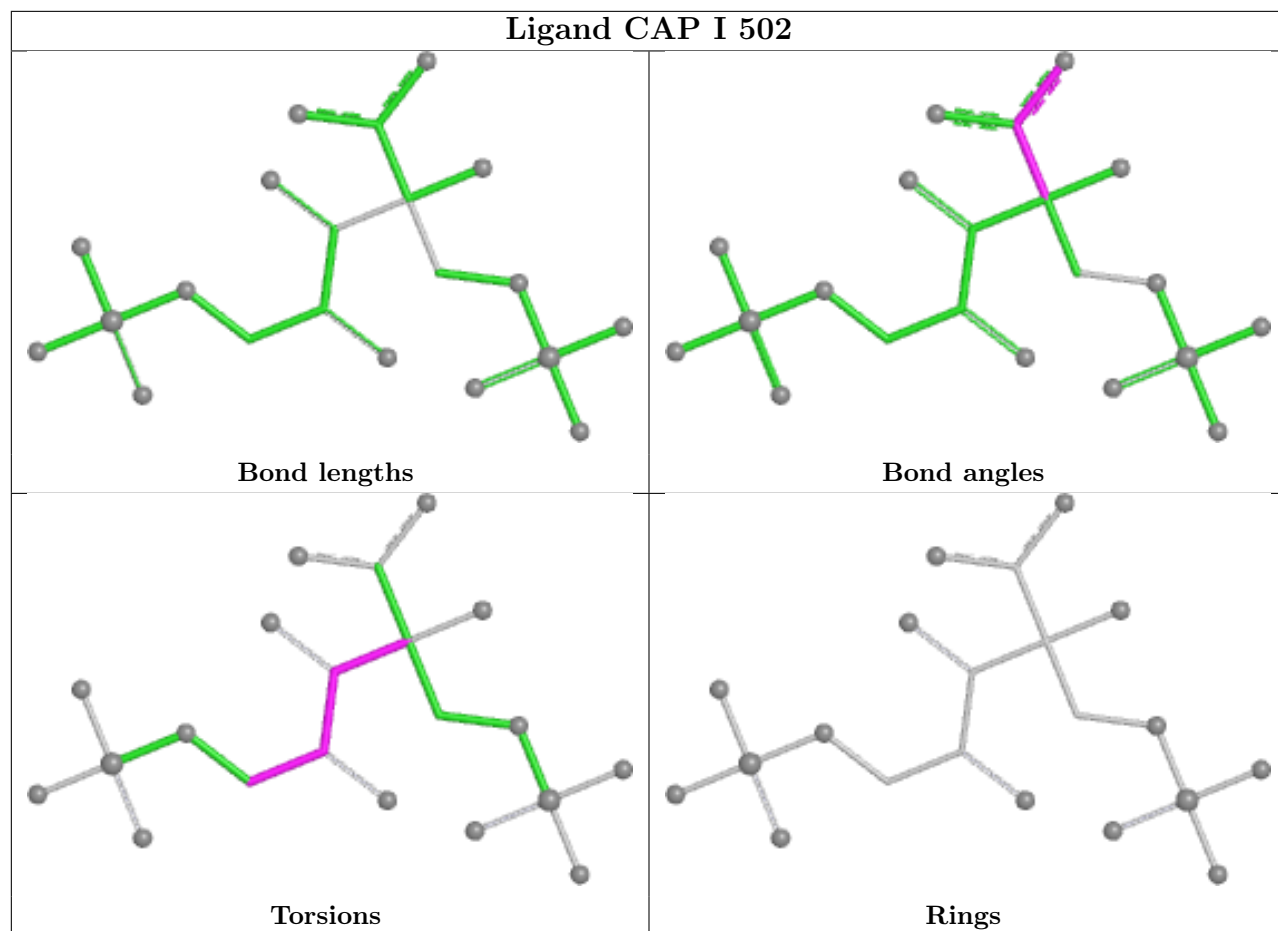


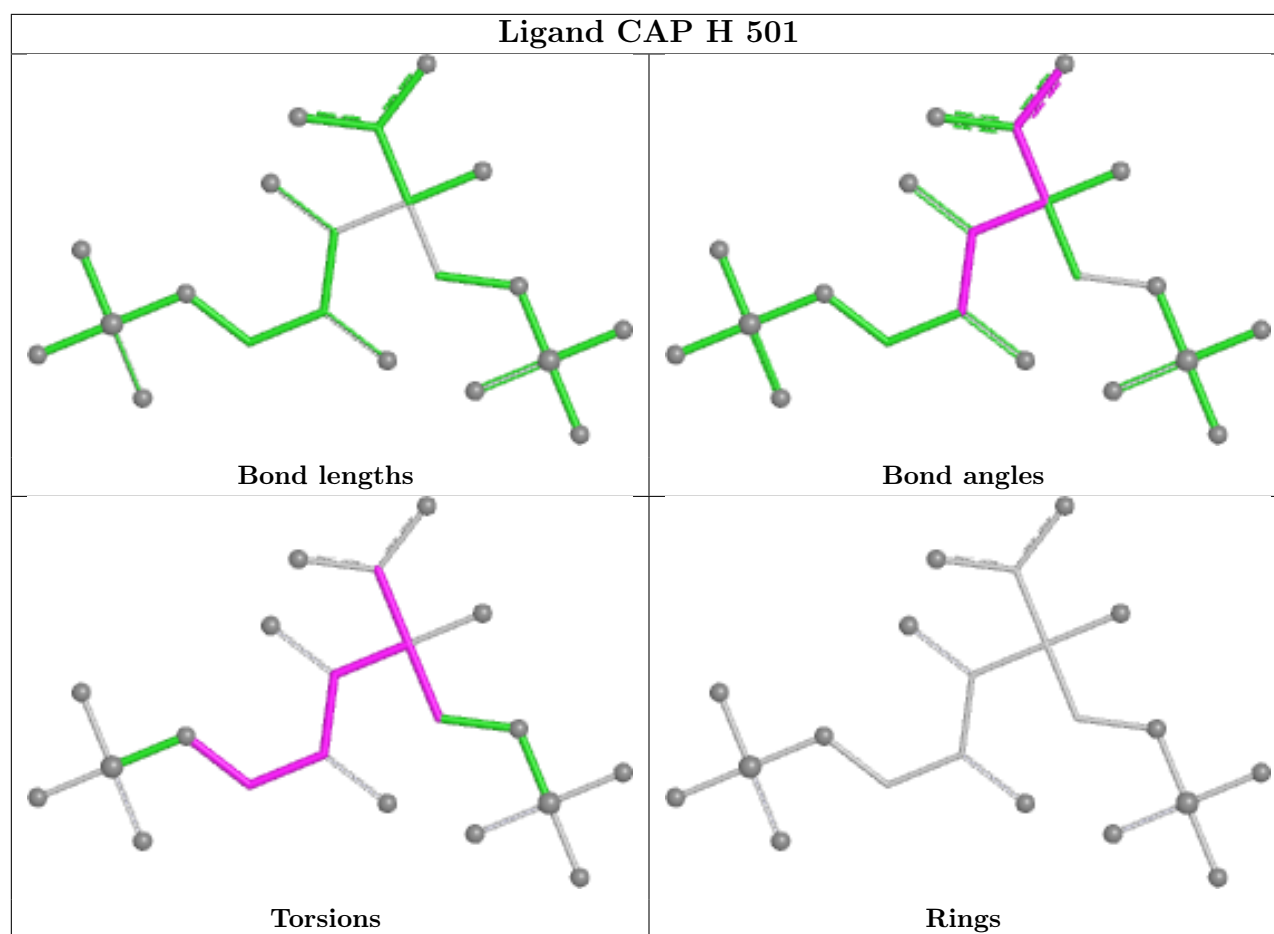


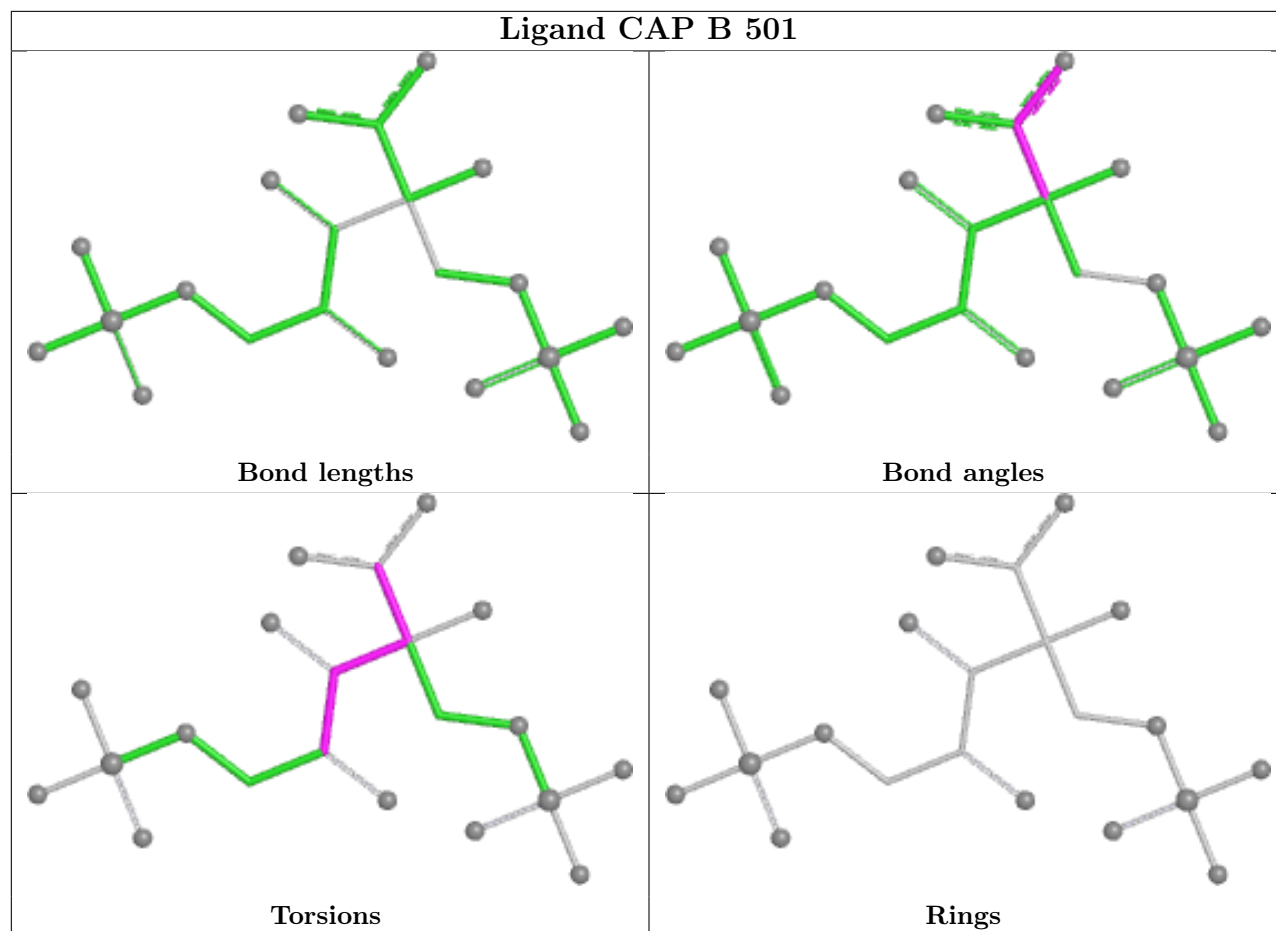
Ligand CAP J 502

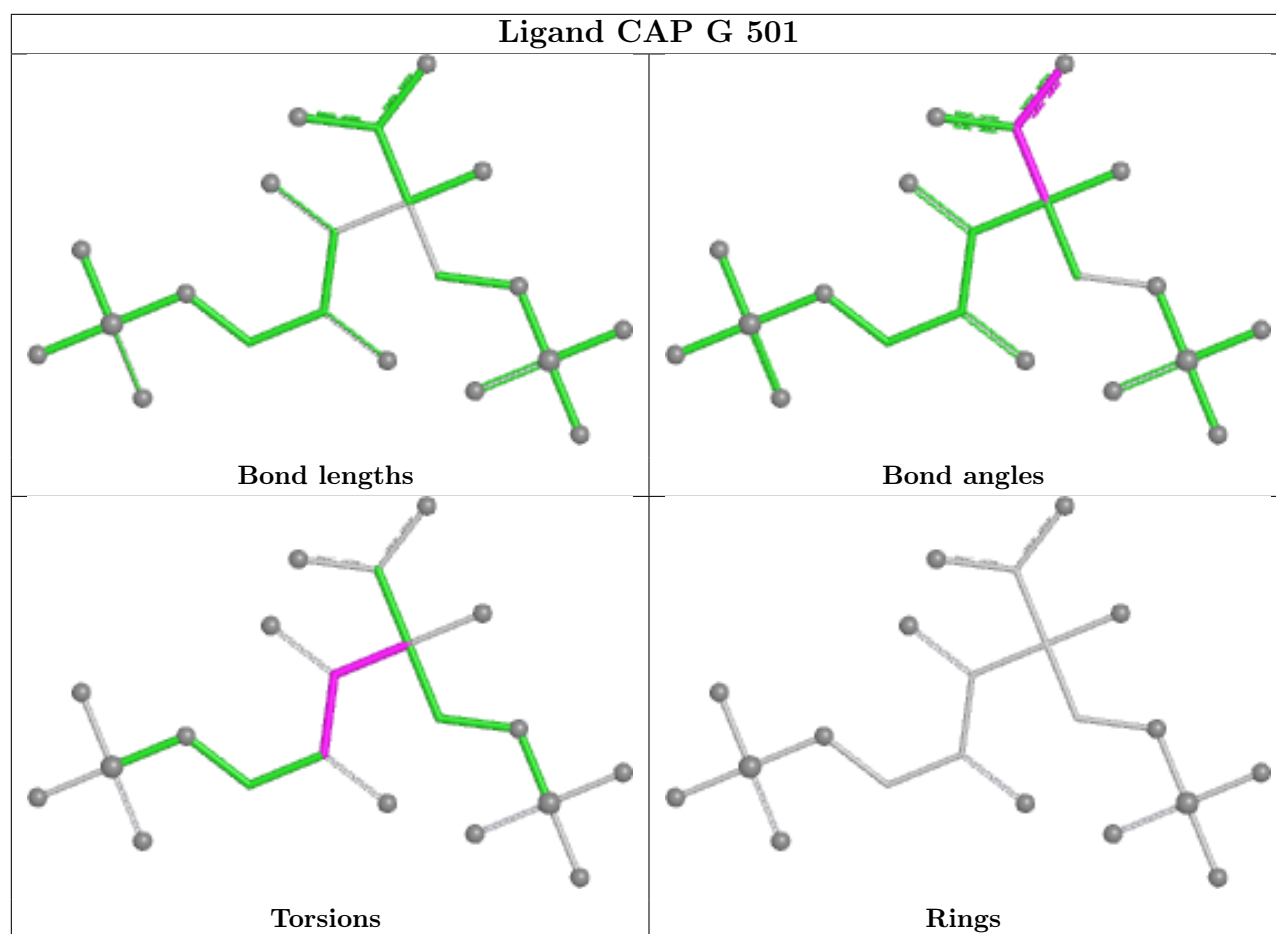


Ligand CAP I 502









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	456/468 (97%)	-0.17	2 (0%) 89 88	21, 34, 54, 114	0
1	B	456/468 (97%)	-0.17	4 (0%) 81 79	20, 34, 61, 104	0
1	C	456/468 (97%)	0.18	4 (0%) 81 79	28, 51, 76, 110	0
1	D	456/468 (97%)	0.84	47 (10%) 13 12	43, 73, 96, 139	0
1	E	456/468 (97%)	0.29	5 (1%) 77 75	32, 55, 78, 123	0
1	F	456/468 (97%)	0.87	29 (6%) 27 24	56, 74, 97, 128	0
1	G	456/468 (97%)	1.81	168 (36%) 1 0	80, 106, 133, 178	0
1	H	456/468 (97%)	2.13	223 (48%) 0 0	90, 105, 134, 169	0
1	I	456/468 (97%)	1.93	200 (43%) 1 0	81, 102, 138, 176	0
1	J	456/468 (97%)	1.84	182 (39%) 1 0	73, 112, 142, 167	0
All	All	4560/4680 (97%)	0.95	864 (18%) 4 4	20, 76, 127, 178	0

