



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

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	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

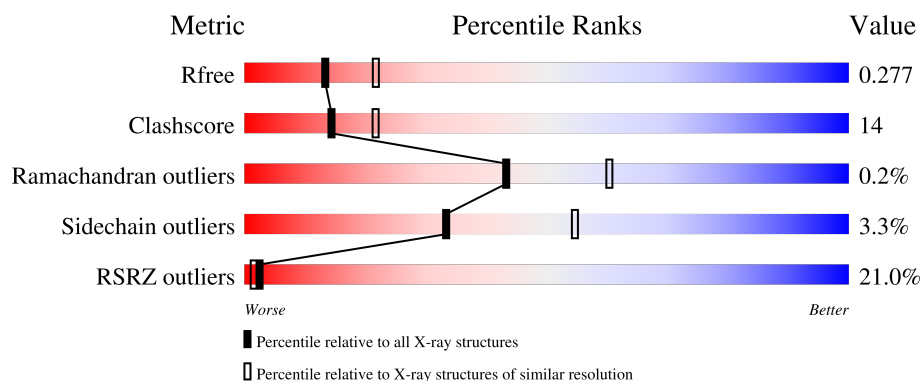
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (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	9% 65% 32% ..
1	G	468	40% 60% 36% ..
1	H	468	51% 59% 38% ..
1	I	468	46% 63% 32% ..
1	J	468	42% 57% 38% ..

2 Entry composition [i](#)

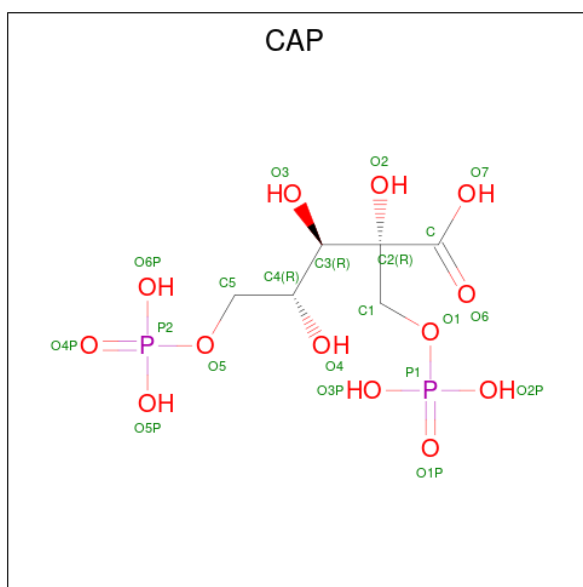
There are 4 unique types of molecules in this entry. The entry contains 36567 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

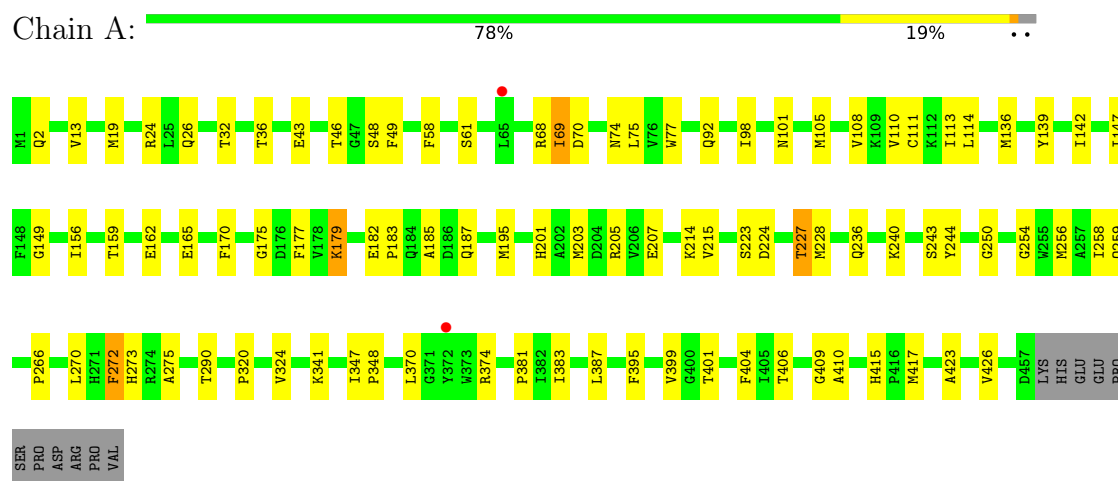
- Molecule 4 is water.

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

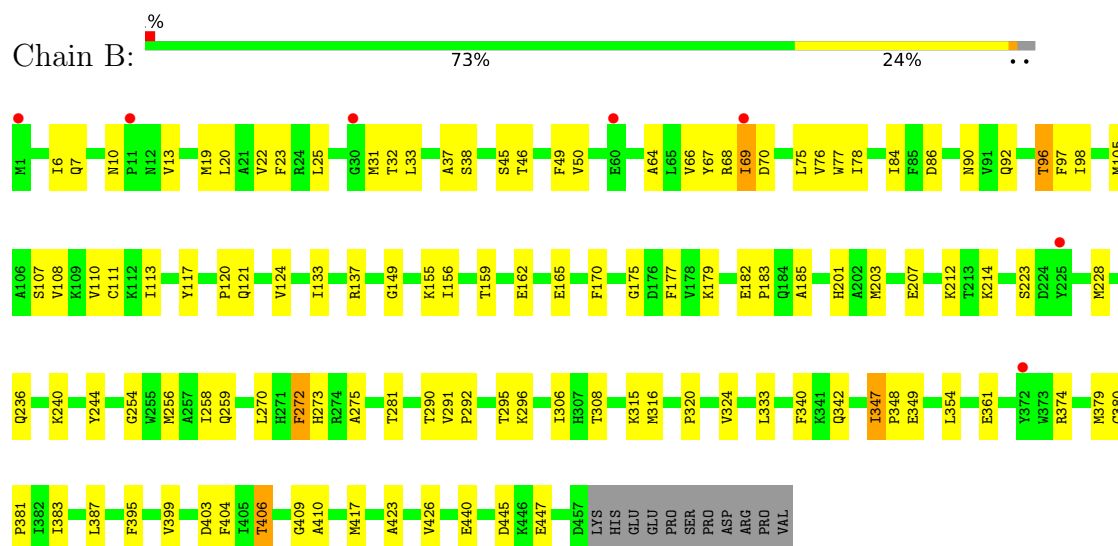
3 Residue-property plots [i](#)

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.

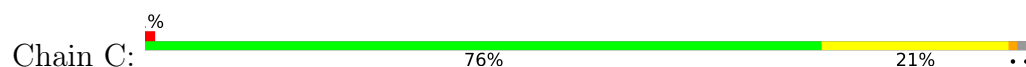
- Molecule 1: ribulose-1,5-bisphosphate carboxylase