All (864) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	301	ALA	8.4
1	G	272	PHE	6.7
1	J	294	LEU	6.0
1	I	250	GLY	5.9
1	H	297	PHE	5.9
1	J	297	PHE	5.8
1	H	16	GLY	5.8
1	J	19	MET	5.7
1	H	294	LEU	5.7
1	H	10	ASN	5.7
1	I	289	TYR	5.6
1	J	372	TYR	5.6
1	J	78	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	J	47	GLY	5.5
1	H	148	PHE	5.4
1	G	297	PHE	5.3
1	H	152	ILE	5.3
1	H	97	PHE	5.3
1	H	96	THR	5.2
1	I	177	PHE	5.2
1	H	275	ALA	5.2
1	I	255	TRP	5.2
1	J	8	ILE	5.1
1	J	275	ALA	5.1
1	H	62	LEU	5.0
1	J	123	LEU	5.0
1	G	372	TYR	5.0
1	H	110	VAL	4.9
1	H	291	VAL	4.9
1	H	91	VAL	4.9
1	H	78	ILE	4.9
1	I	347	ILE	4.9
1	G	25	LEU	4.9
1	G	255	TRP	4.9
1	G	387	LEU	4.8
1	I	373	TRP	4.8
1	J	301	ALA	4.8
1	I	380	CYS	4.8
1	J	439	LEU	4.8
1	J	116	VAL	4.8
1	G	199	VAL	4.8
1	J	65	LEU	4.7
1	H	395	PHE	4.7
1	I	251	ILE	4.7
1	F	372	TYR	4.6
1	H	354	LEU	4.6
1	J	348	PRO	4.6
1	H	372	TYR	4.6
1	H	348	PRO	4.6
1	H	37	ALA	4.6
1	H	380	CYS	4.6
1	H	150	SER	4.5
1	J	56	THR	4.5
1	I	387	LEU	4.5
1	H	295	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	255	TRP	4.5
1	G	166	LEU	4.5
1	J	374	ARG	4.5
1	J	358	ILE	4.5
1	H	123	LEU	4.5
1	J	402	GLN	4.5
1	J	64	ALA	4.5
1	D	18	TYR	4.4
1	G	215	VAL	4.4
1	H	457	ASP	4.4
1	H	58	PHE	4.4
1	G	289	TYR	4.4
1	H	158	LEU	4.3
1	I	248	VAL	4.3
1	I	272	PHE	4.3
1	G	306	ILE	4.3
1	G	177	PHE	4.3
1	I	160	SER	4.3
1	G	102	VAL	4.3
1	H	84	ILE	4.2
1	I	121	GLN	4.2
1	I	91	VAL	4.2
1	H	385	GLY	4.2
1	J	258	ILE	4.1
1	H	157	GLY	4.1
1	H	183	PRO	4.1
1	I	176	ASP	4.1
1	J	343	ILE	4.1
1	J	66	VAL	4.0
1	C	373	TRP	4.0
1	G	158	LEU	4.0
1	H	156	ILE	4.0
1	H	382	ILE	4.0
1	J	91	VAL	4.0
1	G	95	MET	4.0
1	I	97	PHE	4.0
1	H	343	ILE	4.0
1	I	308	THR	4.0
1	D	289	TYR	4.0
1	F	452	ALA	3.9
1	G	410	ALA	3.9
1	J	279	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	426	VAL	3.9
1	I	306	ILE	3.9
1	H	45	SER	3.9
1	H	352	ALA	3.9
1	H	66	VAL	3.9
1	H	248	VAL	3.9
1	J	7	GLN	3.9
1	G	167	CYS	3.9
1	I	412	VAL	3.8
1	J	251	ILE	3.8
1	D	373	TRP	3.8
1	I	166	LEU	3.8
1	H	251	ILE	3.8
1	J	85	PHE	3.8
1	F	275	ALA	3.8
1	J	54	THR	3.8
1	D	25	LEU	3.7
1	H	258	ILE	3.7
1	H	368	SER	3.7
1	I	103	PHE	3.7
1	J	225	TYR	3.7
1	G	84	ILE	3.7
1	I	147	ILE	3.7
1	J	278	GLY	3.7
1	I	25	LEU	3.7
1	J	354	LEU	3.7
1	J	387	LEU	3.7
1	G	120	PRO	3.7
1	G	47	GLY	3.7
1	G	103	PHE	3.7
1	J	378	LYS	3.7
1	H	289	TYR	3.7
1	G	293	VAL	3.7
1	J	255	TRP	3.7
1	H	405	ILE	3.7
1	J	142	ILE	3.7
1	D	275	ALA	3.6
1	C	372	TYR	3.6
1	H	126	TYR	3.6
1	H	49	PHE	3.6
1	G	301	ALA	3.6
1	I	89	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	58	PHE	3.6
1	I	303	ALA	3.6
1	I	22	VAL	3.6
1	J	340	PHE	3.6
1	H	284	GLU	3.6
1	D	64	ALA	3.6
1	H	185	ALA	3.6
1	I	83	ARG	3.6
1	H	54	THR	3.6
1	D	16	GLY	3.6
1	H	177	PHE	3.6
1	I	189	PHE	3.6
1	G	94	ILE	3.5
1	J	98	ILE	3.5
1	H	36	THR	3.5
1	J	373	TRP	3.5
1	J	122	MET	3.5
1	G	299	ARG	3.5
1	I	48	SER	3.5
1	I	293	VAL	3.5
1	H	95	MET	3.5
1	H	44	SER	3.5
1	G	313	ILE	3.5
1	I	372	TYR	3.5
1	H	300	LEU	3.5
1	J	406	THR	3.5
1	E	372	TYR	3.5
1	H	55	ALA	3.4
1	I	125	GLN	3.4
1	H	379	MET	3.4
1	I	257	ALA	3.4
1	G	258	ILE	3.4
1	I	405	ILE	3.4
1	G	300	LEU	3.4
1	H	147	ILE	3.4
1	I	98	ILE	3.4
1	J	6	ILE	3.4
1	J	80	TYR	3.4
1	H	344	TRP	3.4
1	H	298	ALA	3.4
1	I	178	VAL	3.4
1	H	386	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	304	SER	3.4
1	I	32	THR	3.4
1	I	423	ALA	3.3
1	H	306	ILE	3.3
1	H	358	ILE	3.3
1	I	258	ILE	3.3
1	J	34	VAL	3.3
1	H	122	MET	3.3
1	H	435	GLN	3.3
1	J	401	THR	3.3
1	H	77	TRP	3.3
1	J	126	TYR	3.3
1	J	289	TYR	3.3
1	G	98	ILE	3.3
1	I	453	ILE	3.3
1	H	189	PHE	3.3
1	I	29	GLU	3.3
1	G	99	ALA	3.3
1	H	52	ILE	3.3
1	J	52	ILE	3.3
1	I	40	VAL	3.3
1	H	390	LEU	3.3
1	H	146	PRO	3.3
1	H	99	ALA	3.3
1	G	412	VAL	3.3
1	I	124	VAL	3.3
1	I	277	HIS	3.3
1	J	272	PHE	3.3
1	H	142	ILE	3.2
1	J	21	ALA	3.2
1	J	156	ILE	3.2
1	G	373	TRP	3.2
1	J	339	TYR	3.2
1	H	34	VAL	3.2
1	J	40	VAL	3.2
1	D	276	GLY	3.2
1	I	295	THR	3.2
1	G	251	ILE	3.2
1	H	8	ILE	3.2
1	H	387	LEU	3.2
1	D	27	GLY	3.2
1	G	56	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	11	PRO	3.2
1	H	43	GLU	3.2
1	I	275	ALA	3.2
1	I	123	LEU	3.2
1	I	47	GLY	3.2
1	H	351	ASP	3.2
1	G	191	PRO	3.2
1	I	416	PRO	3.2
1	G	407	THR	3.2
1	J	37	ALA	3.2
1	H	184	GLN	3.2
1	J	118	PHE	3.2
1	J	32	THR	3.1
1	J	308	THR	3.1
1	G	44	SER	3.1
1	G	160	SER	3.1
1	I	356	LEU	3.1
1	D	77	TRP	3.1
1	H	98	ILE	3.1
1	J	62	LEU	3.1
1	H	327	ALA	3.1
1	G	189	PHE	3.1
1	H	14	PHE	3.1
1	H	103	PHE	3.1
1	J	280	PHE	3.1
1	E	225	TYR	3.1
1	H	288	GLY	3.1
1	G	380	CYS	3.1
1	J	1	MET	3.1
1	I	52	ILE	3.1
1	J	114	LEU	3.1
1	G	91	VAL	3.1
1	I	164	ALA	3.1
1	J	13	VAL	3.1
1	J	148	PHE	3.1
1	J	404	PHE	3.1
1	H	82	TRP	3.1
1	H	81	PRO	3.1
1	H	119	PRO	3.1
1	H	215	VAL	3.1
1	I	246	PHE	3.1
1	J	177	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	117	TYR	3.1
1	H	437	ILE	3.0
1	H	439	LEU	3.0
1	I	8	ILE	3.0
1	I	84	ILE	3.0
1	I	113	ILE	3.0
1	H	40	VAL	3.0
1	I	202	ALA	3.0
1	I	274	ARG	3.0
1	E	143	GLN	3.0
1	H	280	PHE	3.0
1	I	386	GLY	3.0
1	H	373	TRP	3.0
1	I	43	GLU	3.0
1	J	147	ILE	3.0
1	H	376	THR	3.0
1	H	13	VAL	3.0
1	H	412	VAL	3.0
1	I	327	ALA	3.0
1	J	410	ALA	3.0
1	I	95	MET	3.0
1	G	217	SER	3.0
1	I	309	GLY	3.0
1	J	44	SER	3.0
1	G	147	ILE	3.0
1	G	287	ILE	3.0
1	H	235	ILE	3.0
1	G	37	ALA	3.0
1	E	160	SER	3.0
1	I	77	TRP	3.0
1	B	69	ILE	3.0
1	H	225	TYR	3.0
1	H	383	ILE	3.0
1	I	67	TYR	3.0
1	J	84	ILE	3.0
1	H	32	THR	3.0
1	J	263	ARG	3.0
1	G	50	VAL	3.0
1	I	44	SER	3.0
1	H	144	GLU	2.9
1	G	142	ILE	2.9
1	H	433	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	152	ILE	2.9
1	I	24	ARG	2.9
1	I	56	THR	2.9
1	I	291	VAL	2.9
1	J	79	ALA	2.9
1	J	324	VAL	2.9
1	G	53	GLY	2.9
1	I	276	GLY	2.9
1	H	313	ILE	2.9
1	G	344	TRP	2.9
1	G	430	TYR	2.9
1	I	13	VAL	2.9
1	I	301	ALA	2.9
1	G	26	GLN	2.9
1	J	81	PRO	2.9
1	G	391	LEU	2.9
1	D	107	SER	2.9
1	G	383	ILE	2.9
1	J	295	THR	2.9
1	J	24	ARG	2.9
1	D	67	TYR	2.9
1	G	159	THR	2.9
1	I	159	THR	2.9
1	G	429	ALA	2.9
1	J	55	ALA	2.9
1	D	297	PHE	2.9
1	I	129	PRO	2.9
1	J	183	PRO	2.9
1	G	385	GLY	2.9
1	H	104	GLY	2.9
1	I	111	CYS	2.9
1	I	1	MET	2.8
1	G	156	ILE	2.8
1	H	287	ILE	2.8
1	H	214	LYS	2.8
1	G	339	TYR	2.8
1	G	451	ALA	2.8
1	I	279	ALA	2.8
1	I	330	ALA	2.8
1	I	297	PHE	2.8
1	G	288	GLY	2.8
1	G	354	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	20	LEU	2.8
1	J	144	GLU	2.8
1	H	124	VAL	2.8
1	G	334	TYR	2.8
1	I	294	LEU	2.8
1	G	113	ILE	2.8
1	I	167	CYS	2.8
1	J	108	VAL	2.8
1	I	26	GLN	2.8
1	D	49	PHE	2.8
1	G	292	PRO	2.8
1	I	158	LEU	2.8
1	I	333	LEU	2.8
1	J	33	LEU	2.8
1	H	332	LYS	2.8
1	G	36	THR	2.8
1	G	82	TRP	2.8
1	I	41	ALA	2.8
1	I	406	THR	2.8
1	D	148	PHE	2.8
1	G	395	PHE	2.8
1	D	350	LYS	2.8
1	J	370	LEU	2.8
1	G	453	ILE	2.7
1	D	279	ALA	2.7
1	I	96	THR	2.7
1	I	197	GLN	2.7
1	D	372	TYR	2.7
1	H	328	ARG	2.7
1	J	382	ILE	2.7
1	F	108	VAL	2.7
1	I	253	ALA	2.7
1	H	404	PHE	2.7
1	J	389	PRO	2.7
1	G	411	GLY	2.7
1	G	271	HIS	2.7
1	H	80	TYR	2.7
1	H	367	TYR	2.7
1	I	80	TYR	2.7
1	J	131	TYR	2.7
1	H	113	ILE	2.7
1	I	69	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	287	ILE	2.7
1	I	115	ASP	2.7
1	G	101	ASN	2.7
1	I	101	ASN	2.7
1	H	19	MET	2.7
1	H	324	VAL	2.7
1	F	7	GLN	2.7
1	G	111	CYS	2.7
1	H	303	ALA	2.7
1	J	257	ALA	2.7
1	G	97	PHE	2.7
1	H	132	THR	2.7
1	I	54	THR	2.7
1	J	376	THR	2.7
1	H	48	SER	2.7
1	J	82	TRP	2.7
1	G	83	ARG	2.7
1	H	411	GLY	2.7
1	J	88	GLY	2.7
1	I	346	GLU	2.7
1	H	121	GLN	2.7
1	H	452	ALA	2.7
1	J	298	ALA	2.7
1	I	302	GLY	2.7
1	D	225	TYR	2.6
1	I	388	ASN	2.6
1	H	292	PRO	2.6
1	H	252	THR	2.6
1	J	329	HIS	2.6
1	G	157	GLY	2.6
1	H	438	SER	2.6
1	D	5	TYR	2.6
1	J	316	MET	2.6
1	H	198	ASP	2.6
1	G	206	VAL	2.6
1	G	247	LEU	2.6
1	I	34	VAL	2.6
1	J	399	VAL	2.6
1	J	11	PRO	2.6
1	C	21	ALA	2.6
1	G	58	PHE	2.6
1	G	24	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	30	GLY	2.6
1	J	48	SER	2.6
1	J	261	ILE	2.6
1	I	51	LYS	2.6
1	G	457	ASP	2.6
1	G	219	ASN	2.6
1	G	248	VAL	2.6
1	D	37	ALA	2.6
1	I	148	PHE	2.6
1	H	406	THR	2.6
1	D	47	GLY	2.6
1	G	220	ILE	2.6
1	G	144	GLU	2.6
1	J	43	GLU	2.6
1	H	5	TYR	2.6
1	G	294	LEU	2.6
1	H	180	ASN	2.6
1	I	37	ALA	2.6
1	I	79	ALA	2.6
1	J	395	PHE	2.6
1	G	96	THR	2.6
1	H	407	THR	2.6
1	G	78	ILE	2.6
1	H	168	TYR	2.5
1	J	367	TYR	2.5
1	J	331	LEU	2.5
1	B	11	PRO	2.5
1	J	338	ASP	2.5
1	F	215	VAL	2.5
1	I	299	ARG	2.5
1	J	83	ARG	2.5
1	J	145	ARG	2.5
1	J	342	GLN	2.5
1	G	64	ALA	2.5
1	G	275	ALA	2.5
1	I	57	ALA	2.5
1	G	415	HIS	2.5
1	G	305	GLY	2.5
1	G	386	GLY	2.5
1	H	242	GLY	2.5
1	H	396	ILE	2.5
1	I	36	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	104	GLY	2.5
1	J	154	PRO	2.5
1	G	246	PHE	2.5
1	J	103	PHE	2.5
1	J	388	ASN	2.5
1	F	358	ILE	2.5
1	G	375	ILE	2.5
1	I	287	ILE	2.5
1	H	377	LYS	2.5
1	H	4	GLU	2.5
1	H	39	GLU	2.5
1	H	172	SER	2.5
1	I	150	SER	2.5
1	H	25	LEU	2.5
1	D	120	PRO	2.5
1	J	355	GLN	2.5
1	H	413	HIS	2.5
1	J	23	PHE	2.5
1	G	88	GLY	2.5
1	J	318	GLY	2.5
1	I	221	SER	2.5
1	H	381	PRO	2.5
1	H	389	PRO	2.5
1	I	81	PRO	2.5
1	I	348	PRO	2.5
1	J	120	PRO	2.5
1	D	402	GLN	2.5
1	D	23	PHE	2.5
1	F	456	TYR	2.5
1	H	218	PHE	2.5
1	G	21	ALA	2.5
1	H	249	ASP	2.5
1	I	109	LYS	2.5
1	J	429	ALA	2.5
1	G	27	GLY	2.5
1	J	16	GLY	2.5
1	J	128	GLY	2.5
1	G	348	PRO	2.4
1	H	274	ARG	2.4
1	I	154	PRO	2.4
1	G	291	VAL	2.4
1	J	76	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	2.4
1	H	118	PHE	2.4
1	I	23	PHE	2.4
1	I	452	ALA	2.4
1	J	57	ALA	2.4
1	H	27	GLY	2.4
1	H	314	GLY	2.4
1	H	46	THR	2.4
1	I	419	THR	2.4
1	G	416	PRO	2.4
1	H	241	PRO	2.4
1	G	223	SER	2.4
1	I	102	VAL	2.4
1	J	22	VAL	2.4
1	D	111	CYS	2.4
1	G	8	ILE	2.4
1	H	334	TYR	2.4
1	D	346	GLU	2.4
1	D	33	LEU	2.4
1	H	65	LEU	2.4
1	I	427	LEU	2.4
1	J	247	LEU	2.4
1	D	3	LYS	2.4
1	G	22	VAL	2.4
1	I	116	VAL	2.4
1	J	368	SER	2.4
1	G	404	PHE	2.4
1	G	152	ILE	2.4
1	H	410	ALA	2.4
1	I	133	ILE	2.4
1	I	156	ILE	2.4
1	I	451	ALA	2.4
1	G	456	TYR	2.4
1	H	12	ASN	2.4
1	I	100	GLY	2.4
1	I	403	ASP	2.4
1	G	406	THR	2.4
1	G	270	LEU	2.4
1	H	370	LEU	2.4
1	I	33	LEU	2.4
1	J	346	GLU	2.4
1	G	381	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	408	MET	2.4
1	G	116	VAL	2.4
1	H	171	TRP	2.4
1	H	329	HIS	2.4
1	F	160	SER	2.4
1	F	395	PHE	2.4
1	I	455	PHE	2.4
1	J	14	PHE	2.4
1	G	6	ILE	2.4
1	I	55	ALA	2.4
1	I	64	ALA	2.4
1	I	358	ILE	2.4
1	I	126	TYR	2.4
1	J	30	GLY	2.4
1	H	140	LEU	2.3
1	G	196	VAL	2.3
1	H	116	VAL	2.3
1	I	426	VAL	2.3
1	J	50	VAL	2.3
1	I	85	PHE	2.3
1	J	121	GLN	2.3
1	F	313	ILE	2.3
1	G	38	SER	2.3
1	G	232	ALA	2.3
1	G	317	ALA	2.3
1	H	133	ILE	2.3
1	H	276	GLY	2.3
1	H	409	GLY	2.3
1	J	364	GLY	2.3
1	H	188	ASP	2.3
1	J	15	ASN	2.3
1	H	356	LEU	2.3
1	I	20	LEU	2.3
1	I	310	THR	2.3
1	J	96	THR	2.3
1	J	300	LEU	2.3
1	I	365	GLU	2.3
1	D	34	VAL	2.3
1	G	40	VAL	2.3
1	I	108	VAL	2.3
1	G	52	ILE	2.3
1	H	229	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	113	ILE	2.3
1	H	326	ALA	2.3
1	I	16	GLY	2.3
1	A	65	LEU	2.3
1	B	225	TYR	2.3
1	H	117	TYR	2.3
1	I	62	LEU	2.3
1	J	270	LEU	2.3
1	J	456	TYR	2.3
1	I	219	ASN	2.3
1	I	227	THR	2.3
1	J	10	ASN	2.3
1	H	136	MET	2.3
1	I	50	VAL	2.3
1	I	66	VAL	2.3
1	J	269	PHE	2.3
1	J	152	ILE	2.3
1	J	453	ILE	2.3
1	H	317	ALA	2.3
1	G	48	SER	2.3
1	H	345	SER	2.3
1	I	414	SER	2.3
1	H	302	GLY	2.3
1	I	371	GLY	2.3
1	I	140	LEU	2.3
1	D	1	MET	2.3
1	H	394	LYS	2.3
1	I	378	LYS	2.3
1	G	401	THR	2.3
1	G	280	PHE	2.3
1	I	395	PHE	2.3
1	I	375	ILE	2.3
1	I	396	ILE	2.3
1	H	202	ALA	2.3
1	H	309	GLY	2.3
1	D	123	LEU	2.3
1	F	414	SER	2.3
1	I	411	GLY	2.3
1	G	114	LEU	2.3
1	H	194	LYS	2.2
1	I	114	LEU	2.3
1	J	95	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	32	THR	2.2
1	G	192	TYR	2.2
1	H	131	TYR	2.2
1	H	159	THR	2.2
1	J	457	ASP	2.2
1	F	167	CYS	2.2
1	H	216	HIS	2.2
1	J	293	VAL	2.2
1	H	6	ILE	2.2
1	H	375	ILE	2.2
1	I	49	PHE	2.2
1	I	94	ILE	2.2
1	I	404	PHE	2.2
1	J	97	PHE	2.2
1	G	253	ALA	2.2
1	H	79	ALA	2.2
1	H	164	ALA	2.2
1	G	333	LEU	2.2
1	G	243	SER	2.2
1	G	162	GLU	2.2
1	F	295	THR	2.2
1	J	5	TYR	2.2
1	G	108	VAL	2.2
1	G	324	VAL	2.2
1	I	280	PHE	2.2
1	I	383	ILE	2.2
1	D	112	LYS	2.2
1	J	326	ALA	2.2
1	H	316	MET	2.2
1	I	344	TRP	2.2
1	F	309	GLY	2.2
1	H	100	GLY	2.2
1	H	400	GLY	2.2
1	J	166	LEU	2.2
1	H	137	ARG	2.2
1	G	161	SER	2.2
1	J	345	SER	2.2
1	D	39	GLU	2.2
1	G	252	THR	2.2
1	G	310	THR	2.2
1	G	10	ASN	2.2
1	H	67	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	456	TYR	2.2
1	H	127	ASP	2.2
1	J	86	ASP	2.2
1	H	50	VAL	2.2
1	H	102	VAL	2.2
1	H	340	PHE	2.2
1	I	269	PHE	2.2
1	J	313	ILE	2.2
1	G	212	LYS	2.2
1	G	41	ALA	2.2
1	G	327	ALA	2.2
1	G	330	ALA	2.2
1	H	423	ALA	2.2
1	I	106	ALA	2.2
1	J	330	ALA	2.2
1	H	449	LEU	2.2
1	I	449	LEU	2.2
1	J	356	LEU	2.2
1	C	364	GLY	2.2
1	F	30	GLY	2.2
1	J	276	GLY	2.2
1	J	411	GLY	2.2
1	F	154	PRO	2.2
1	J	292	PRO	2.2
1	G	403	ASP	2.2
1	H	339	TYR	2.2
1	I	367	TYR	2.2
1	I	369	ASN	2.2
1	J	63	ASP	2.2
1	D	6	ILE	2.2
1	F	196	VAL	2.2
1	H	69	ILE	2.2
1	H	143	GLN	2.2
1	H	220	ILE	2.2
1	H	293	VAL	2.2
1	I	14	PHE	2.2
1	J	92	GLN	2.2
1	J	3	LYS	2.2
1	J	230	LYS	2.2
1	G	55	ALA	2.2
1	G	75	LEU	2.2
1	H	21	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	370	LEU	2.2
1	J	357	ALA	2.2
1	G	276	GLY	2.2
1	H	88	GLY	2.2
1	H	200	ARG	2.2
1	I	128	GLY	2.2
1	G	384	SER	2.1
1	H	59	SER	2.1
1	I	415	HIS	2.1
1	G	225	TYR	2.1
1	D	116	VAL	2.1
1	G	153	LYS	2.1
1	H	399	VAL	2.1
1	J	58	PHE	2.1
1	J	377	LYS	2.1
1	I	31	MET	2.1
1	D	65	LEU	2.1
1	G	62	LEU	2.1
1	I	21	ALA	2.1
1	F	386	GLY	2.1
1	D	348	PRO	2.1
1	G	183	PRO	2.1
1	J	381	PRO	2.1
1	G	414	SER	2.1
1	H	398	THR	2.1
1	I	2	GLN	2.1
1	I	6	ILE	2.1
1	I	180	ASN	2.1
1	A	372	TYR	2.1
1	D	102	VAL	2.1
1	D	126	TYR	2.1
1	G	454	GLN	2.1
1	I	430	TYR	2.1
1	J	136	MET	2.1
1	H	272	PHE	2.1
1	I	118	PHE	2.1
1	I	249	ASP	2.1
1	J	248	VAL	2.1
1	I	311	ALA	2.1
1	I	374	ARG	2.1
1	J	42	ALA	2.1
1	G	174	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	400	GLY	2.1
1	J	309	GLY	2.1
1	J	380	CYS	2.1
1	G	43	GLU	2.1
1	J	146	PRO	2.1
1	J	365	GLU	2.1
1	D	54	THR	2.1
1	G	172	SER	2.1
1	I	107	SER	2.1
1	I	222	SER	2.1
1	J	107	SER	2.1
1	D	98	ILE	2.1
1	H	26	GLN	2.1
1	H	269	PHE	2.1
1	H	33	LEU	2.1
1	I	270	LEU	2.1
1	J	25	LEU	2.1
1	F	37	ALA	2.1
1	F	164	ALA	2.1
1	G	100	GLY	2.1
1	J	371	GLY	2.1
1	I	292	PRO	2.1
1	I	322	GLU	2.1
1	I	72	LYS	2.1
1	G	195	MET	2.1
1	G	290	THR	2.1
1	J	252	THR	2.1
1	H	199	VAL	2.1
1	I	435	GLN	2.1
1	G	449	LEU	2.1
1	H	93	ASN	2.1
1	H	114	LEU	2.1
1	H	166	LEU	2.1
1	H	391	LEU	2.1
1	G	35	ASP	2.1
1	G	145	ARG	2.1
1	G	181	ASP	2.1
1	I	338	ASP	2.1
1	G	279	ALA	2.1
1	I	232	ALA	2.1
1	D	30	GLY	2.1
1	G	173	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	385	GLY	2.1
1	H	271	HIS	2.0
1	B	1	MET	2.0
1	F	95	MET	2.0
1	H	1	MET	2.0
1	I	228	MET	2.0
1	I	417	MET	2.0
1	F	419	THR	2.0
1	H	56	THR	2.0
1	I	407	THR	2.0
1	I	392	ILE	2.0
1	J	69	ILE	2.0
1	J	306	ILE	2.0
1	F	150	SER	2.0
1	G	34	VAL	2.0
1	H	160	SER	2.0
1	H	170	PHE	2.0
1	H	208	GLN	2.0
1	I	384	SER	2.0
1	J	49	PHE	2.0
1	J	455	PHE	2.0
1	F	333	LEU	2.0
1	I	65	LEU	2.0
1	J	449	LEU	2.0
1	H	388	ASN	2.0
1	I	90	ASN	2.0
1	J	274	ARG	2.0
1	J	299	ARG	2.0
1	G	186	ASP	2.0
1	J	362	ALA	2.0
1	H	89	GLY	2.0
1	J	418	GLY	2.0
1	D	11	PRO	2.0
1	J	266	PRO	2.0
1	H	201	HIS	2.0
1	H	415	HIS	2.0
1	G	1	MET	2.0
1	G	379	MET	2.0
1	J	344	TRP	2.0
1	G	405	ILE	2.0
1	H	401	THR	2.0
1	D	85	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	7	GLN	2.0
1	H	85	PHE	2.0
1	J	189	PHE	2.0
1	D	44	SER	2.0
1	D	87	ARG	2.0
1	F	202	ALA	2.0
1	F	367	TYR	2.0
1	G	198	ASP	2.0
1	I	225	TYR	2.0
1	I	457	ASP	2.0
1	J	188	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	H	179	12/13	0.77	0.14	96,97,106,106	0
1	KCX	G	179	12/13	0.82	0.20	100,103,105,106	0
1	KCX	I	179	12/13	0.84	0.20	87,89,91,92	0
1	KCX	F	179	12/13	0.88	0.15	66,66,67,70	0
1	KCX	J	179	12/13	0.89	0.12	86,91,94,94	0
1	KCX	B	179	12/13	0.90	0.10	20,25,27,30	0
1	KCX	E	179	12/13	0.91	0.11	50,51,53,60	0
1	KCX	D	179	12/13	0.92	0.11	49,51,56,61	0
1	KCX	A	179	12/13	0.93	0.08	24,27,31,32	0
1	KCX	C	179	12/13	0.95	0.09	31,34,39,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

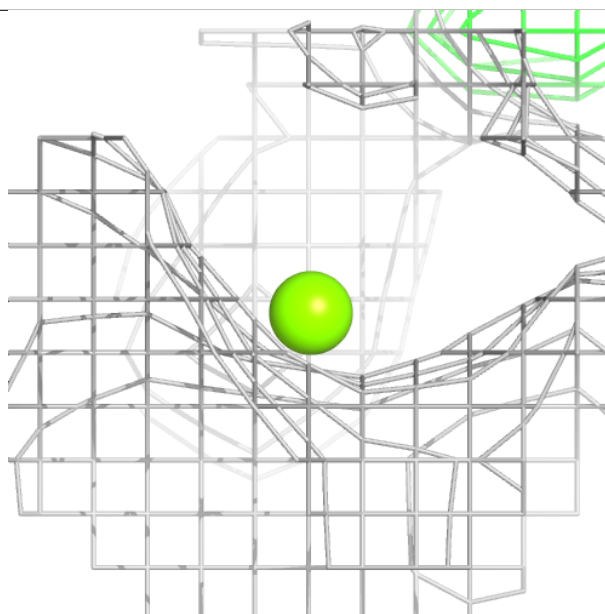
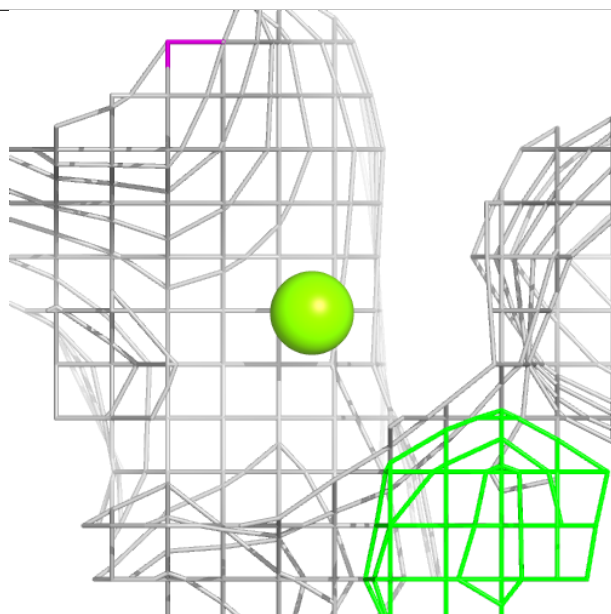
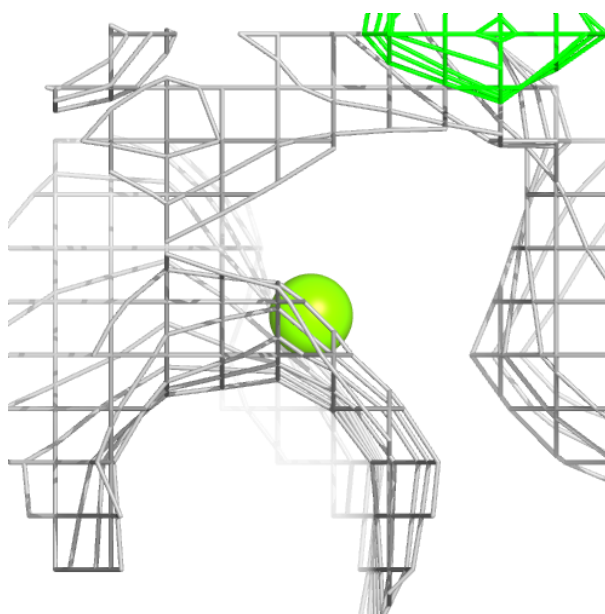
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	F	503	1/1	0.43	0.15	95,95,95,95	0
3	MG	E	503	1/1	0.55	0.15	88,88,88,88	0
3	MG	H	503	1/1	0.74	0.18	103,103,103,103	0
2	CAP	G	501	21/21	0.75	0.15	94,102,109,112	0
2	CAP	H	501	21/21	0.75	0.15	91,100,109,122	0
2	CAP	J	502	21/21	0.75	0.15	82,98,107,112	0
2	CAP	F	501	21/21	0.83	0.13	49,67,76,79	0
2	CAP	I	502	21/21	0.83	0.15	74,88,94,100	0
3	MG	A	504	1/1	0.87	0.06	53,53,53,53	0
3	MG	J	503	1/1	0.87	0.07	105,105,105,105	0
3	MG	G	503	1/1	0.89	0.11	97,97,97,97	0
2	CAP	D	502	21/21	0.89	0.11	44,58,67,68	0
3	MG	I	503	1/1	0.89	0.08	92,92,92,92	0
3	MG	B	503	1/1	0.89	0.09	43,43,43,43	0
2	CAP	E	501	21/21	0.92	0.09	35,50,57,65	0
2	CAP	A	501	21/21	0.92	0.10	31,36,47,112	0
3	MG	G	502	1/1	0.93	0.08	109,109,109,109	0
3	MG	A	503	1/1	0.94	0.05	34,34,34,34	0
2	CAP	B	501	21/21	0.95	0.07	24,30,39,73	0
3	MG	J	501	1/1	0.96	0.07	86,86,86,86	0
2	CAP	C	501	21/21	0.96	0.06	31,40,45,47	0
3	MG	H	502	1/1	0.97	0.07	86,86,86,86	0
3	MG	I	501	1/1	0.98	0.09	60,60,60,60	0
3	MG	F	502	1/1	0.98	0.07	54,54,54,54	0
3	MG	A	502	1/1	0.98	0.04	35,35,35,35	0
3	MG	B	502	1/1	0.98	0.13	46,46,46,46	0
3	MG	E	502	1/1	0.99	0.04	47,47,47,47	0
3	MG	C	502	1/1	0.99	0.02	35,35,35,35	0
3	MG	D	501	1/1	0.99	0.02	34,34,34,34	0
3	MG	D	503	1/1	0.99	0.03	49,49,49,49	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.