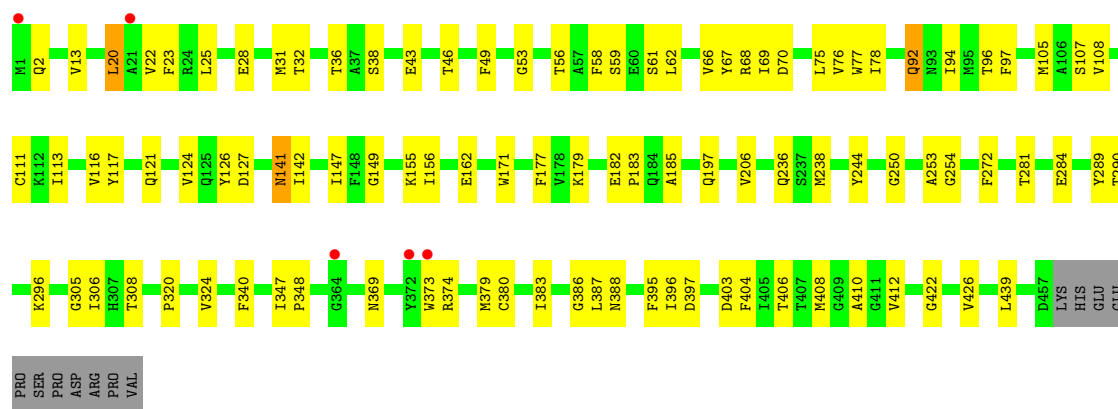


- Molecule 1: ribulose-1,5-bisphosphate carboxylase

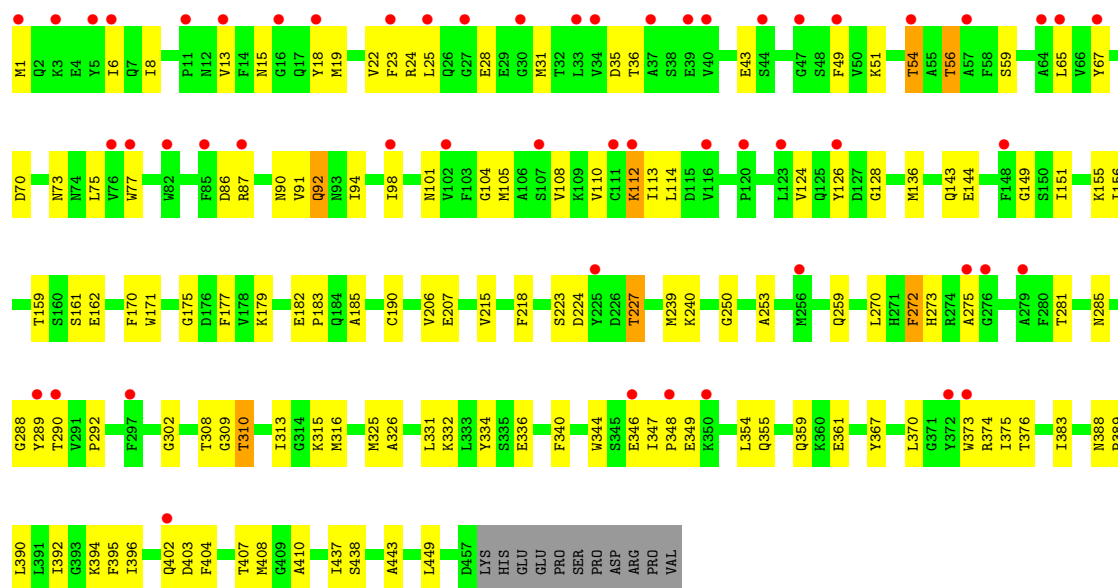


- Molecule 1: ribulose-1,5-bisphosphate carboxylase

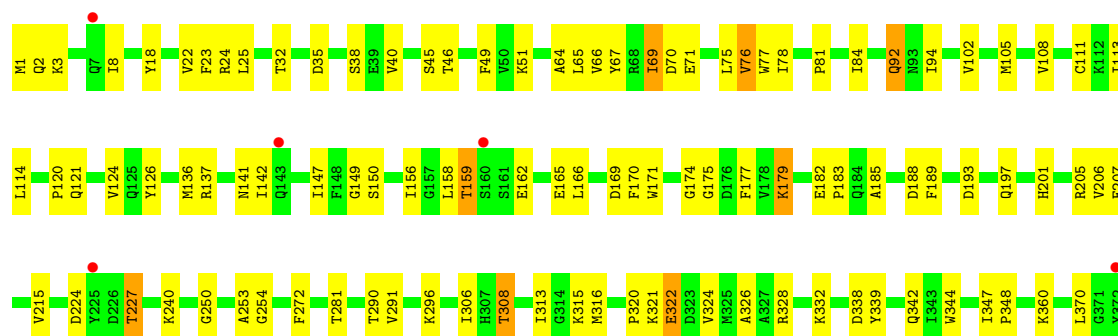


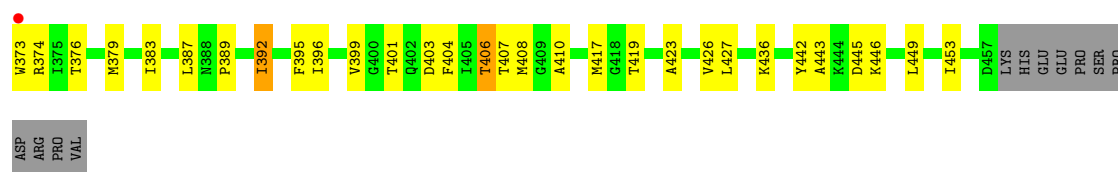


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

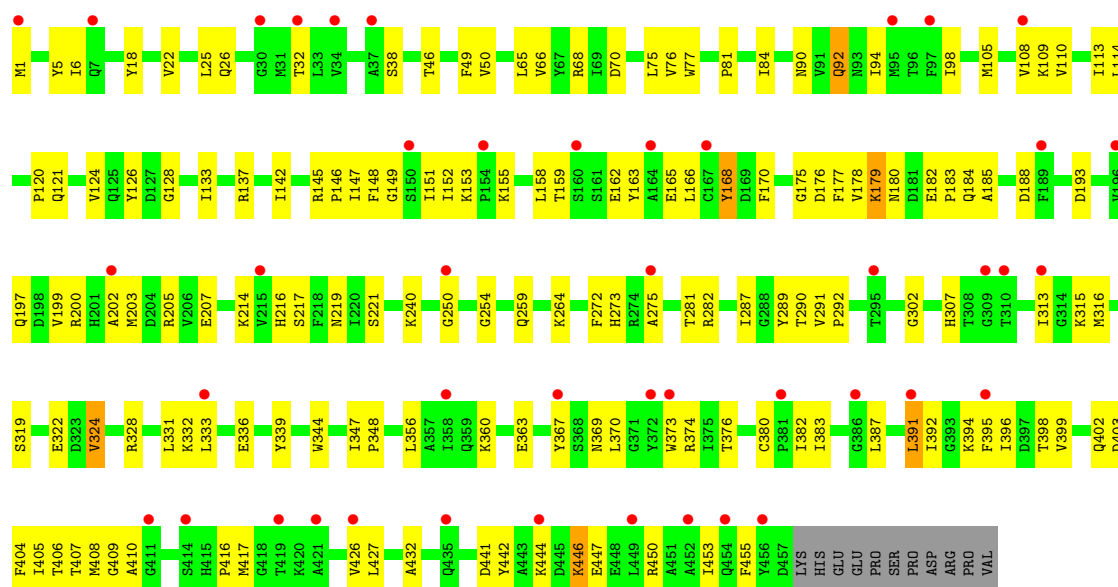


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

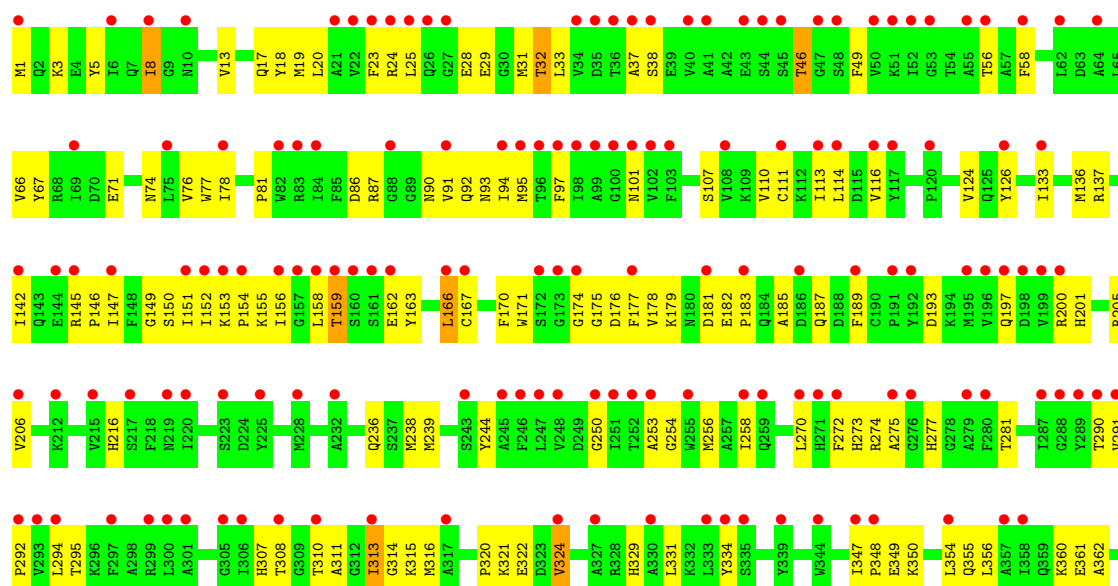
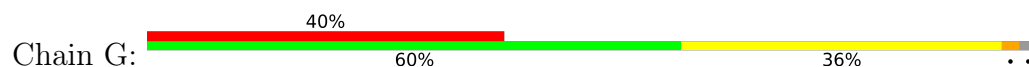