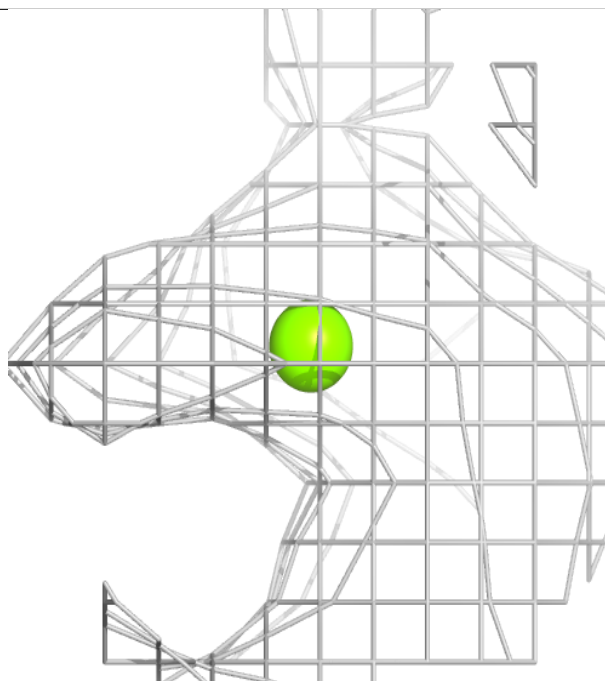
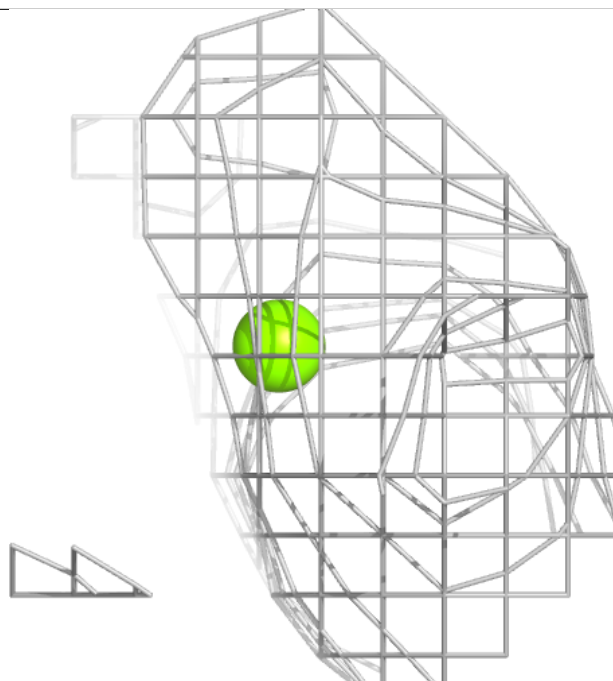
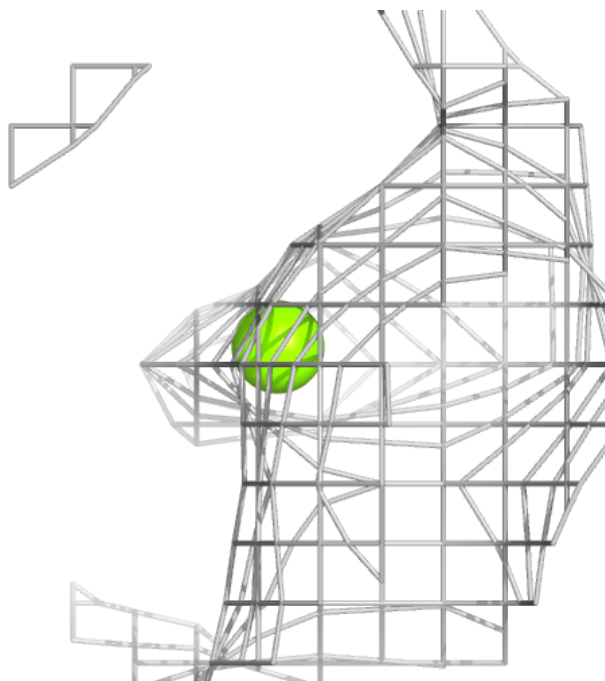
Electron density around MG F 503:

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



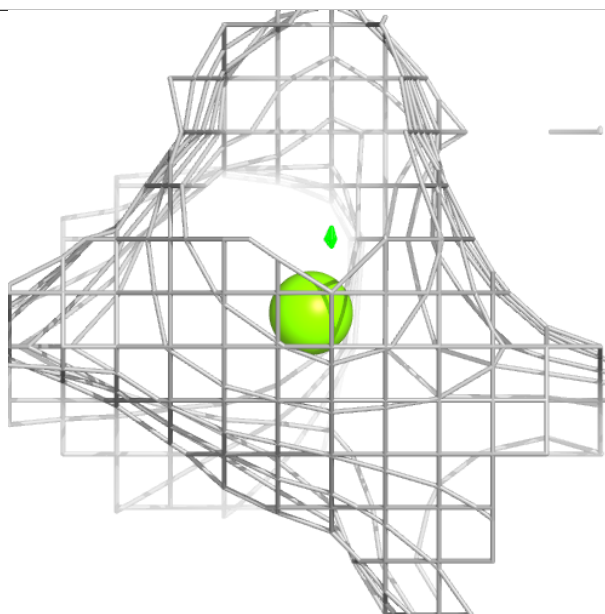
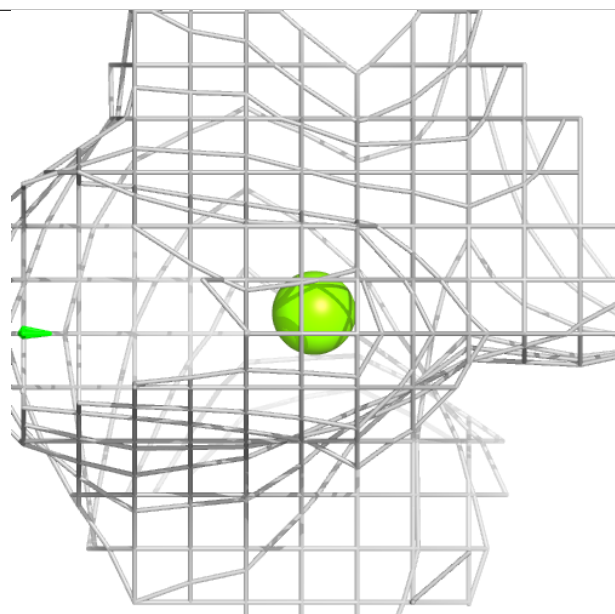
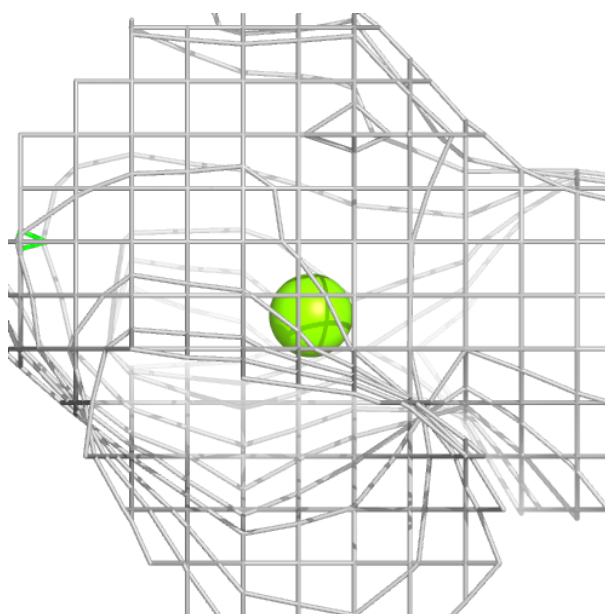
Electron density around MG E 503:

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



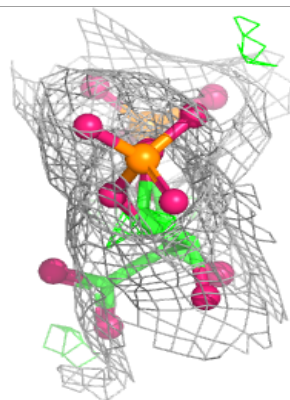
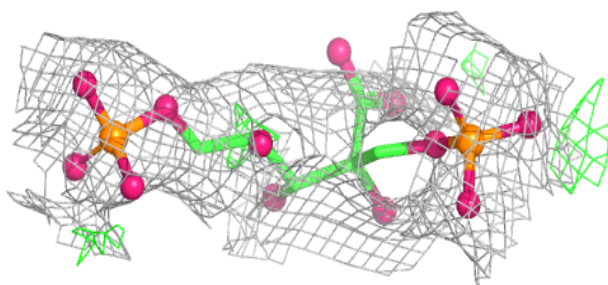
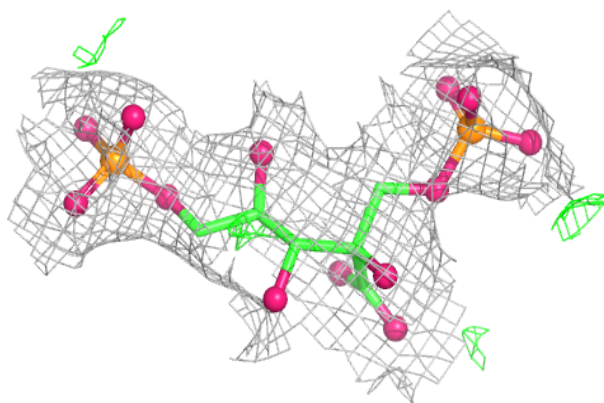
Electron density around MG H 503:

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

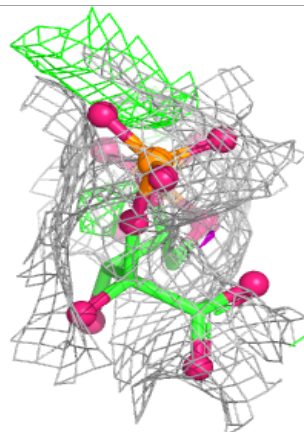
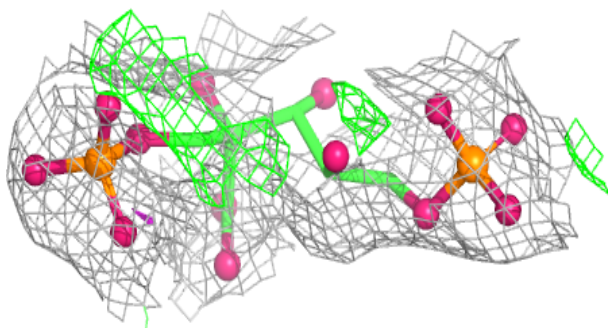
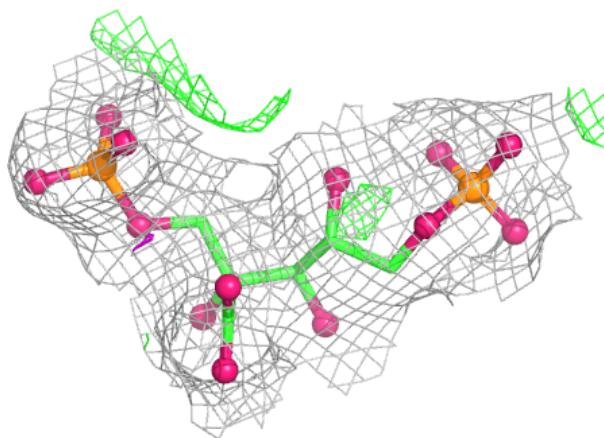


Electron density around CAP G 501:

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

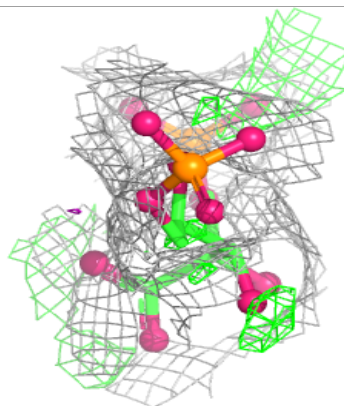
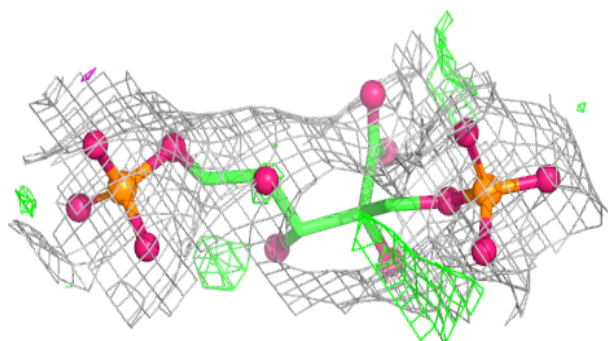
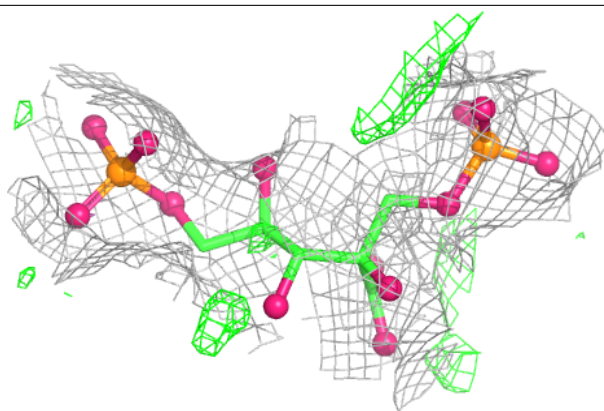
**Electron density around CAP H 501:**

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

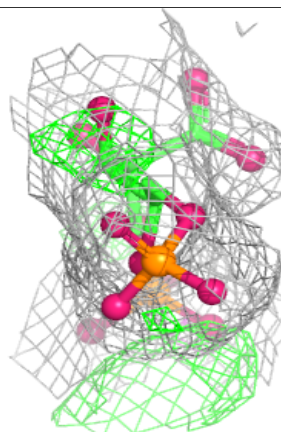
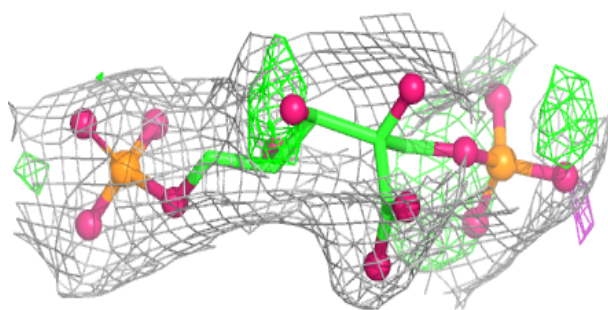
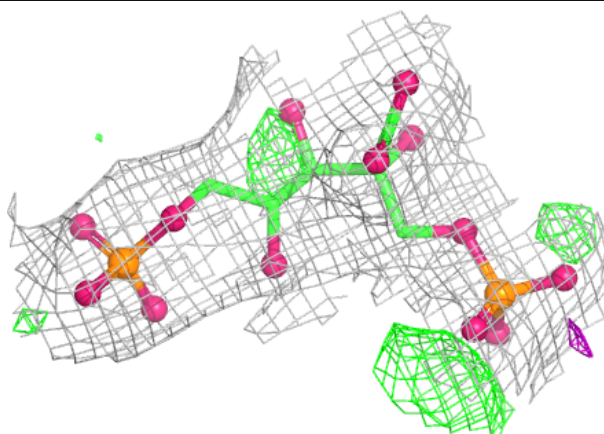