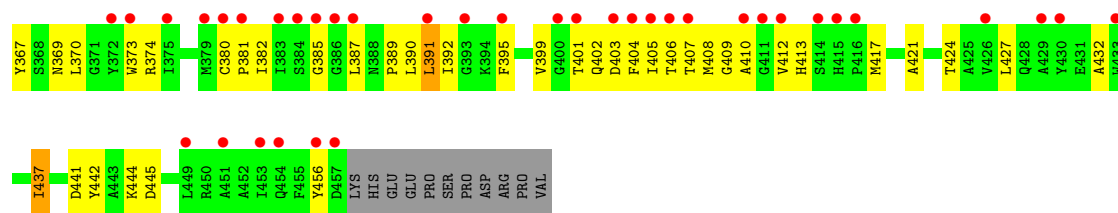


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

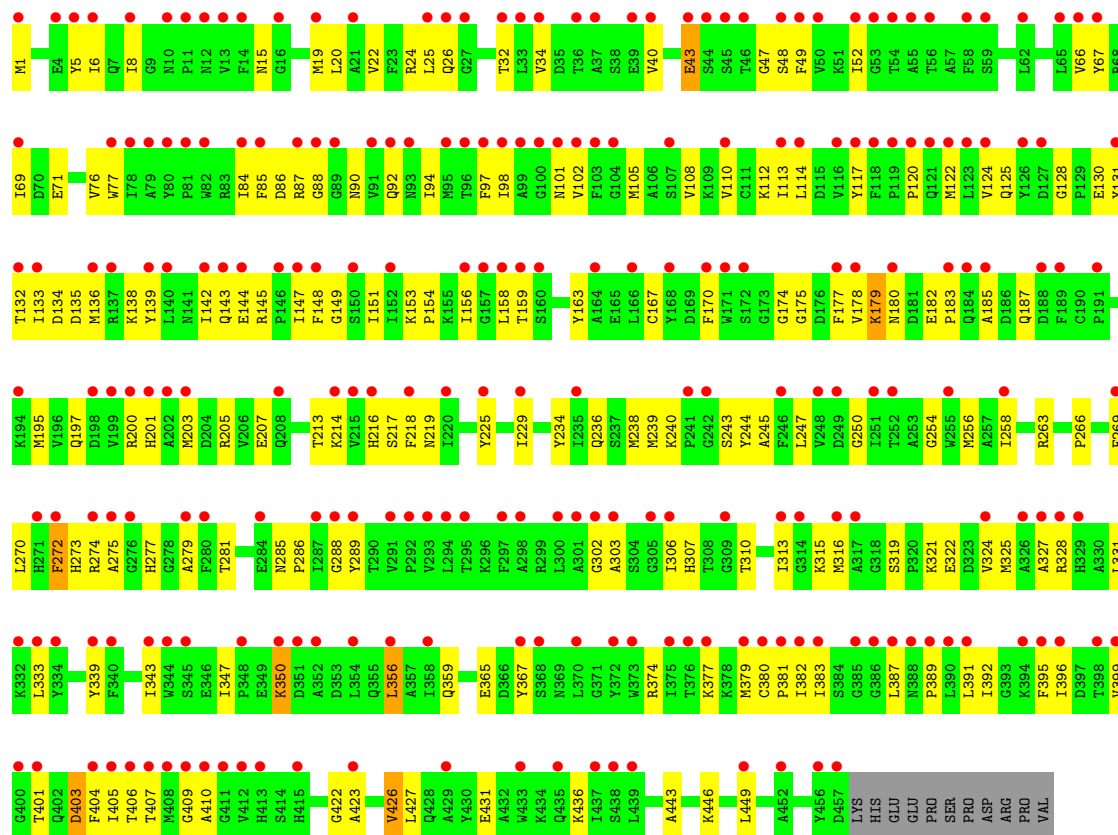


• Molecule 1: ribulose-1,5-bisphosphate carboxylase

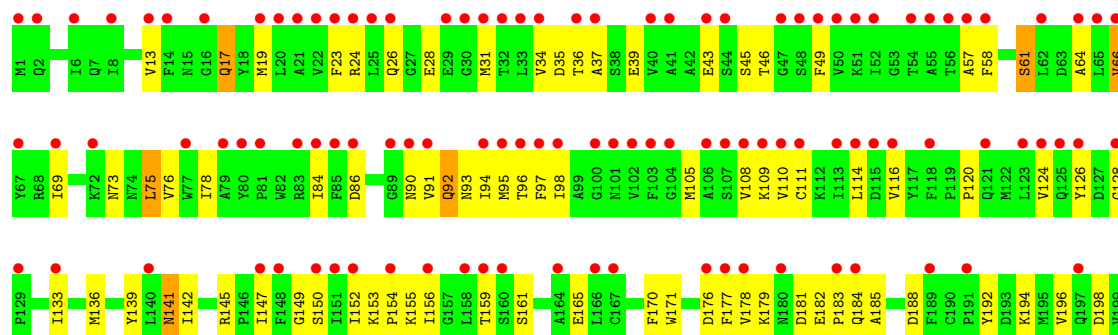


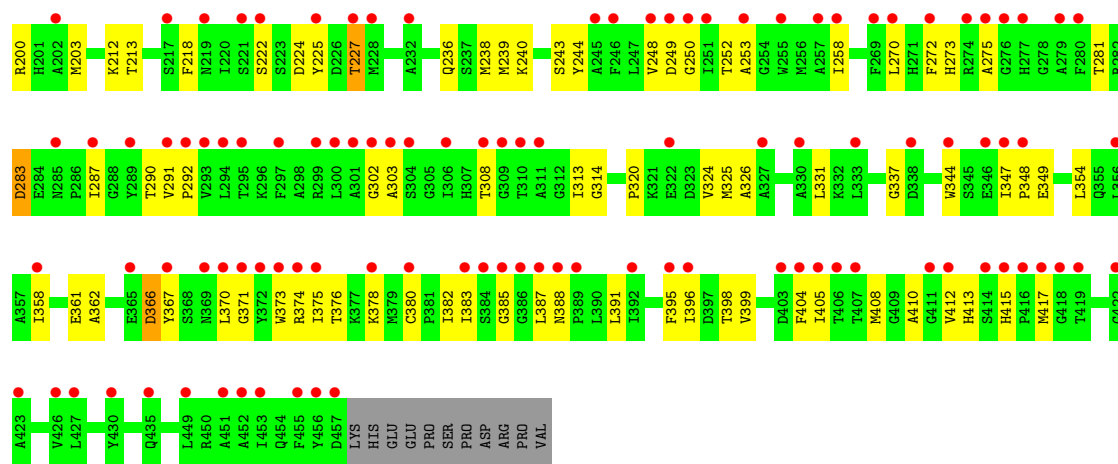


● Molecule 1: ribulose-1,5-bisphosphate carboxylase

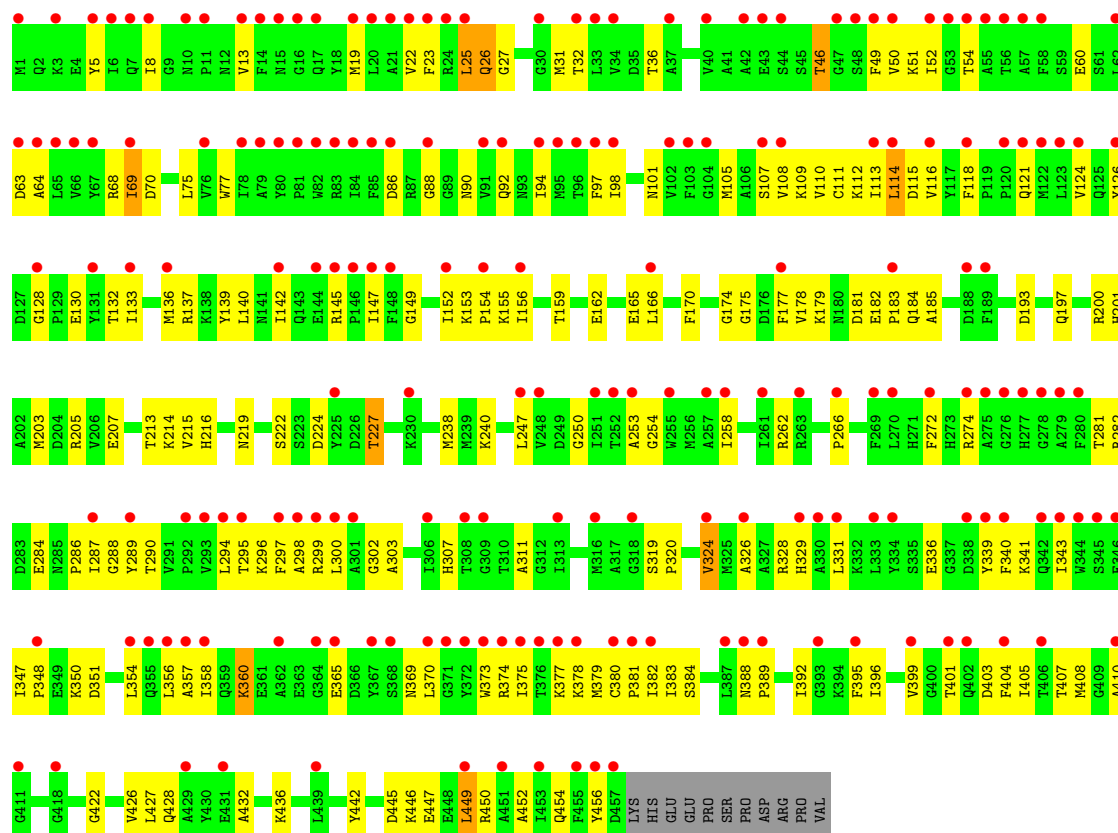
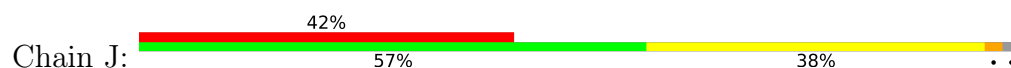


● Molecule 1: ribulose-1,5-bisphosphate carboxylase





• 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: MG, CAP, KCX

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%)	43	60
1	B	454/468 (97%)	441 (97%)	12 (3%)	1 (0%)	43	60
1	C	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	43	60
1	D	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	43	60
1	E	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	43	60
1	F	454/468 (97%)	439 (97%)	14 (3%)	1 (0%)	43	60
1	G	454/468 (97%)	441 (97%)	12 (3%)	1 (0%)	43	60
1	H	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	43	60
1	I	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	43	60
1	J	454/468 (97%)	440 (97%)	13 (3%)	1 (0%)	43	60
All	All	4540/4680 (97%)	4398 (97%)	132 (3%)	10 (0%)	43	60

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%)	50	71
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	53
1	E	377/388 (97%)	366 (97%)	11 (3%)	37	58
1	F	377/388 (97%)	364 (97%)	13 (3%)	32	53
1	G	377/388 (97%)	359 (95%)	18 (5%)	23	39
1	H	377/388 (97%)	365 (97%)	12 (3%)	34	55
1	I	377/388 (97%)	363 (96%)	14 (4%)	30	50
1	J	377/388 (97%)	364 (97%)	13 (3%)	32	53
All	All	3770/3880 (97%)	3647 (97%)	123 (3%)	33	55

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	D	179	1,3	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	1,3	10,11,12	2.01	2 (20%)	6,12,14	1.65	1 (16%)
1	KCX	F	179	1,3	10,11,12	2.17	2 (20%)	6,12,14	2.33	3 (50%)
1	KCX	B	179	1,3	10,11,12	1.98	2 (20%)	6,12,14	1.75	1 (16%)
1	KCX	C	179	1,3	10,11,12	2.08	2 (20%)	6,12,14	1.33	1 (16%)
1	KCX	G	179	1,3	10,11,12	2.09	2 (20%)	6,12,14	1.62	1 (16%)
1	KCX	H	179	1,3	10,11,12	2.09	2 (20%)	6,12,14	1.34	1 (16%)
1	KCX	E	179	1,3	10,11,12	2.02	2 (20%)	6,12,14	1.94	2 (33%)
1	KCX	I	179	1,3	10,11,12	2.15	2 (20%)	6,12,14	1.58	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	D	179	1,3	-	0/9/10/12	-
1	KCX	J	179	1	-	0/9/10/12	-
1	KCX	A	179	1,3	-	0/9/10/12	-
1	KCX	F	179	1,3	-	0/9/10/12	-
1	KCX	B	179	1,3	-	0/9/10/12	-
1	KCX	C	179	1,3	-	1/9/10/12	-
1	KCX	G	179	1,3	-	1/9/10/12	-

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

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	-3.65	119.38	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	A	179	KCX	1	0
1	F	179	KCX	3	0
1	H	179	KCX	1	0
1	E	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	C	501	3	18,20,20	1.04	0	23,31,31	1.06	1 (4%)
2	CAP	E	501	3	18,20,20	1.07	0	23,31,31	1.04	1 (4%)
2	CAP	B	501	3	18,20,20	1.03	0	23,31,31	1.23	1 (4%)

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	I	502	3	18,20,20	1.07	0	23,31,31	1.05	1 (4%)
2	CAP	G	501	3	18,20,20	1.06	0	23,31,31	1.07	1 (4%)
2	CAP	J	502	3	18,20,20	1.07	0	23,31,31	1.08	1 (4%)
2	CAP	H	501	3	18,20,20	1.07	0	23,31,31	1.09	2 (8%)
2	CAP	A	501	3	18,20,20	1.06	0	23,31,31	1.13	2 (8%)
2	CAP	F	501	3	18,20,20	1.07	0	23,31,31	1.15	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	C	501	3	-	13/29/29/29	-
2	CAP	E	501	3	-	7/29/29/29	-
2	CAP	B	501	3	-	9/29/29/29	-
2	CAP	D	502	3	-	11/29/29/29	-
2	CAP	I	502	3	-	5/29/29/29	-
2	CAP	G	501	3	-	3/29/29/29	-
2	CAP	J	502	3	-	11/29/29/29	-
2	CAP	H	501	3	-	14/29/29/29	-
2	CAP	A	501	3	-	10/29/29/29	-
2	CAP	F	501	3	-	7/29/29/29	-