Electron density around CAP J 502:

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

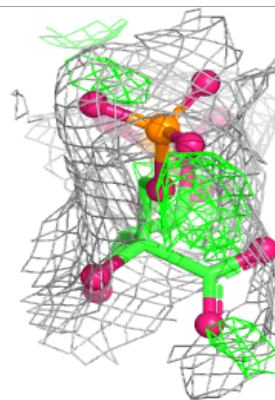
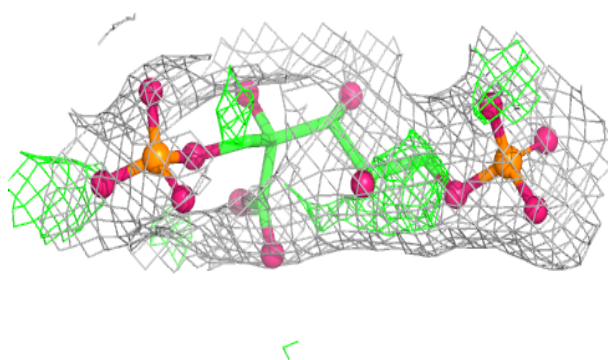
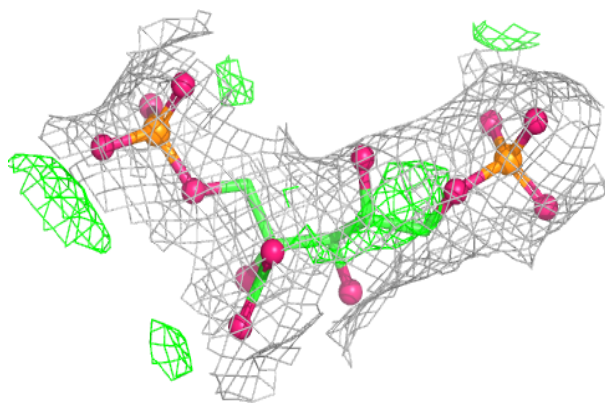
**Electron density around CAP F 501:**

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



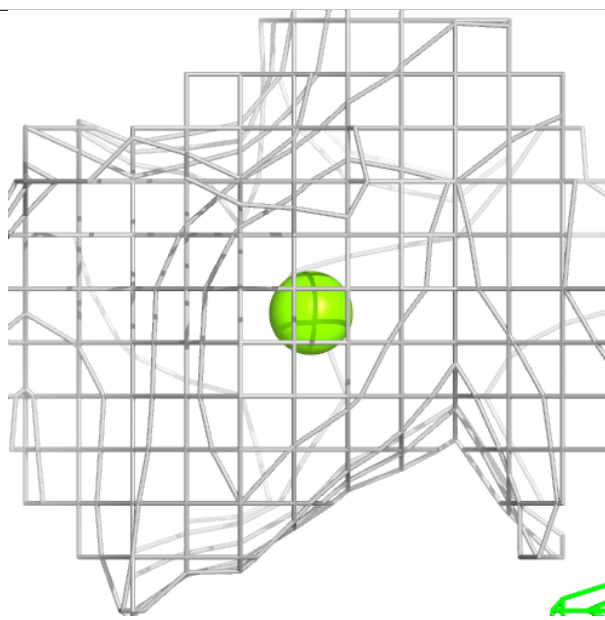
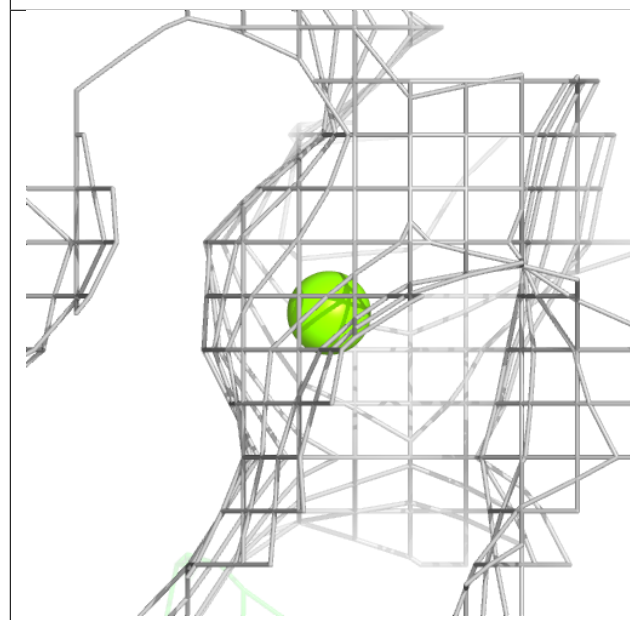
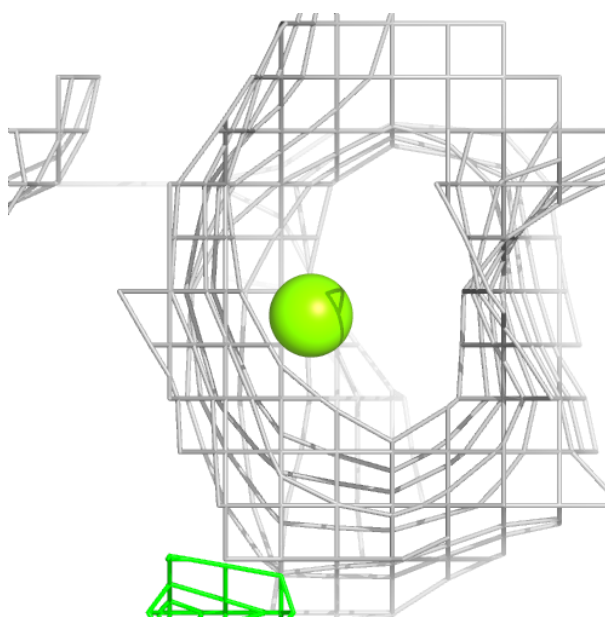
Electron density around CAP I 502:

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



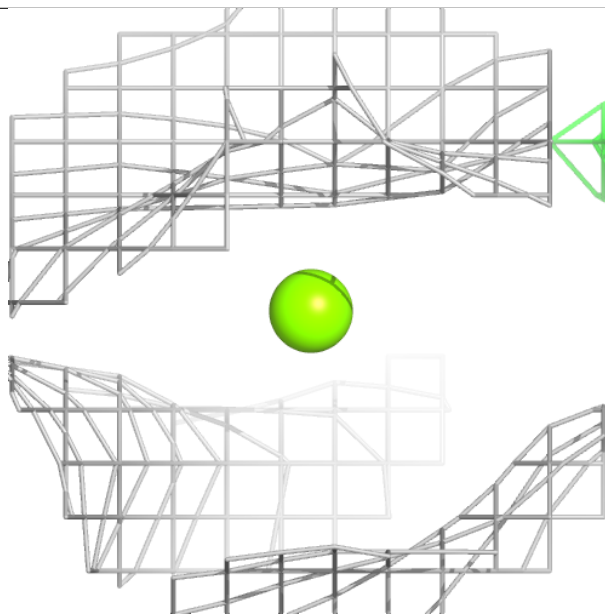
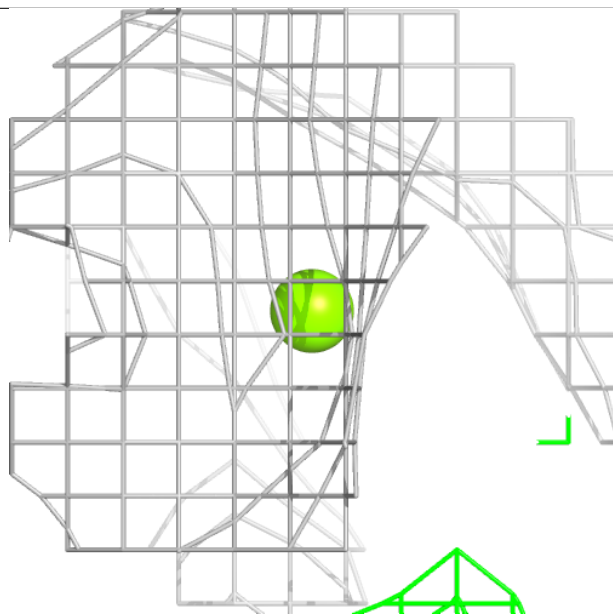
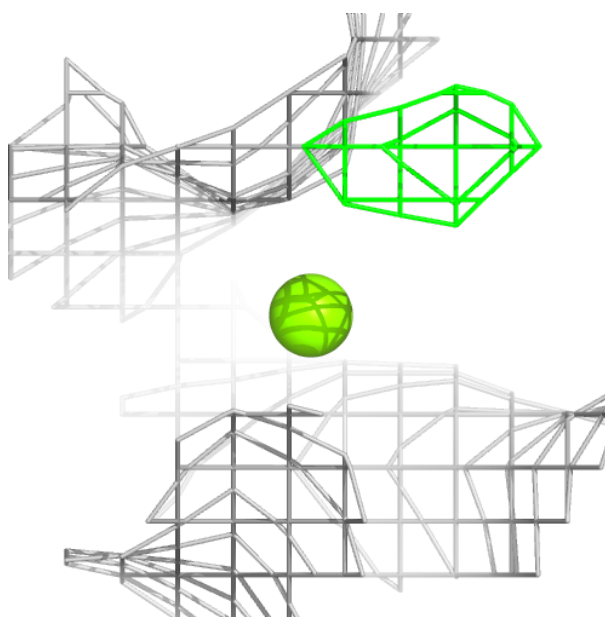
Electron density around MG A 504:

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



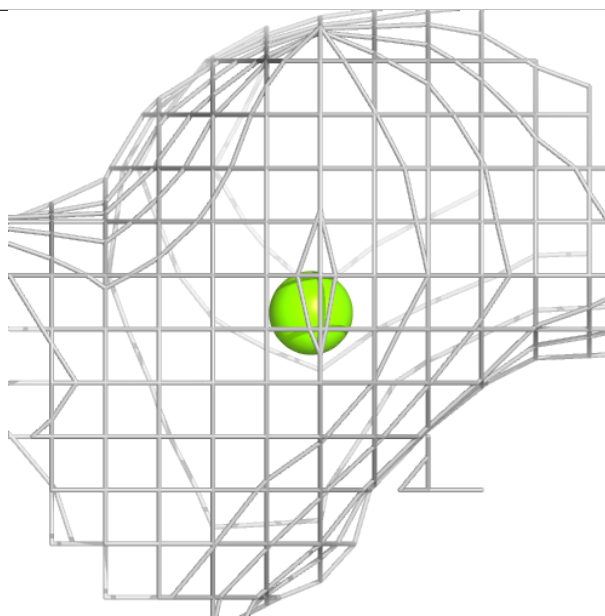
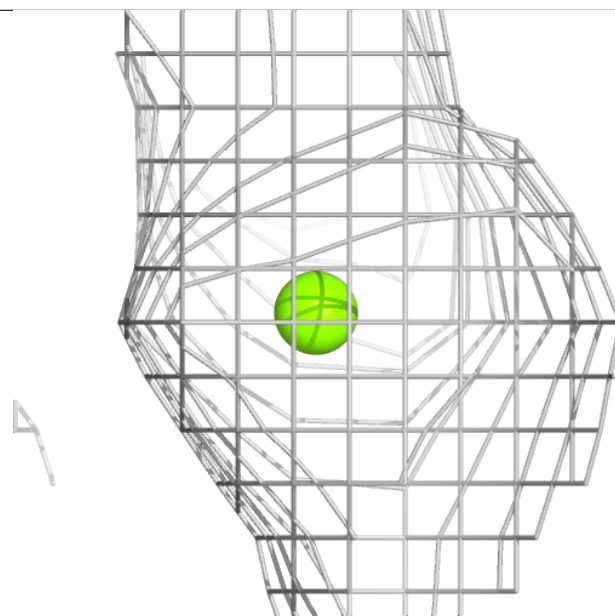
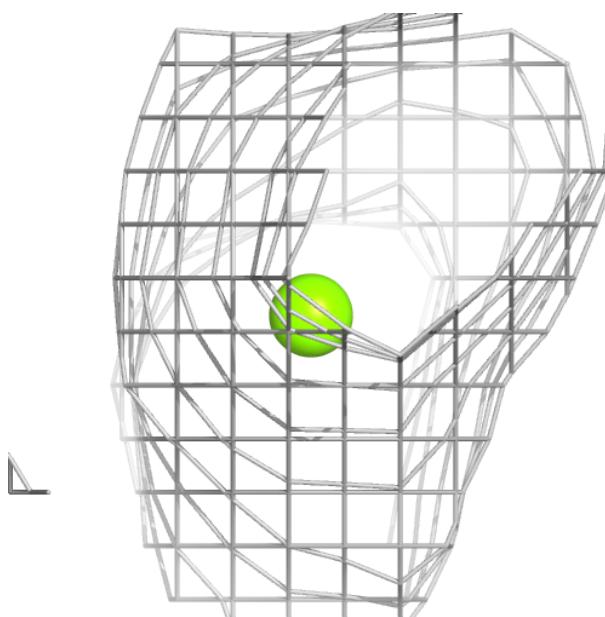
Electron density around MG J 503:

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



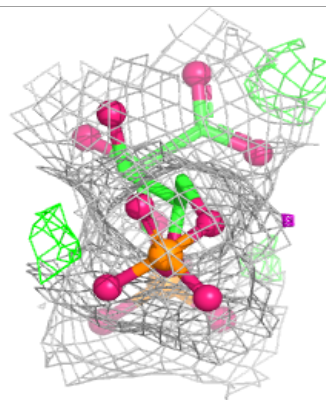
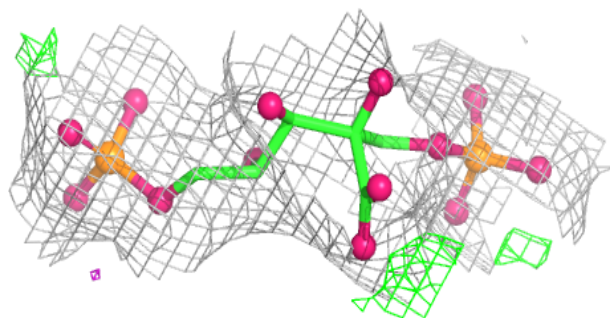
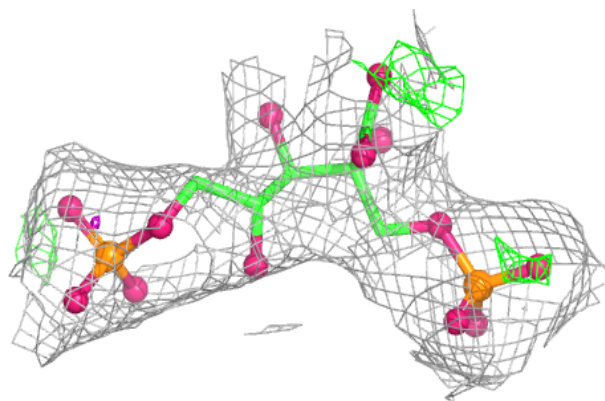
Electron density around MG G 503:

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



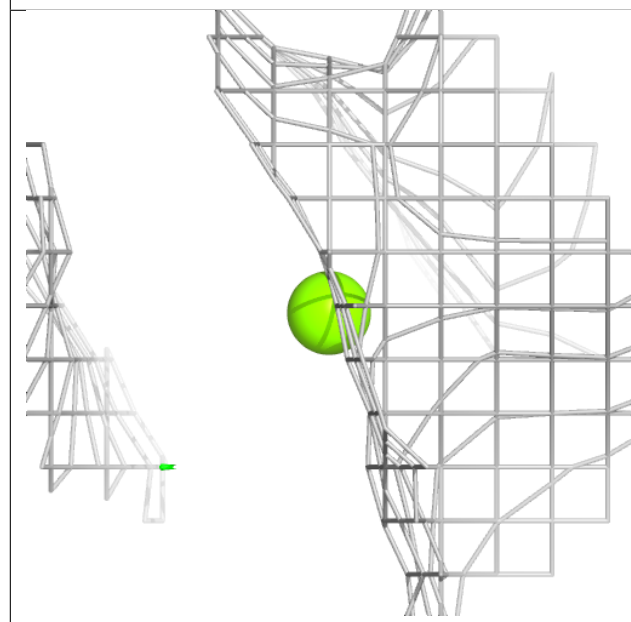
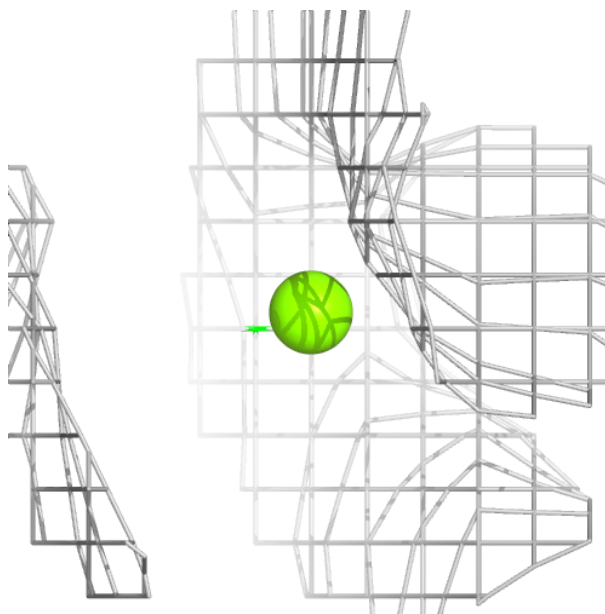
Electron density around CAP D 502:

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



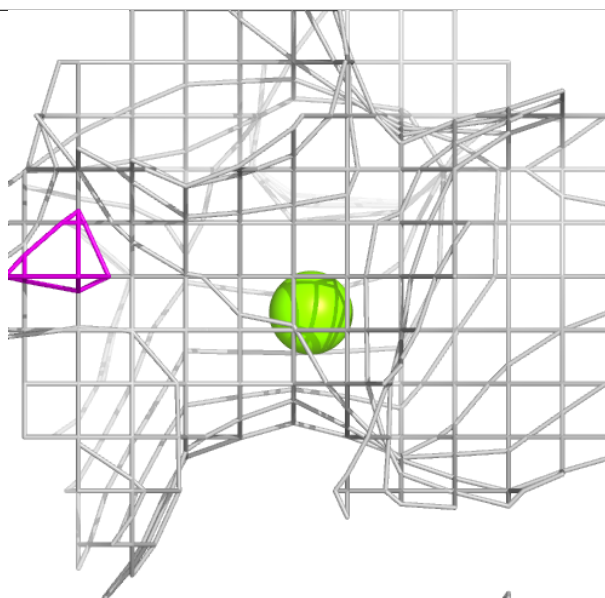
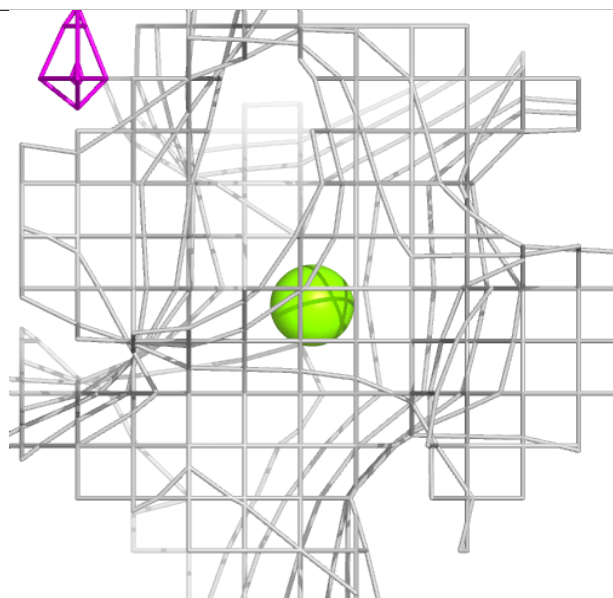
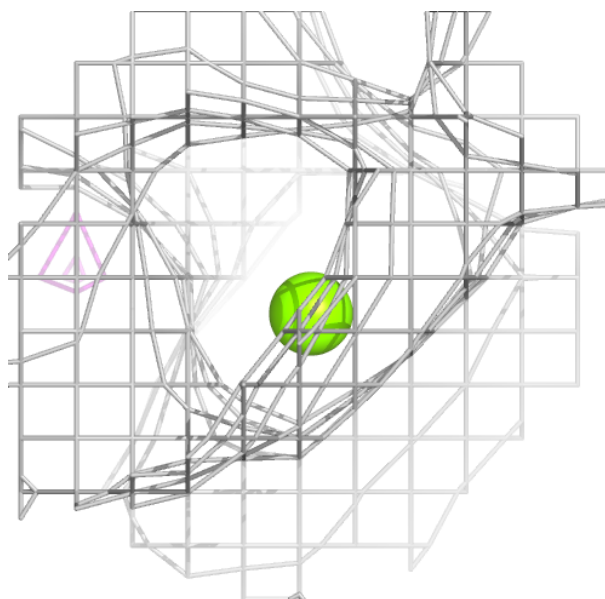
Electron density around MG I 503:

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



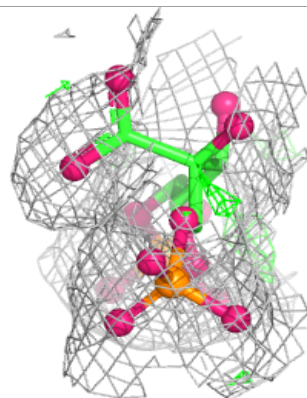
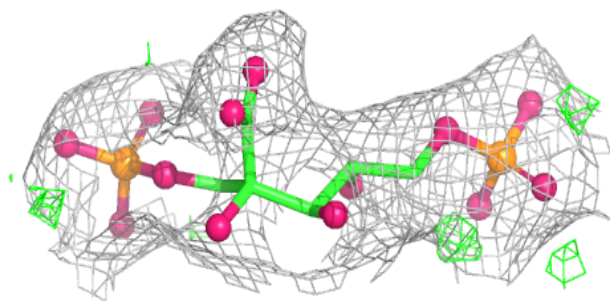
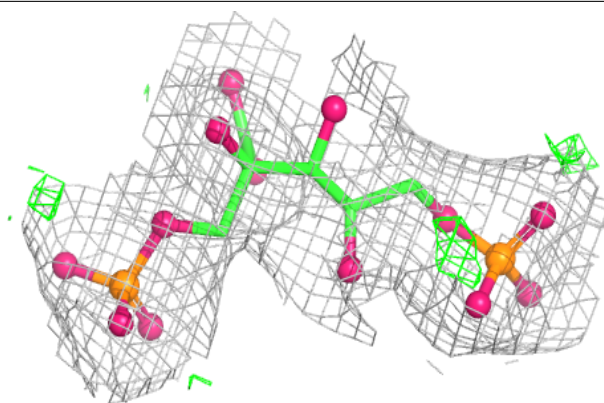
Electron density around MG B 503:

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

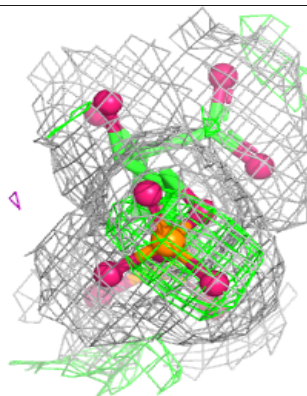
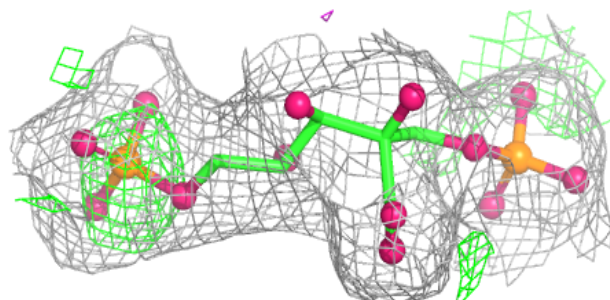
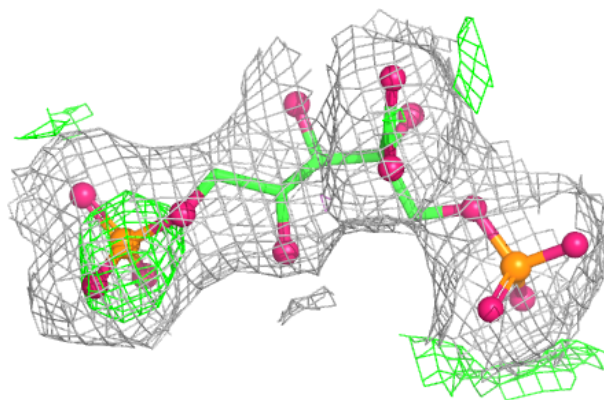


Electron density around CAP E 501:

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

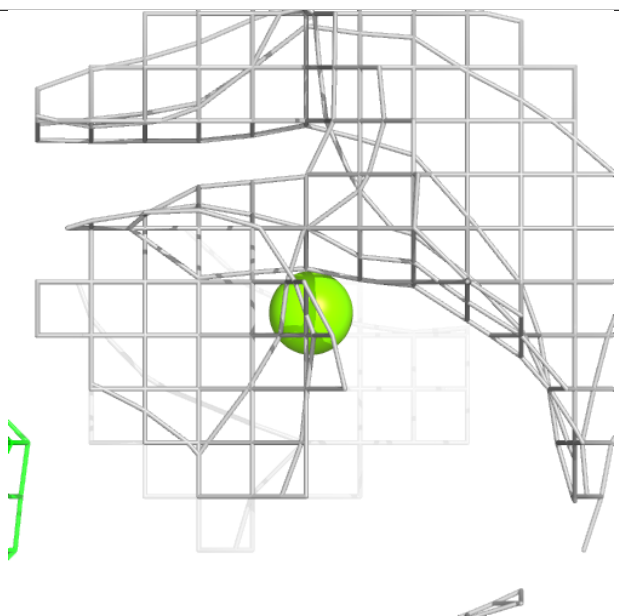
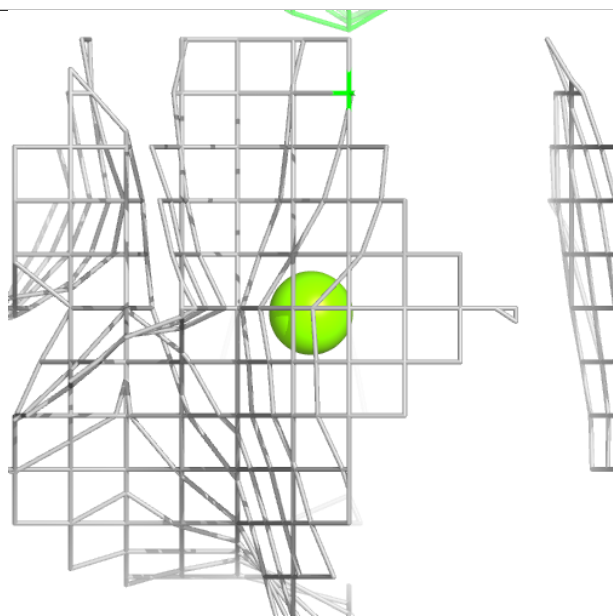
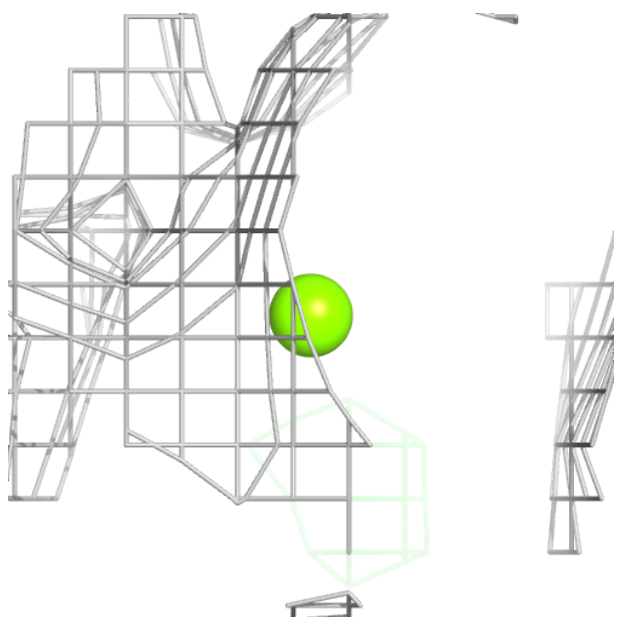
**Electron density around CAP A 501:**

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



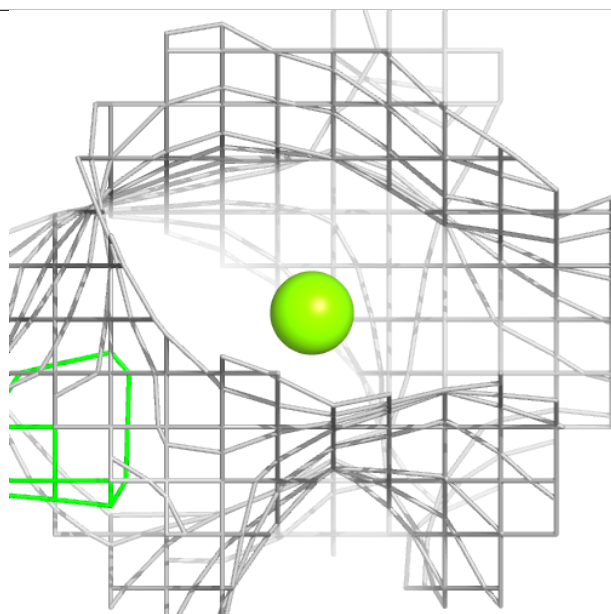
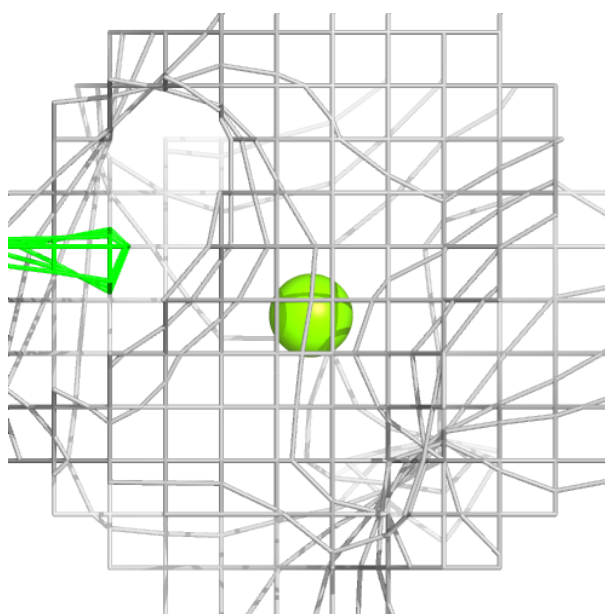
Electron density around MG G 502:

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



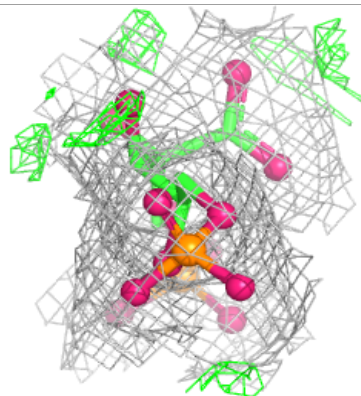
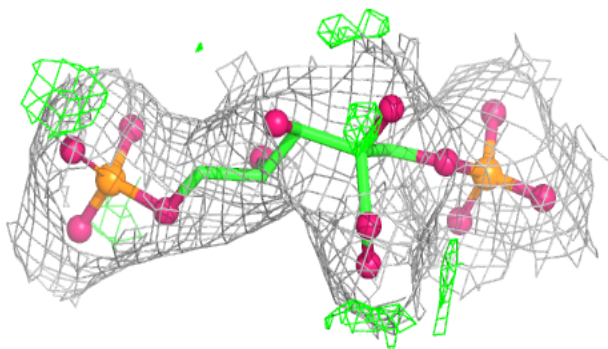
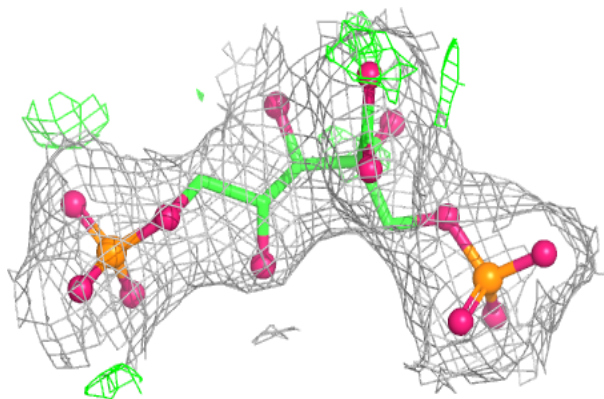
Electron density around MG A 503:

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



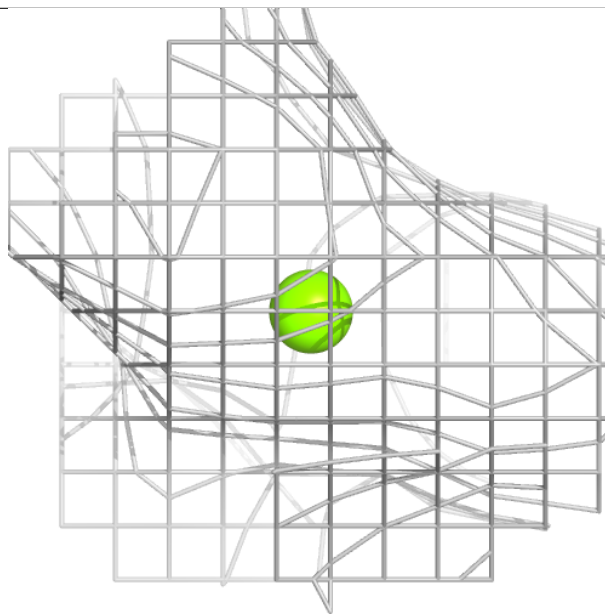
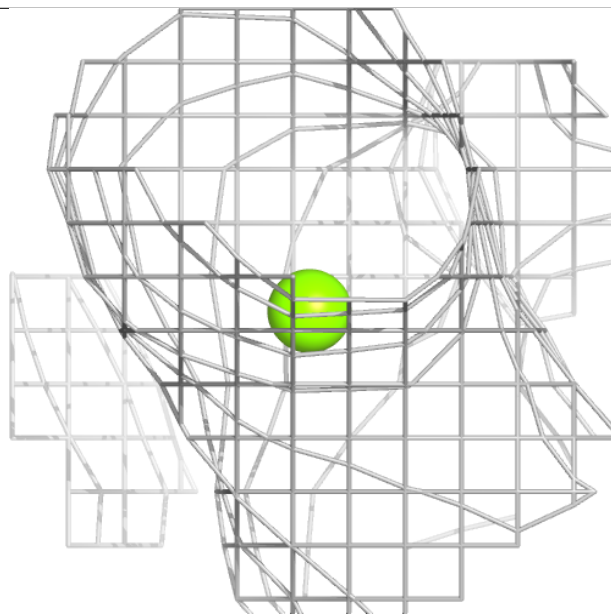
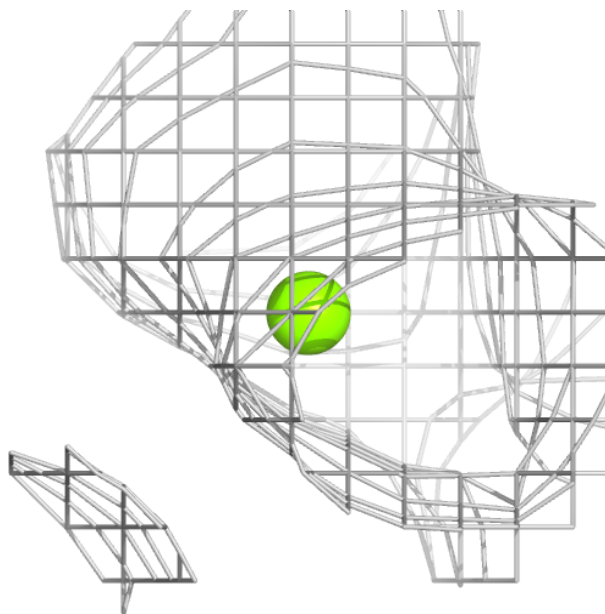
Electron density around CAP B 501:

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



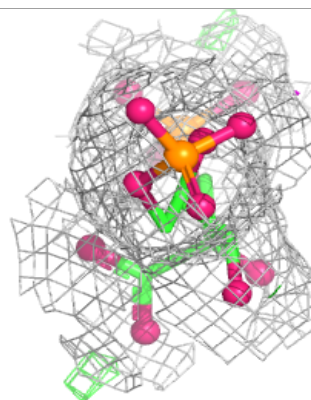
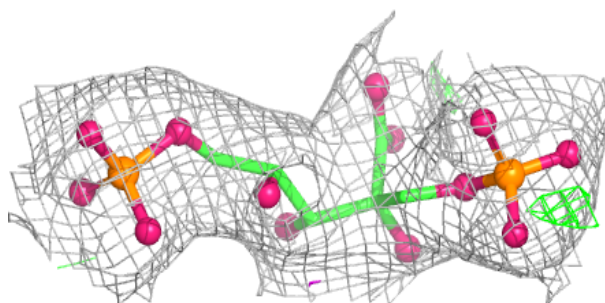
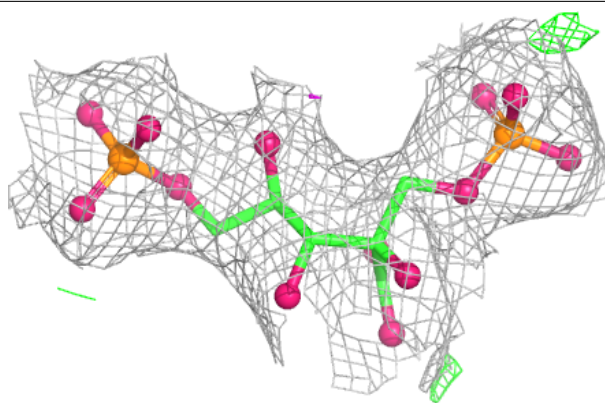
Electron density around MG J 501:

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



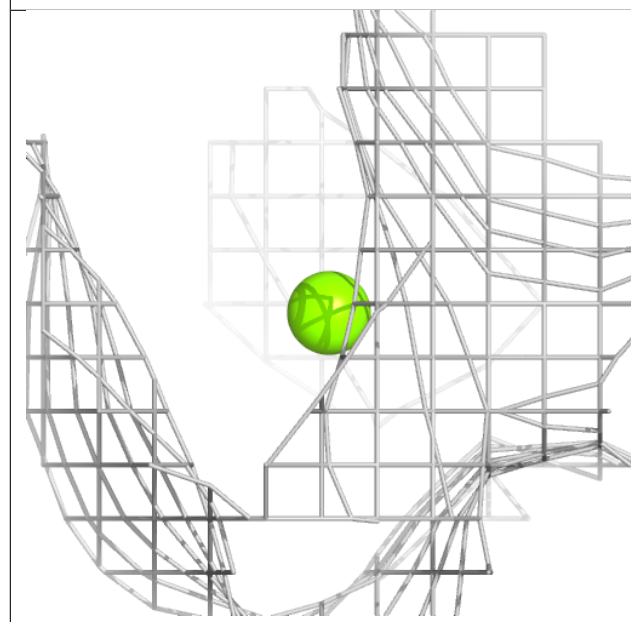
Electron density around CAP C 501:

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



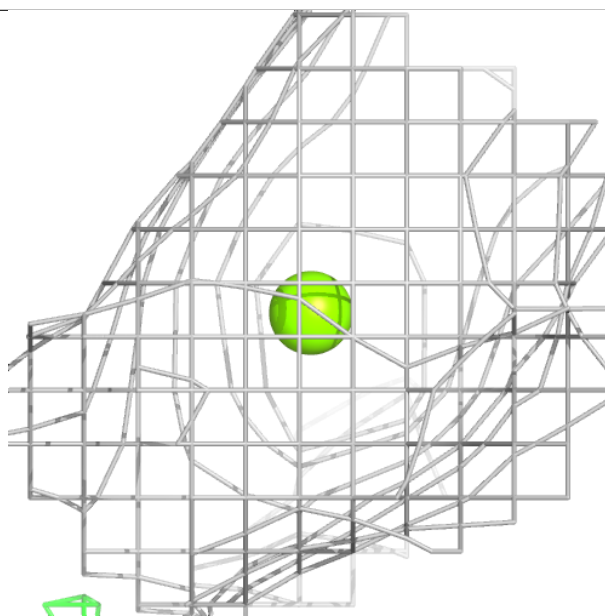
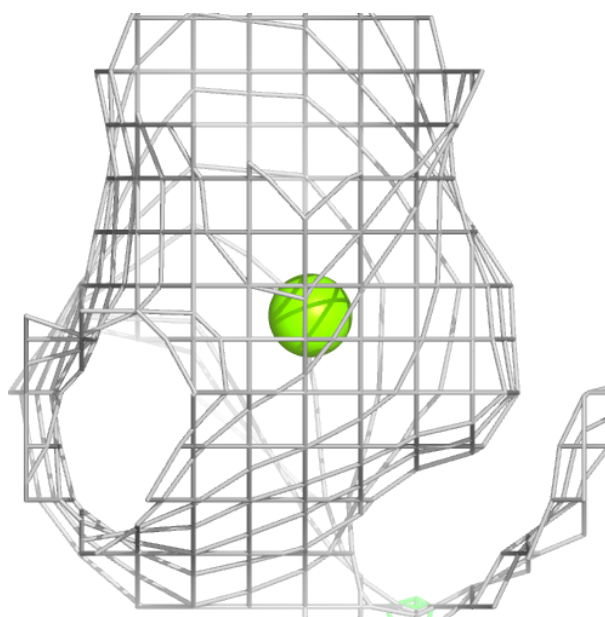
Electron density around MG H 502:

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



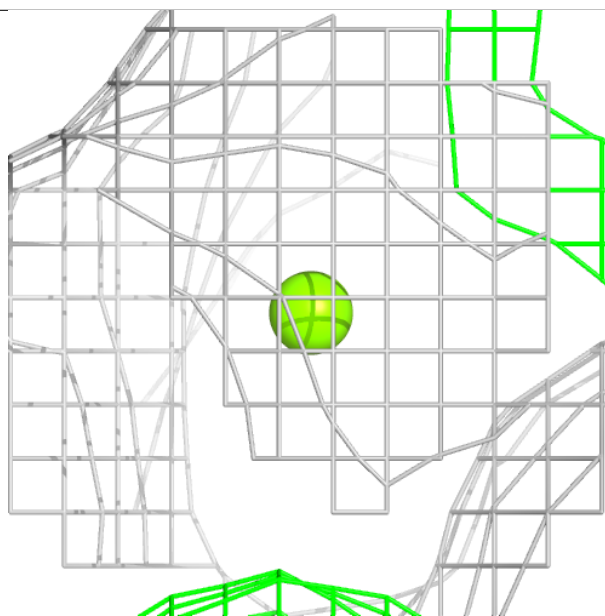
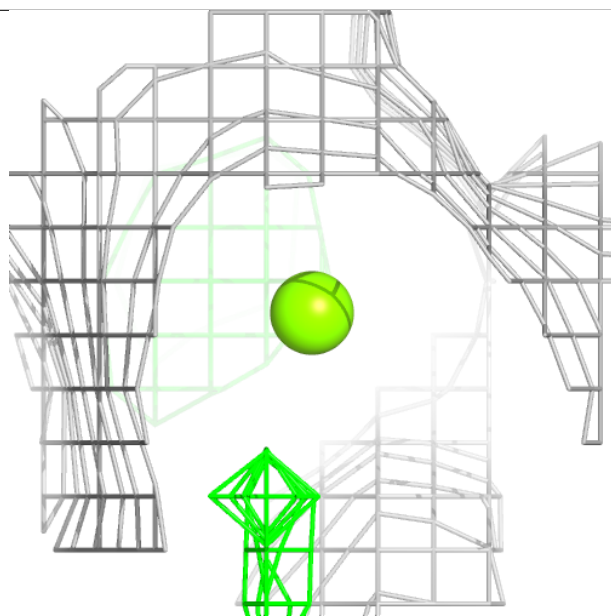
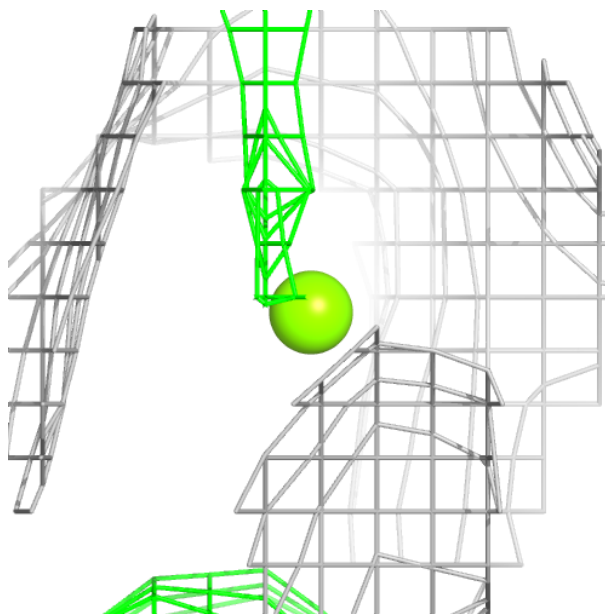
Electron density around MG I 501:

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



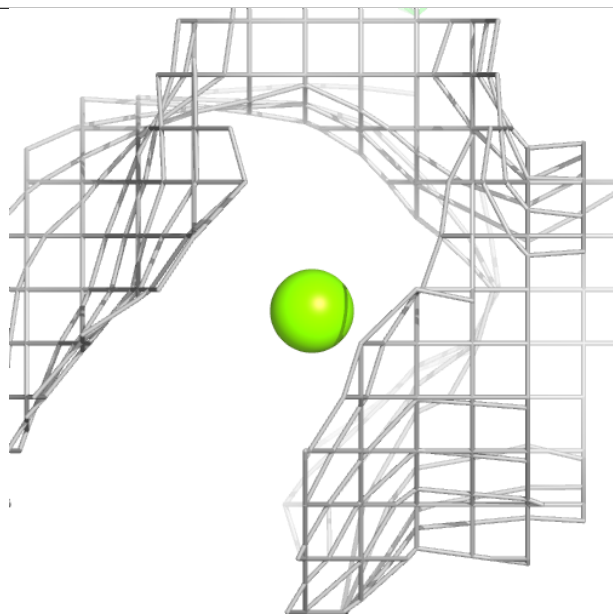
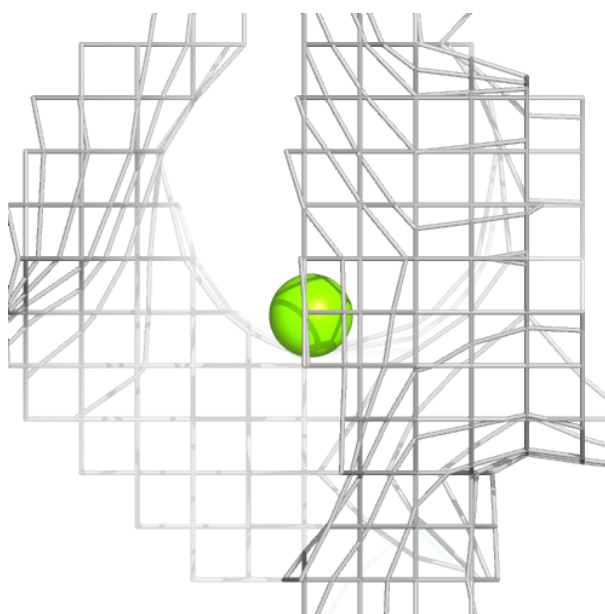
Electron density around MG F 502:

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



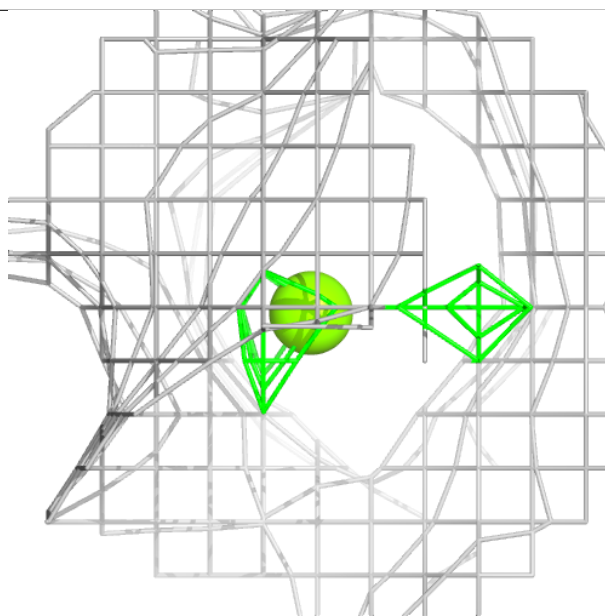
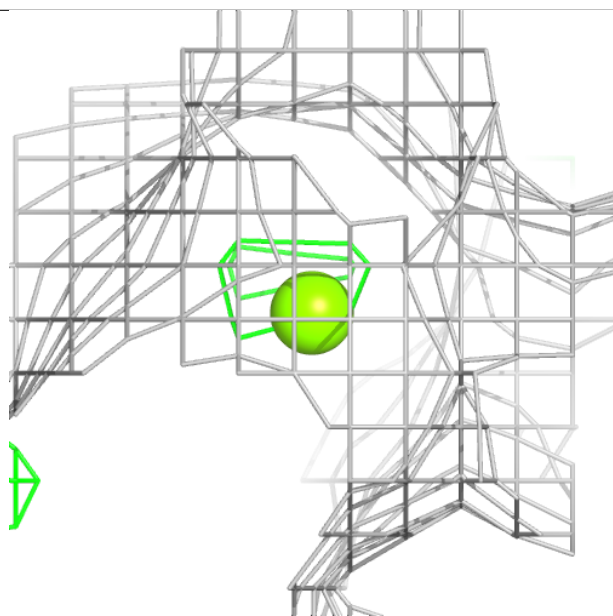
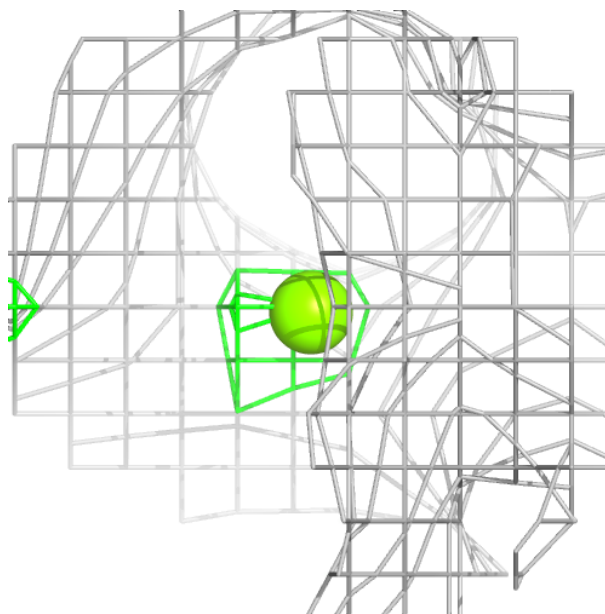
Electron density around MG A 502:

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



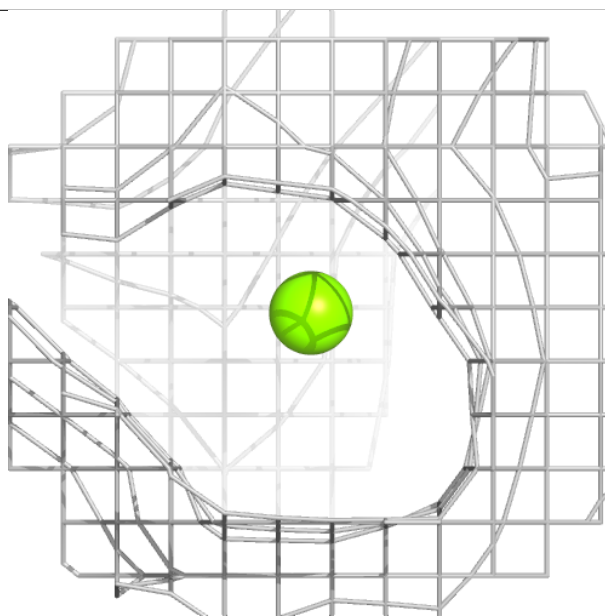
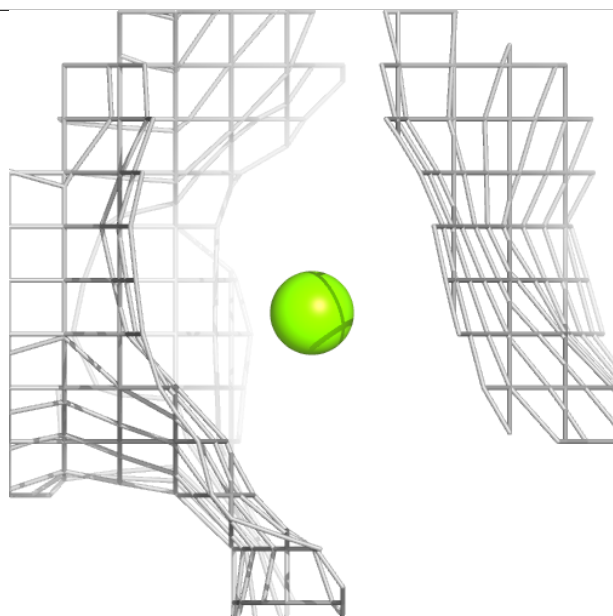
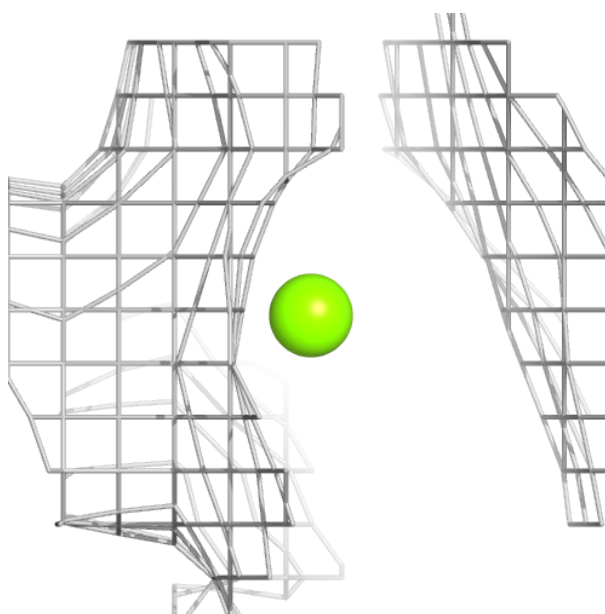
Electron density around MG B 502:

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



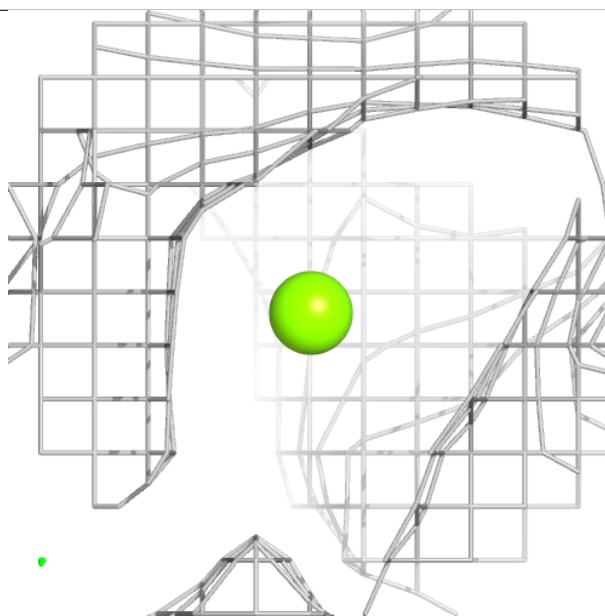
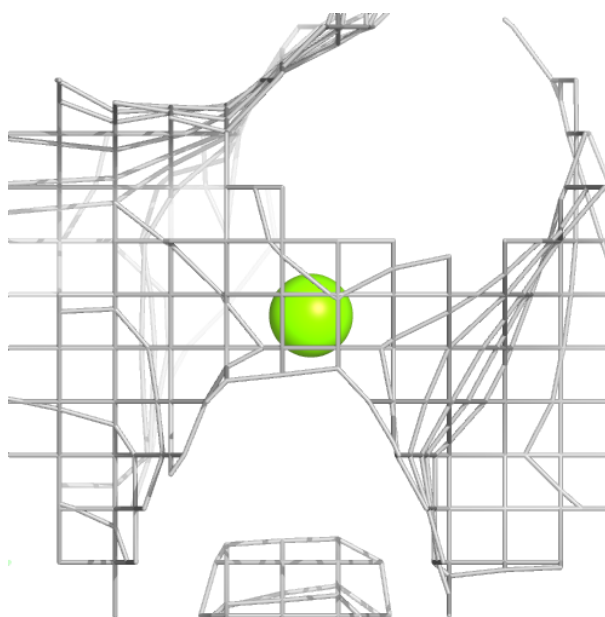
Electron density around MG E 502:

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



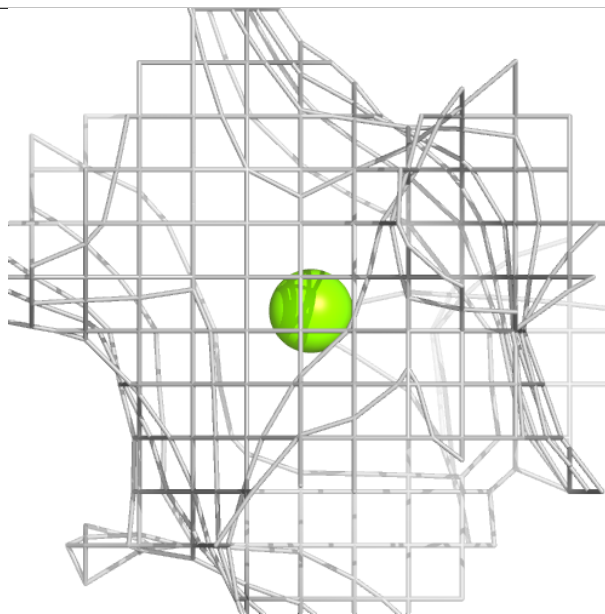
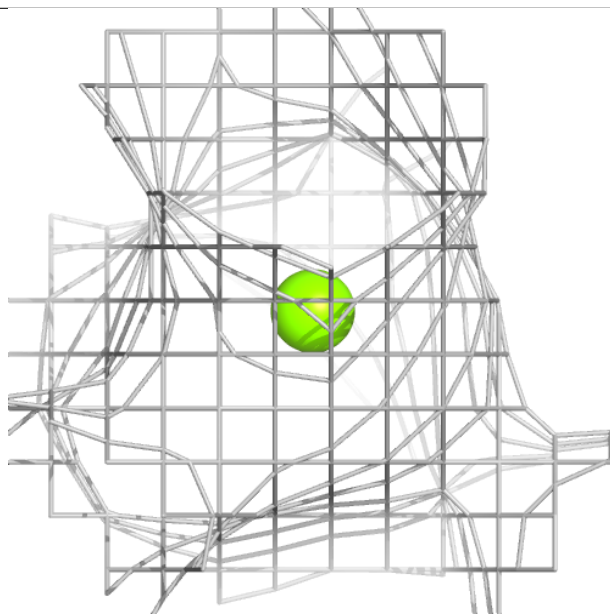
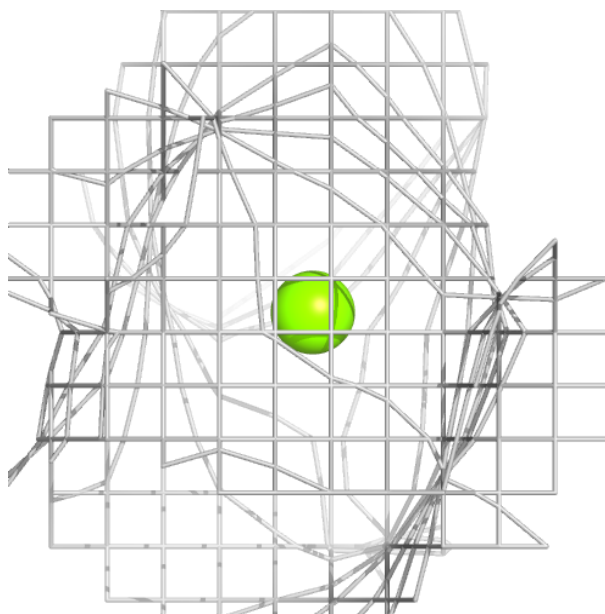
Electron density around MG C 502:

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



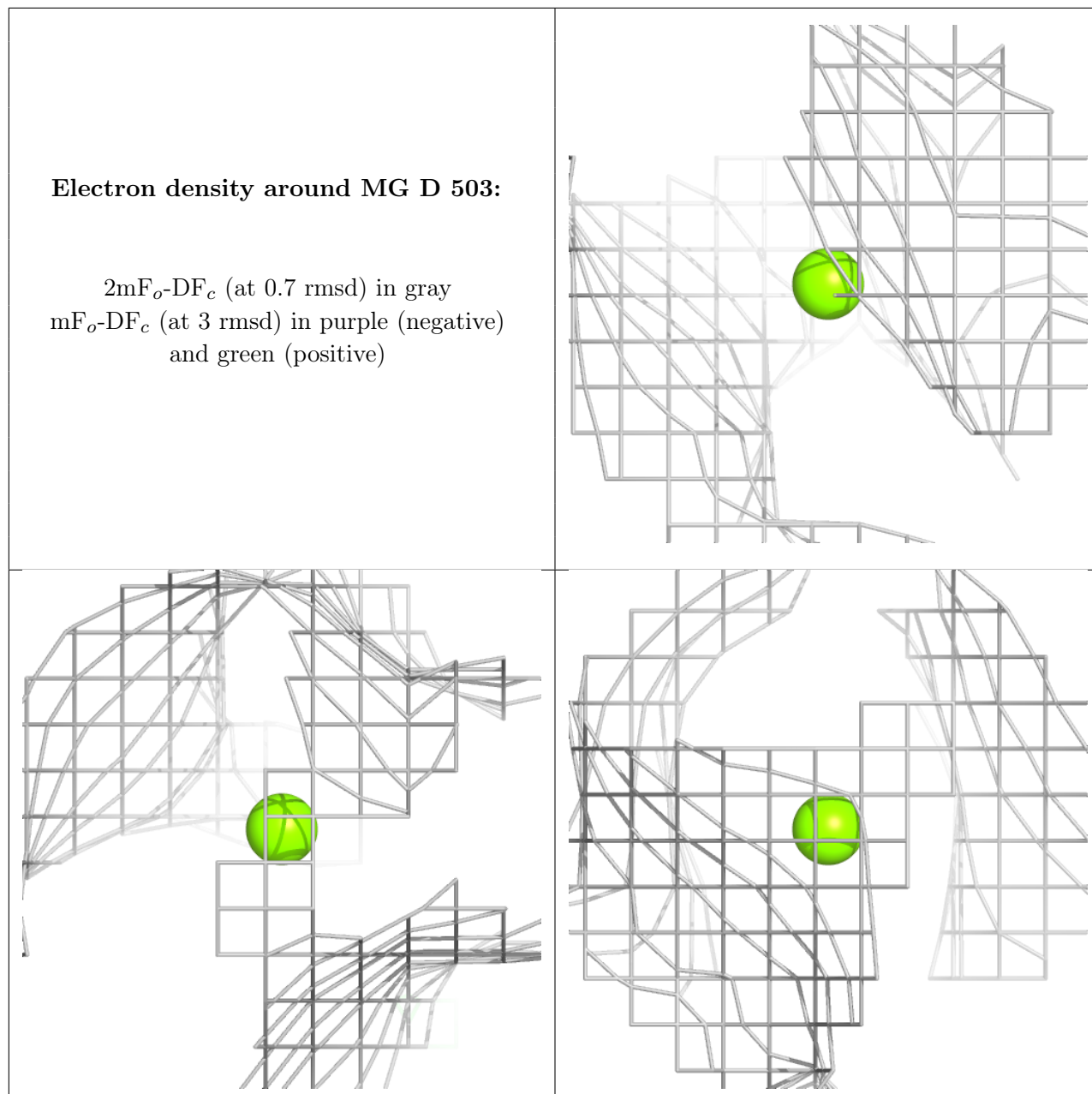
Electron density around MG D 501:

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



Electron density around MG D 503:

$2mF_o-DF_c$ (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.