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	3.46	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	3.04	119.15	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	112.86	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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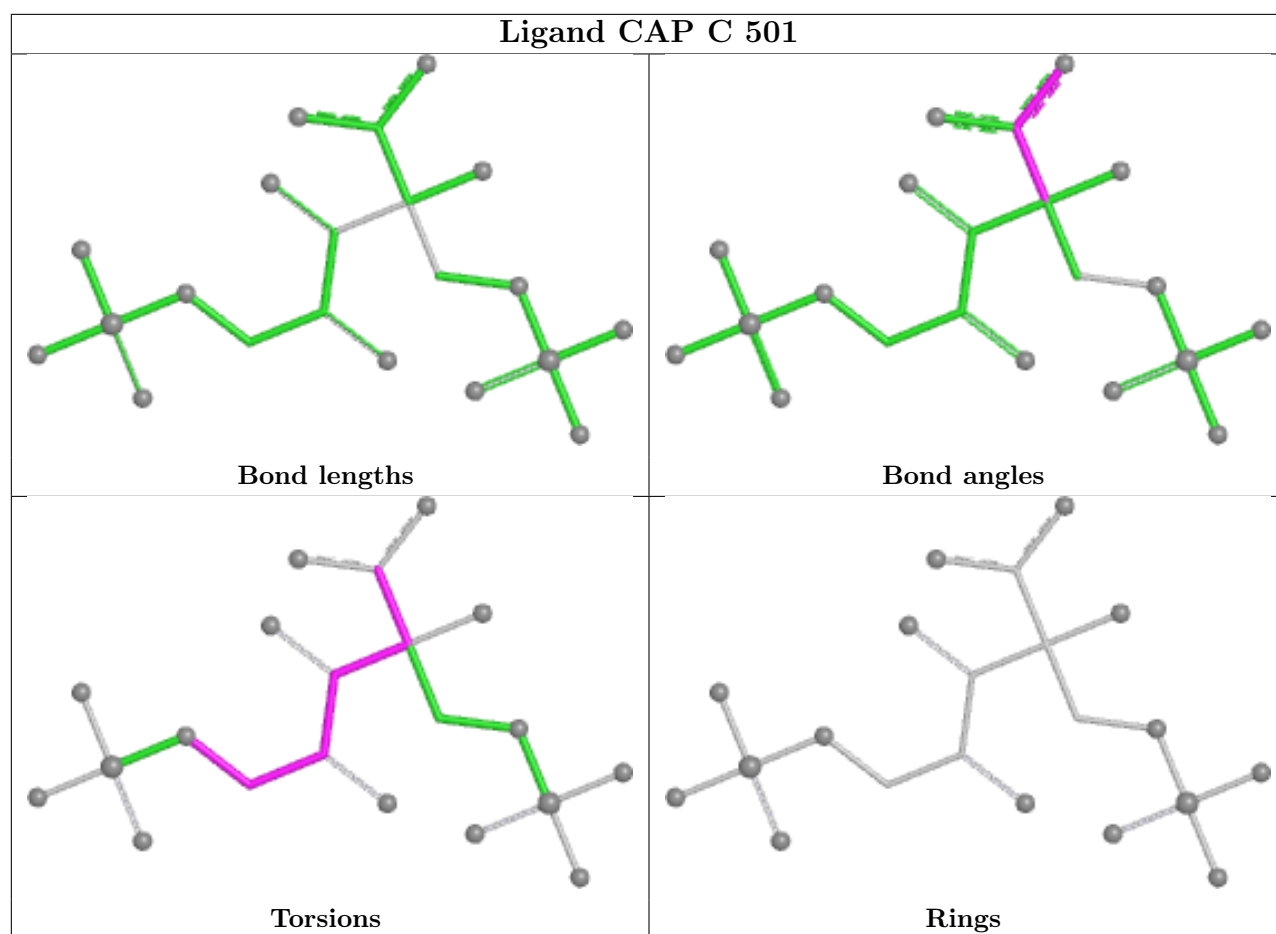
Mol	Chain	Res	Type	Atoms
2	D	502	CAP	O6-C-C2-C3
2	E	501	CAP	O6-C-C2-C3
2	F	501	CAP	O6-C-C2-C3
2	E	501	CAP	O7-C-C2-C1
2	F	501	CAP	O7-C-C2-C1
2	D	502	CAP	C3-C4-C5-O5
2	J	502	CAP	C3-C4-C5-O5
2	D	502	CAP	C4-C5-O5-P2
2	C	501	CAP	O3-C3-C4-C5
2	F	501	CAP	C4-C5-O5-P2
2	C	501	CAP	C2-C3-C4-C5
2	H	501	CAP	C2-C3-C4-C5
2	A	501	CAP	C1-C2-C3-O3
2	G	501	CAP	C2-C3-C4-O4

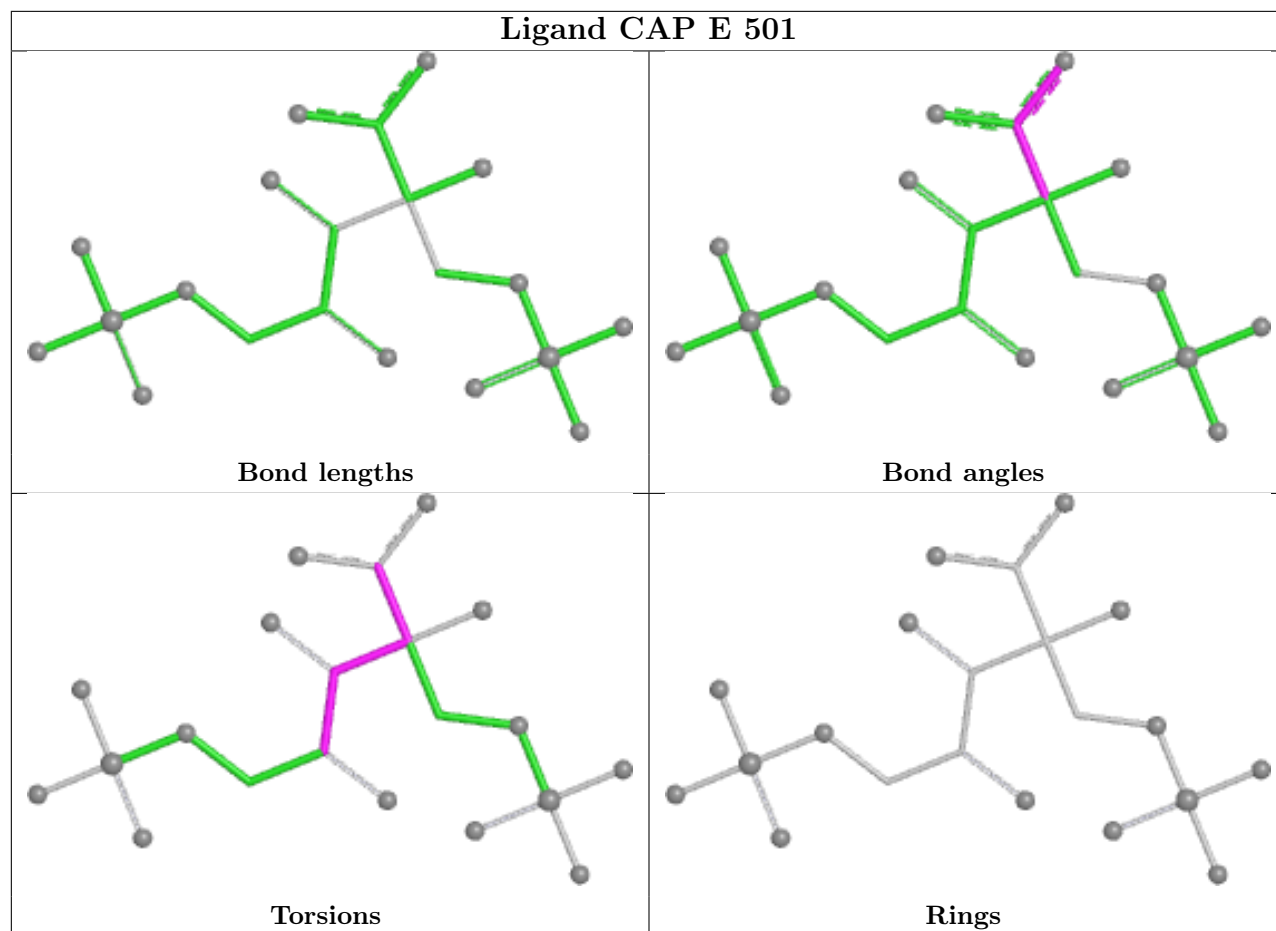
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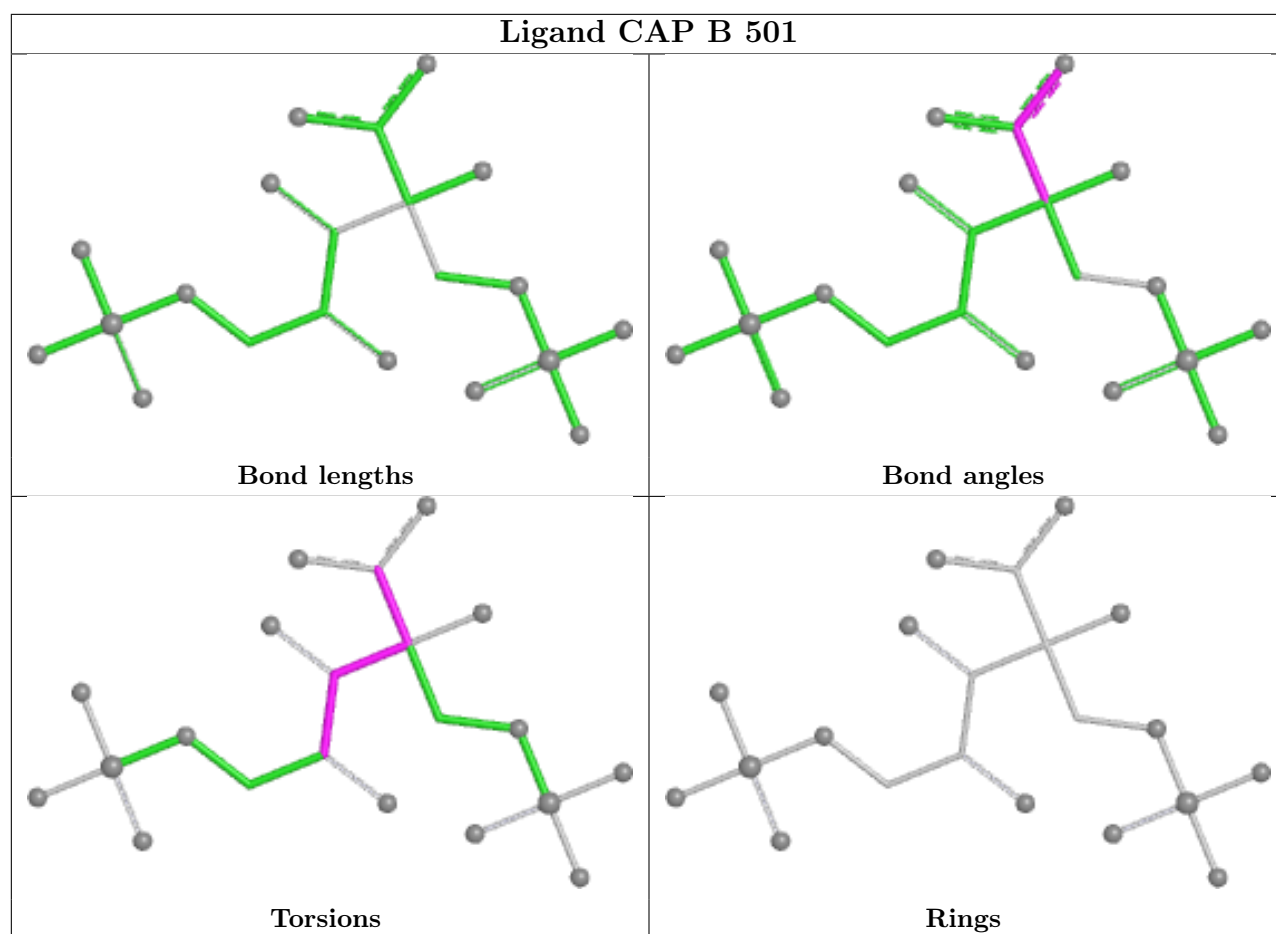
7 monomers are involved in 13 short contacts:

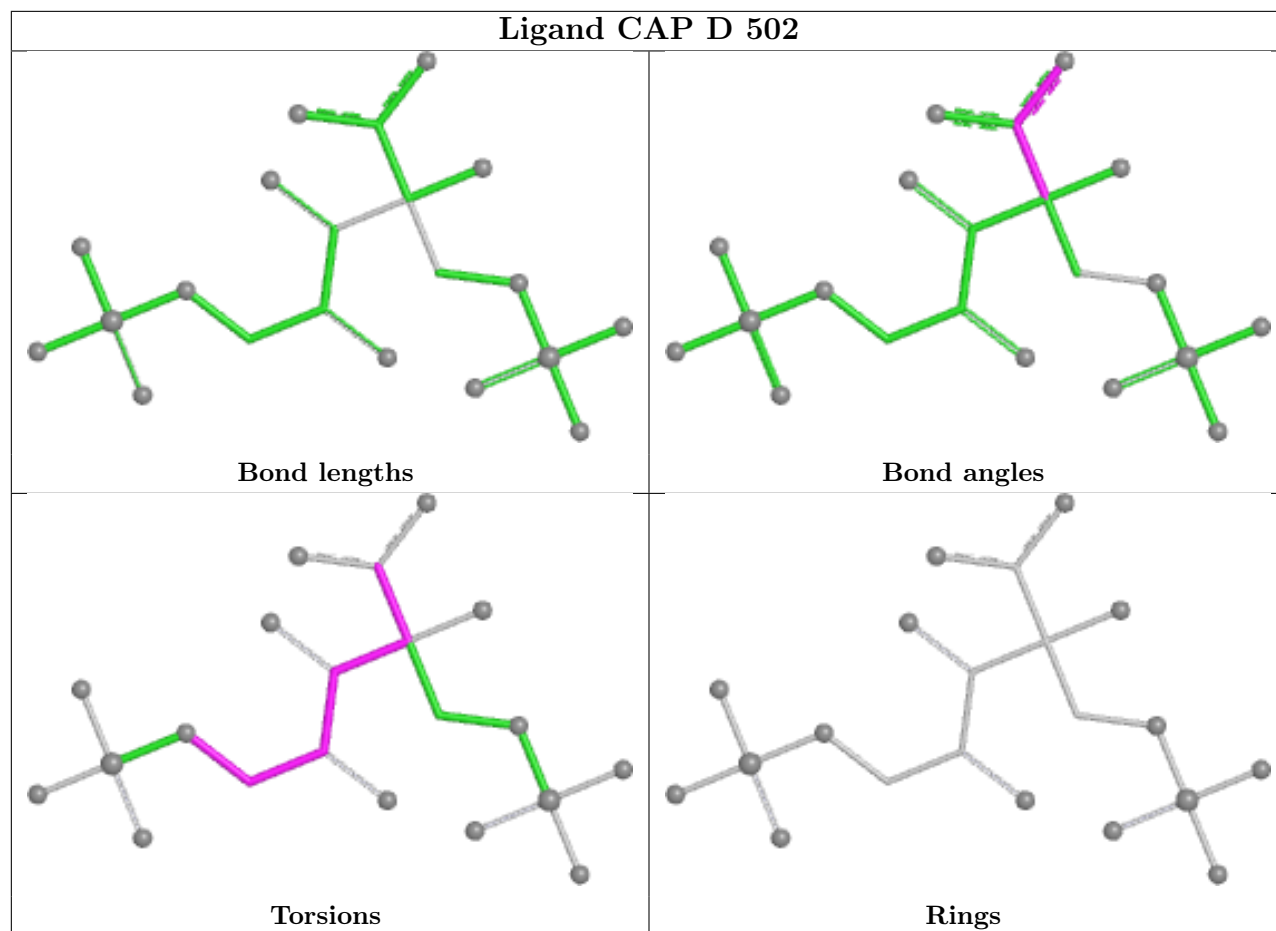
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CAP	1	0
2	D	502	CAP	1	0
2	I	502	CAP	2	0
2	J	502	CAP	2	0
2	H	501	CAP	3	0
2	A	501	CAP	2	0
2	F	501	CAP	2	0

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.

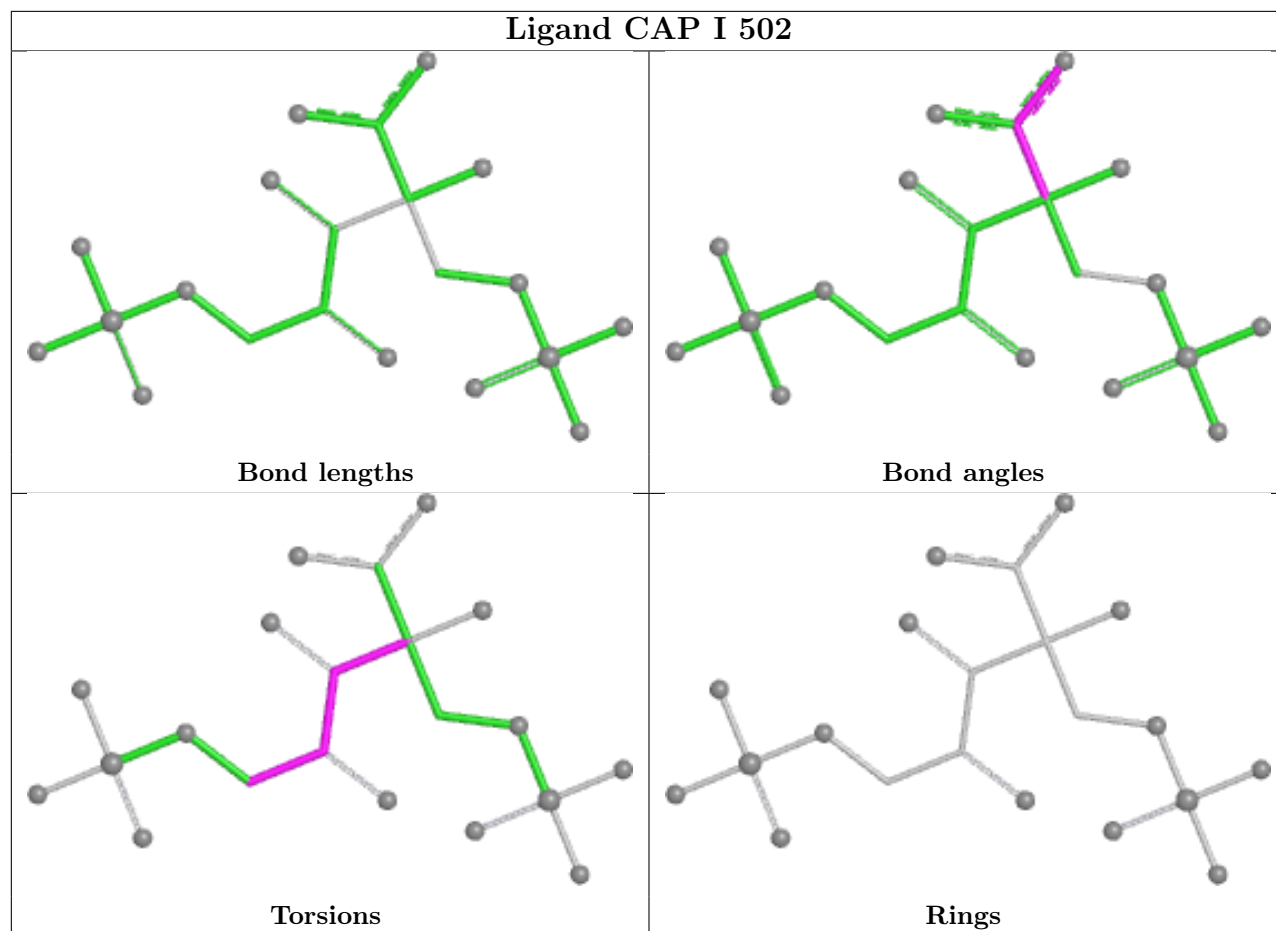


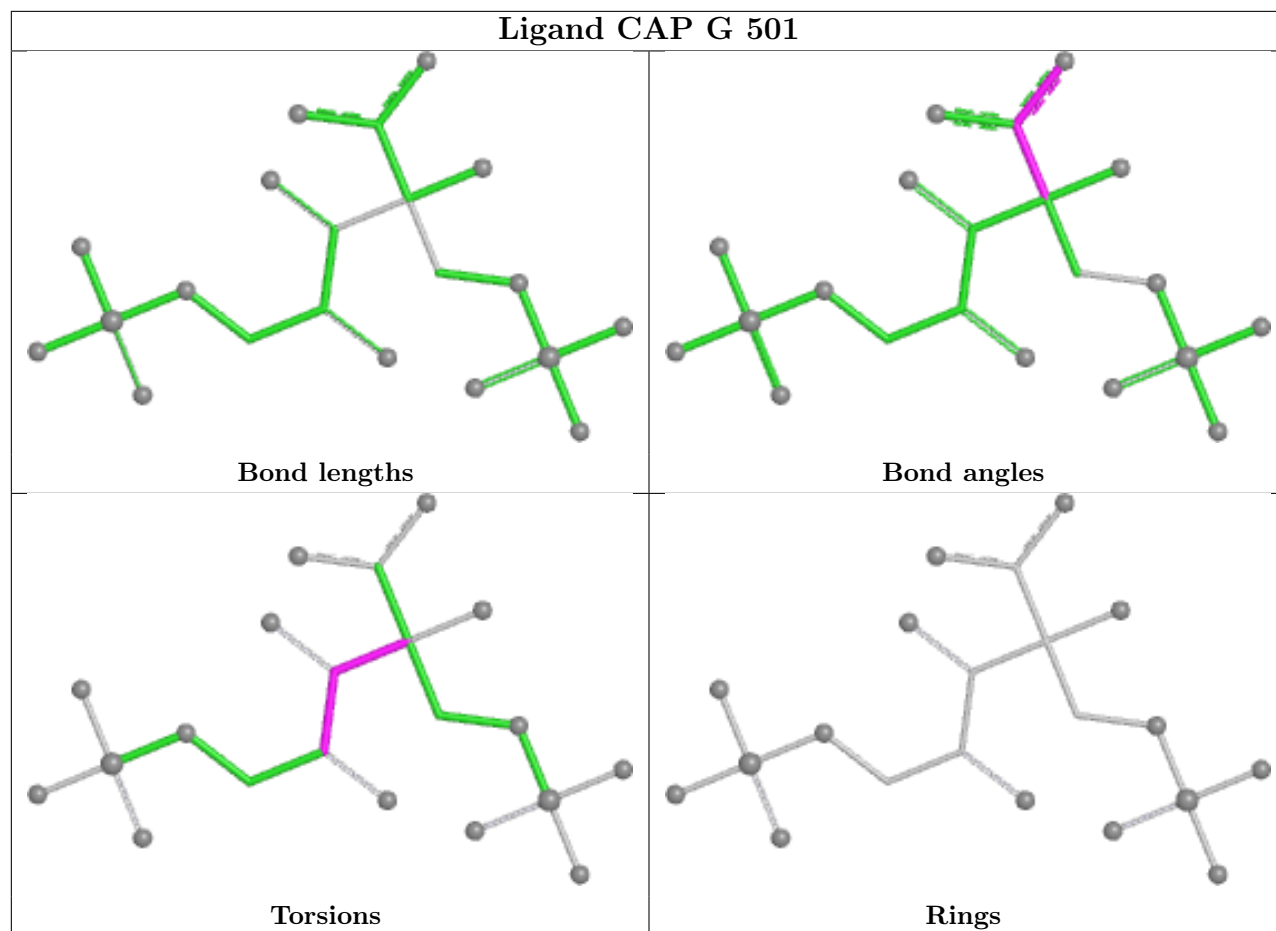




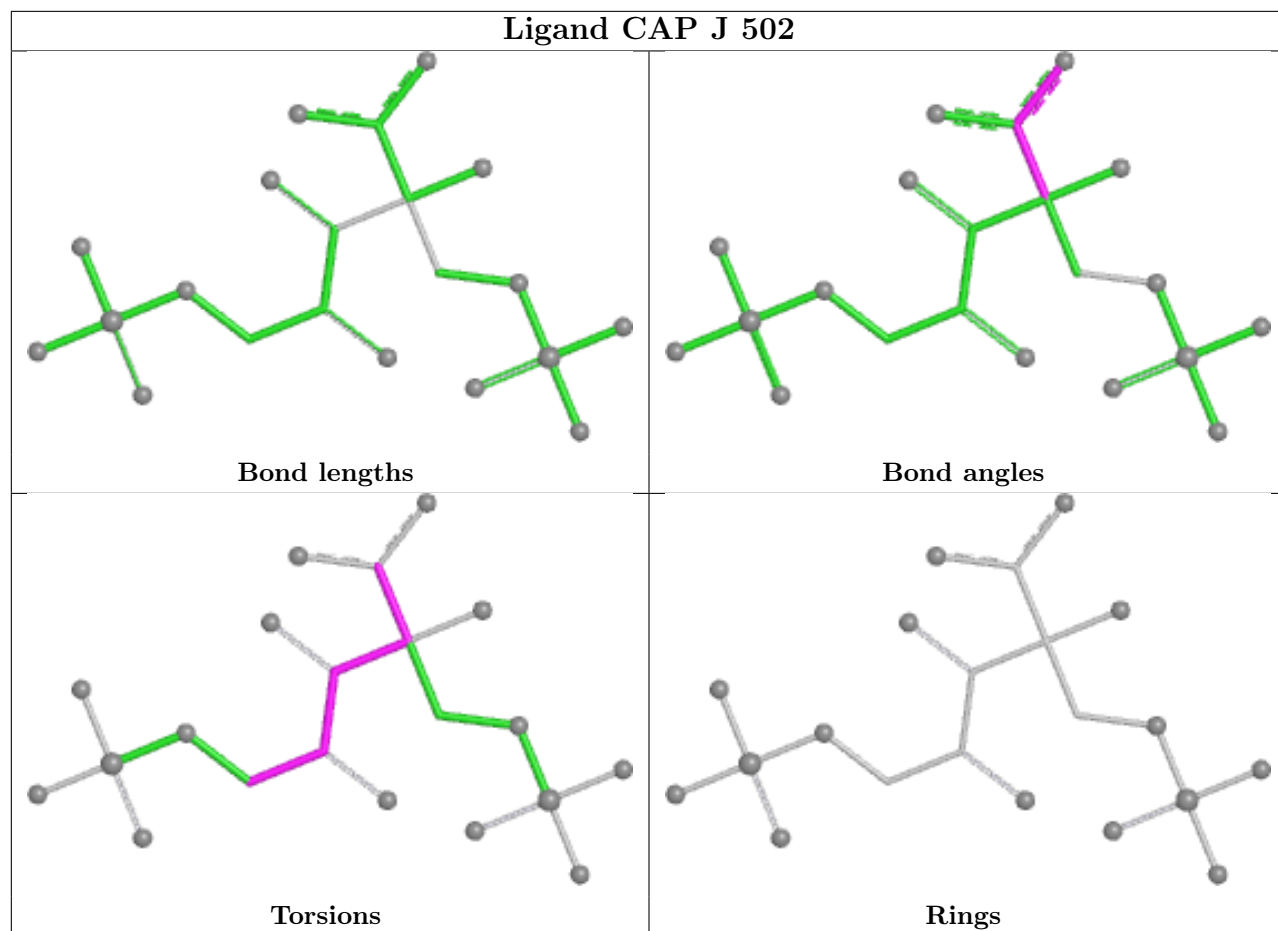


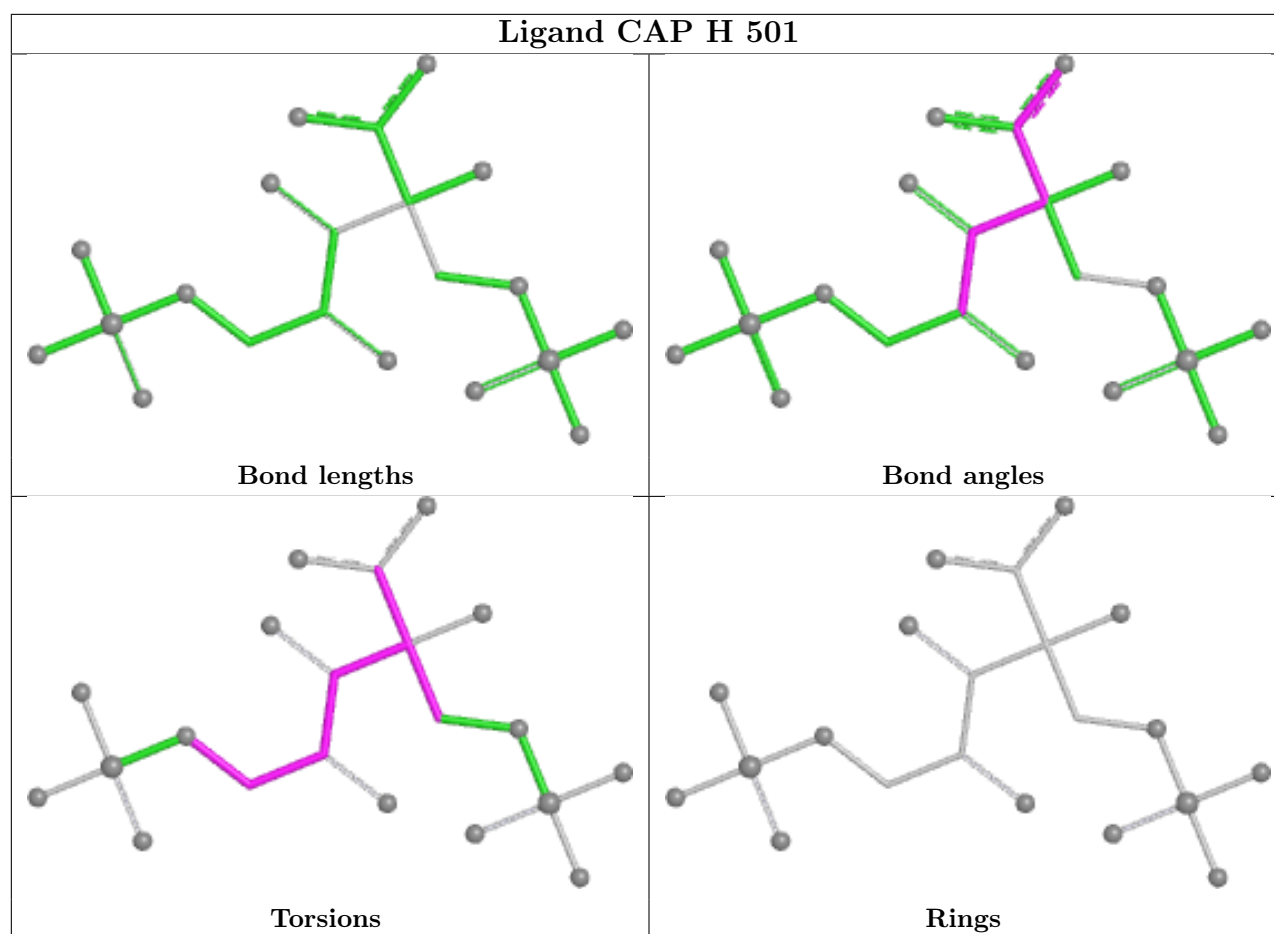
Ligand CAP I 502

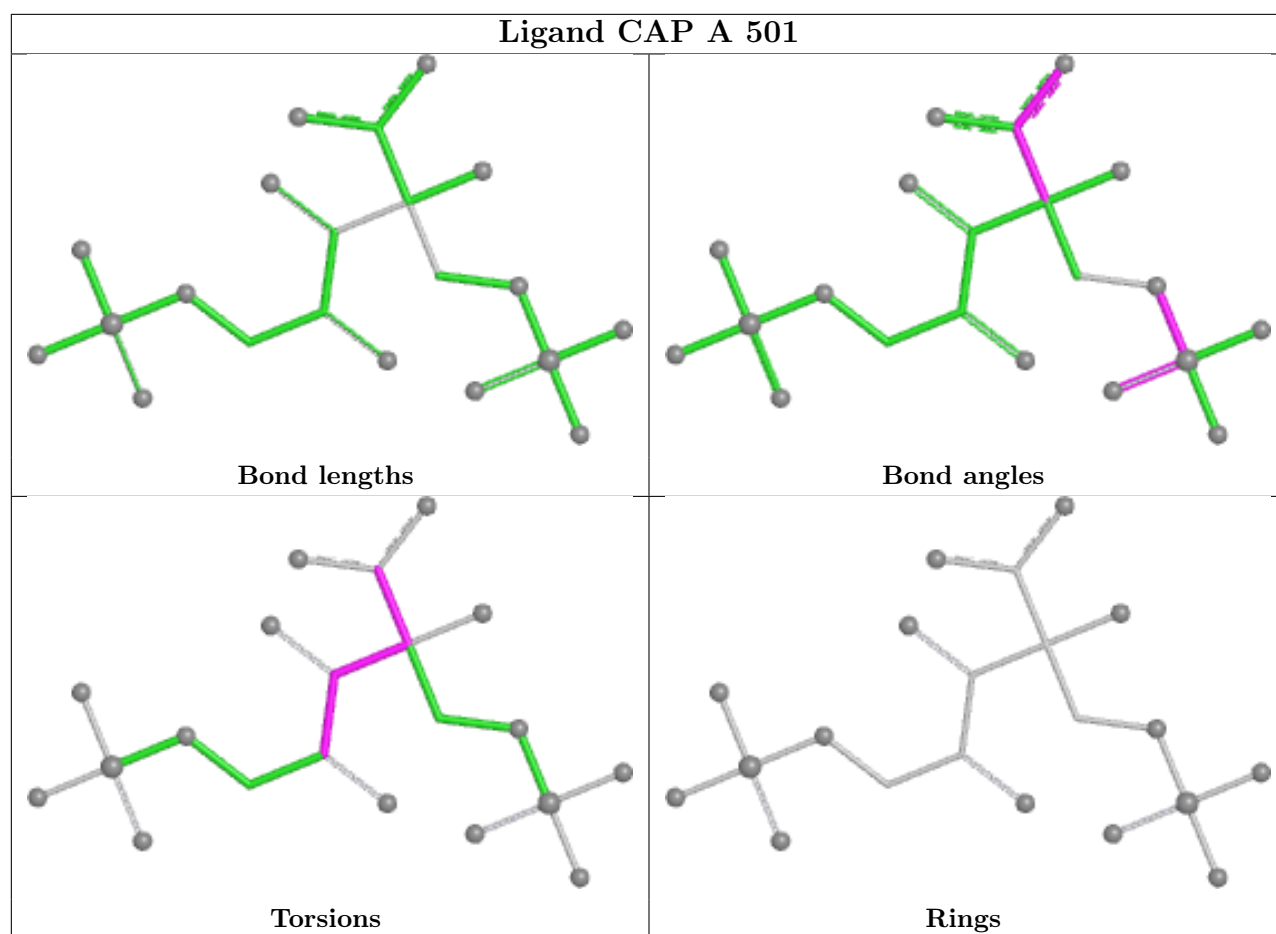


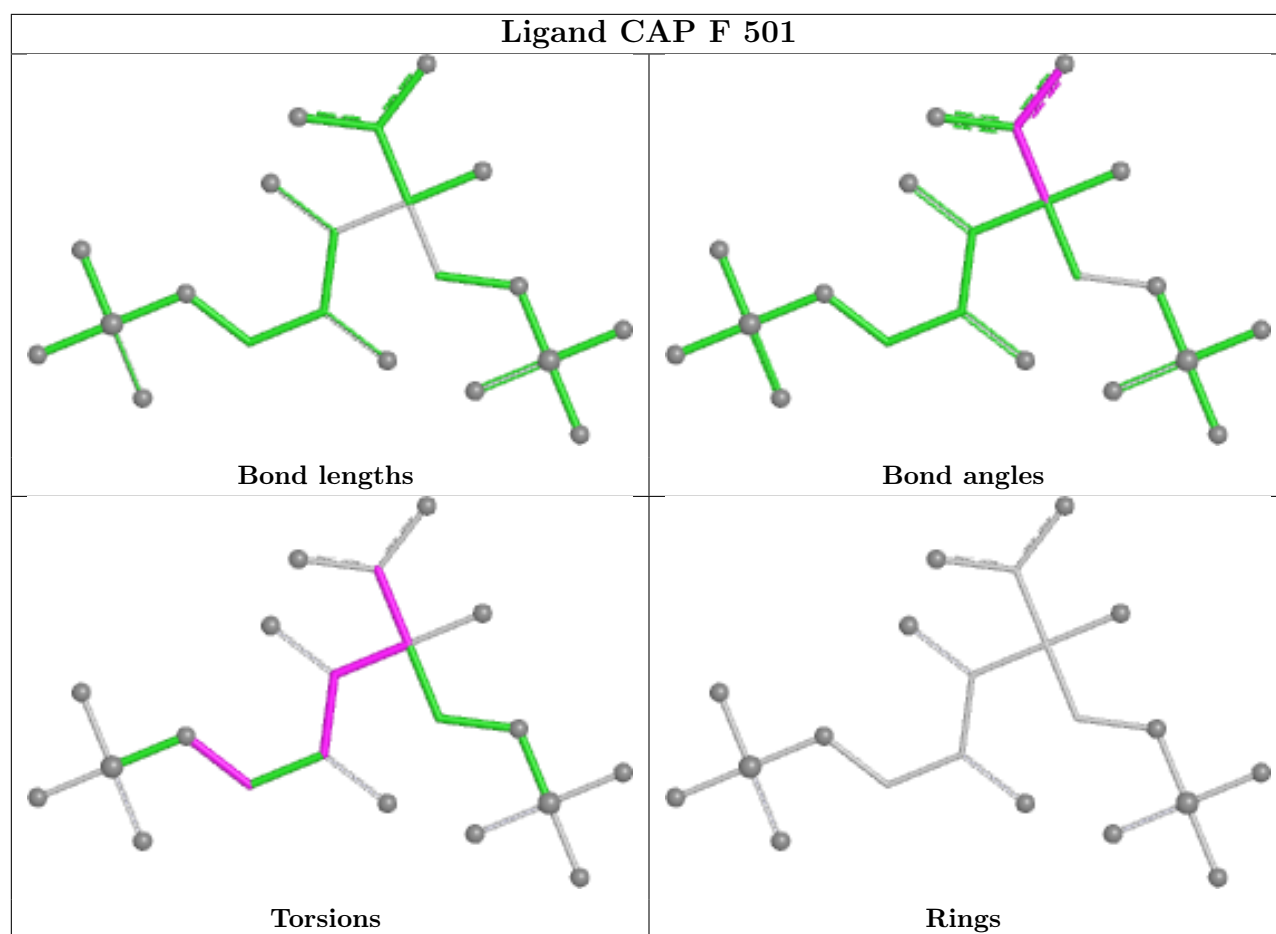


Ligand CAP J 502









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%)	-0.03	2 (0%) 88 87	21, 34, 54, 114	0
1	B	456/468 (97%)	-0.04	7 (1%) 72 67	20, 34, 61, 104	0
1	C	456/468 (97%)	0.31	5 (1%) 78 75	28, 51, 76, 110	0
1	D	456/468 (97%)	0.97	54 (11%) 9 7	43, 73, 96, 139	0
1	E	456/468 (97%)	0.42	6 (1%) 75 71	32, 55, 78, 123	0
1	F	456/468 (97%)	0.99	44 (9%) 13 11	56, 74, 97, 128	0
1	G	456/468 (97%)	1.92	189 (41%) 0 0	80, 106, 133, 178	0
1	H	456/468 (97%)	2.24	240 (52%) 0 0	90, 105, 134, 169	0
1	I	456/468 (97%)	2.05	214 (46%) 0 0	81, 102, 138, 176	0
1	J	456/468 (97%)	1.95	198 (43%) 0 0	73, 112, 142, 167	0
All	All	4560/4680 (97%)	1.08	959 (21%) 2 1	20, 76, 127, 178	0

All (959) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	301	ALA	8.5
1	G	272	PHE	6.8
1	J	294	LEU	6.1
1	I	250	GLY	6.0
1	H	297	PHE	6.0
1	J	297	PHE	6.0
1	H	16	GLY	5.9
1	H	294	LEU	5.9
1	J	19	MET	5.8
1	I	289	TYR	5.7
1	J	372	TYR	5.7
1	H	10	ASN	5.7
1	J	78	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	J	47	GLY	5.6
1	H	148	PHE	5.5
1	G	297	PHE	5.5
1	H	97	PHE	5.4
1	H	152	ILE	5.4
1	I	177	PHE	5.4
1	H	96	THR	5.3
1	H	275	ALA	5.3
1	I	255	TRP	5.3
1	J	8	ILE	5.2
1	J	275	ALA	5.2
1	H	62	LEU	5.2
1	J	123	LEU	5.2
1	G	372	TYR	5.1
1	H	110	VAL	5.1
1	H	291	VAL	5.1
1	H	91	VAL	5.0
1	G	255	TRP	5.0
1	G	25	LEU	5.0
1	H	78	ILE	5.0
1	I	347	ILE	5.0
1	G	387	LEU	5.0
1	I	373	TRP	5.0
1	J	301	ALA	4.9
1	J	439	LEU	4.9
1	I	380	CYS	4.9
1	J	116	VAL	4.9
1	G	199	VAL	4.9
1	H	395	PHE	4.8
1	J	65	LEU	4.8
1	I	251	ILE	4.8
1	F	372	TYR	4.8
1	H	354	LEU	4.8
1	H	372	TYR	4.7
1	J	348	PRO	4.7
1	H	348	PRO	4.7
1	H	37	ALA	4.7
1	H	380	CYS	4.7
1	I	387	LEU	4.7
1	H	255	TRP	4.6
1	J	56	THR	4.6
1	G	166	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	295	THR	4.6
1	H	123	LEU	4.6
1	H	150	SER	4.6
1	D	18	TYR	4.6
1	J	358	ILE	4.6
1	J	64	ALA	4.6
1	H	58	PHE	4.5
1	G	215	VAL	4.5
1	J	402	GLN	4.5
1	G	289	TYR	4.5
1	I	272	PHE	4.5
1	J	374	ARG	4.5
1	H	158	LEU	4.5
1	I	248	VAL	4.5
1	G	177	PHE	4.4
1	G	306	ILE	4.4
1	H	457	ASP	4.4
1	G	102	VAL	4.4
1	I	160	SER	4.3
1	H	84	ILE	4.3
1	H	385	GLY	4.3
1	I	91	VAL	4.3
1	H	157	GLY	4.3
1	J	258	ILE	4.3
1	I	121	GLN	4.2
1	H	183	PRO	4.2
1	C	373	TRP	4.2
1	J	343	ILE	4.2
1	J	66	VAL	4.2
1	G	158	LEU	4.2
1	H	156	ILE	4.1
1	H	382	ILE	4.1
1	I	97	PHE	4.1
1	I	176	ASP	4.1
1	J	91	VAL	4.1
1	D	289	TYR	4.1
1	G	95	MET	4.1
1	H	343	ILE	4.1
1	F	452	ALA	4.1
1	G	410	ALA	4.1
1	I	308	THR	4.1
1	J	279	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	426	VAL	4.0
1	I	306	ILE	4.0
1	H	352	ALA	4.0
1	H	66	VAL	4.0
1	H	248	VAL	4.0
1	G	167	CYS	4.0
1	I	412	VAL	4.0
1	H	45	SER	3.9
1	J	251	ILE	3.9
1	D	373	TRP	3.9
1	J	85	PHE	3.9
1	J	7	GLN	3.9
1	I	166	LEU	3.9
1	F	275	ALA	3.9
1	H	251	ILE	3.9
1	I	103	PHE	3.9
1	D	25	LEU	3.9
1	J	225	TYR	3.8
1	J	54	THR	3.8
1	H	258	ILE	3.8
1	J	278	GLY	3.8
1	G	103	PHE	3.8
1	G	84	ILE	3.8
1	I	25	LEU	3.8
1	I	147	ILE	3.8
1	J	354	LEU	3.8
1	J	387	LEU	3.8
1	G	47	GLY	3.8
1	G	120	PRO	3.8
1	J	255	TRP	3.8
1	H	289	TYR	3.8
1	H	368	SER	3.8
1	H	49	PHE	3.8
1	G	293	VAL	3.8
1	C	372	TYR	3.8
1	H	126	TYR	3.8
1	H	405	ILE	3.8
1	J	142	ILE	3.8
1	D	275	ALA	3.8
1	I	58	PHE	3.8
1	G	301	ALA	3.7
1	I	89	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	378	LYS	3.7
1	J	340	PHE	3.7
1	I	303	ALA	3.7
1	H	177	PHE	3.7
1	I	189	PHE	3.7
1	I	22	VAL	3.7
1	D	16	GLY	3.7
1	D	64	ALA	3.7
1	H	185	ALA	3.7
1	J	373	TRP	3.7
1	G	94	ILE	3.6
1	H	54	THR	3.6
1	J	98	ILE	3.6
1	J	122	MET	3.6
1	I	293	VAL	3.6
1	H	36	THR	3.6
1	I	372	TYR	3.6
1	H	95	MET	3.6
1	H	284	GLU	3.6
1	H	300	LEU	3.6
1	G	313	ILE	3.6
1	I	83	ARG	3.6
1	E	372	TYR	3.6
1	I	48	SER	3.6
1	H	55	ALA	3.6
1	H	44	SER	3.6
1	G	299	ARG	3.5
1	J	406	THR	3.5
1	H	379	MET	3.5
1	I	257	ALA	3.5
1	G	300	LEU	3.5
1	G	258	ILE	3.5
1	I	405	ILE	3.5
1	H	344	TRP	3.5
1	I	125	GLN	3.5
1	J	80	TYR	3.5
1	H	147	ILE	3.5
1	I	98	ILE	3.5
1	J	6	ILE	3.5
1	H	298	ALA	3.5
1	H	386	GLY	3.5
1	I	178	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	423	ALA	3.5
1	H	189	PHE	3.5
1	H	77	TRP	3.5
1	J	34	VAL	3.5
1	H	306	ILE	3.4
1	H	358	ILE	3.4
1	I	258	ILE	3.4
1	J	126	TYR	3.4
1	J	289	TYR	3.4
1	H	122	MET	3.4
1	I	32	THR	3.4
1	G	98	ILE	3.4
1	I	453	ILE	3.4
1	I	304	SER	3.4
1	J	401	THR	3.4
1	G	99	ALA	3.4
1	H	390	LEU	3.4
1	H	435	GLN	3.4
1	J	272	PHE	3.4
1	I	40	VAL	3.4
1	H	52	ILE	3.4
1	J	52	ILE	3.4
1	H	99	ALA	3.4
1	H	146	PRO	3.4
1	G	412	VAL	3.4
1	I	124	VAL	3.4
1	G	373	TRP	3.4
1	J	339	TYR	3.4
1	D	276	GLY	3.4
1	J	21	ALA	3.4
1	I	277	HIS	3.4
1	H	34	VAL	3.4
1	J	40	VAL	3.4
1	H	142	ILE	3.3
1	J	156	ILE	3.3
1	D	27	GLY	3.3
1	H	387	LEU	3.3
1	I	29	GLU	3.3
1	G	251	ILE	3.3
1	H	8	ILE	3.3
1	I	295	THR	3.3
1	H	11	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	123	LEU	3.3
1	I	47	GLY	3.3
1	I	275	ALA	3.3
1	J	118	PHE	3.3
1	G	56	THR	3.3
1	G	191	PRO	3.3
1	I	416	PRO	3.3
1	J	37	ALA	3.3
1	D	77	TRP	3.3
1	G	407	THR	3.3
1	I	356	LEU	3.3
1	G	189	PHE	3.3
1	H	14	PHE	3.3
1	H	103	PHE	3.3
1	J	280	PHE	3.3
1	H	351	ASP	3.3
1	H	43	GLU	3.2
1	J	62	LEU	3.2
1	J	32	THR	3.2
1	J	308	THR	3.2
1	H	184	GLN	3.2
1	E	225	TYR	3.2
1	H	288	GLY	3.2
1	H	327	ALA	3.2
1	H	98	ILE	3.2
1	J	148	PHE	3.2
1	J	404	PHE	3.2
1	G	380	CYS	3.2
1	J	1	MET	3.2
1	J	114	LEU	3.2
1	H	82	TRP	3.2
1	G	44	SER	3.2
1	G	160	SER	3.2
1	I	164	ALA	3.2
1	G	91	VAL	3.2
1	I	52	ILE	3.2
1	I	246	PHE	3.2
1	J	13	VAL	3.2
1	J	177	PHE	3.2
1	H	81	PRO	3.2
1	H	119	PRO	3.2
1	G	117	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	215	VAL	3.2
1	H	280	PHE	3.2
1	H	439	LEU	3.2
1	H	373	TRP	3.2
1	I	386	GLY	3.2
1	I	202	ALA	3.2
1	H	437	ILE	3.2
1	I	8	ILE	3.2
1	I	84	ILE	3.2
1	I	113	ILE	3.2
1	H	40	VAL	3.2
1	I	309	GLY	3.1
1	I	327	ALA	3.1
1	J	410	ALA	3.1
1	J	147	ILE	3.1
1	H	13	VAL	3.1
1	H	412	VAL	3.1
1	I	95	MET	3.1
1	E	143	GLN	3.1
1	H	376	THR	3.1
1	G	37	ALA	3.1
1	I	77	TRP	3.1
1	G	147	ILE	3.1
1	G	287	ILE	3.1
1	H	235	ILE	3.1
1	H	225	TYR	3.1
1	I	67	TYR	3.1
1	B	69	ILE	3.1
1	H	383	ILE	3.1
1	H	433	TRP	3.1
1	J	84	ILE	3.1
1	G	50	VAL	3.1
1	G	217	SER	3.1
1	I	274	ARG	3.1
1	J	44	SER	3.1
1	I	43	GLU	3.1
1	G	53	GLY	3.1
1	H	32	THR	3.1
1	I	276	GLY	3.1
1	G	142	ILE	3.1
1	I	152	ILE	3.1
1	J	79	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	344	TRP	3.1
1	I	291	VAL	3.1
1	J	324	VAL	3.1
1	E	160	SER	3.1
1	G	430	TYR	3.0
1	I	56	THR	3.0
1	H	313	ILE	3.0
1	I	301	ALA	3.0
1	I	13	VAL	3.0
1	I	44	SER	3.0
1	G	391	LEU	3.0
1	J	81	PRO	3.0
1	G	383	ILE	3.0
1	J	263	ARG	3.0
1	D	297	PHE	3.0
1	H	144	GLU	3.0
1	D	67	TYR	3.0
1	G	26	GLN	3.0
1	I	24	ARG	3.0
1	G	385	GLY	3.0
1	H	104	GLY	3.0
1	J	295	THR	3.0
1	G	429	ALA	3.0
1	J	55	ALA	3.0
1	I	297	PHE	3.0
1	D	107	SER	3.0
1	I	111	CYS	3.0
1	I	129	PRO	3.0
1	J	183	PRO	3.0
1	G	339	TYR	3.0
1	I	1	MET	3.0
1	G	156	ILE	3.0
1	H	287	ILE	3.0
1	G	159	THR	3.0
1	G	288	GLY	3.0
1	I	159	THR	3.0
1	G	451	ALA	3.0
1	I	279	ALA	3.0
1	I	330	ALA	3.0
1	G	354	LEU	2.9
1	J	20	LEU	2.9
1	G	334	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	49	PHE	2.9
1	H	124	VAL	2.9
1	I	294	LEU	2.9
1	H	214	LYS	2.9
1	I	167	CYS	2.9
1	J	24	ARG	2.9
1	G	113	ILE	2.9
1	D	148	PHE	2.9
1	G	395	PHE	2.9
1	J	108	VAL	2.9
1	I	158	LEU	2.9
1	I	333	LEU	2.9
1	J	33	LEU	2.9
1	G	292	PRO	2.9
1	G	82	TRP	2.9
1	I	41	ALA	2.9
1	J	370	LEU	2.9
1	J	144	GLU	2.9
1	I	26	GLN	2.9
1	G	453	ILE	2.9
1	D	372	TYR	2.9
1	G	36	THR	2.9
1	I	406	THR	2.9
1	D	279	ALA	2.9
1	H	332	LYS	2.9
1	H	404	PHE	2.9
1	J	382	ILE	2.8
1	D	350	LYS	2.8
1	G	411	GLY	2.8
1	H	80	TYR	2.8
1	H	367	TYR	2.8
1	I	80	TYR	2.8
1	J	131	TYR	2.8
1	I	96	THR	2.8
1	I	253	ALA	2.8
1	F	108	VAL	2.8
1	G	97	PHE	2.8
1	J	389	PRO	2.8
1	I	197	GLN	2.8
1	J	82	TRP	2.8
1	H	113	ILE	2.8
1	I	69	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	287	ILE	2.8
1	H	411	GLY	2.8
1	J	88	GLY	2.8
1	G	111	CYS	2.8
1	H	303	ALA	2.8
1	J	257	ALA	2.8
1	G	271	HIS	2.8
1	H	324	VAL	2.8
1	H	19	MET	2.8
1	G	101	ASN	2.8
1	I	101	ASN	2.8
1	I	302	GLY	2.8
1	I	115	ASP	2.8
1	H	132	THR	2.8
1	D	225	TYR	2.8
1	H	452	ALA	2.8
1	I	54	THR	2.8
1	J	298	ALA	2.8
1	J	376	THR	2.8
1	H	328	ARG	2.8
1	F	7	GLN	2.8
1	H	48	SER	2.8
1	G	157	GLY	2.8
1	G	58	PHE	2.8
1	D	5	TYR	2.8
1	H	292	PRO	2.7
1	H	121	GLN	2.7
1	G	247	LEU	2.7
1	I	30	GLY	2.7
1	I	388	ASN	2.7
1	J	316	MET	2.7
1	J	329	HIS	2.7
1	C	21	ALA	2.7
1	G	83	ARG	2.7
1	G	206	VAL	2.7
1	H	252	THR	2.7
1	I	34	VAL	2.7
1	I	346	GLU	2.7
1	I	148	PHE	2.7
1	J	399	VAL	2.7
1	J	11	PRO	2.7
1	J	261	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	47	GLY	2.7
1	H	438	SER	2.7
1	D	37	ALA	2.7
1	G	248	VAL	2.7
1	H	198	ASP	2.7
1	J	395	PHE	2.7
1	H	5	TYR	2.7
1	G	220	ILE	2.7
1	G	294	LEU	2.7
1	G	219	ASN	2.7
1	J	48	SER	2.7
1	G	457	ASP	2.7
1	H	406	THR	2.7
1	I	37	ALA	2.7
1	I	79	ALA	2.7
1	I	51	LYS	2.7
1	H	168	TYR	2.7
1	J	367	TYR	2.7
1	G	78	ILE	2.7
1	J	331	LEU	2.7
1	G	24	ARG	2.7
1	G	305	GLY	2.7
1	G	386	GLY	2.7
1	H	242	GLY	2.7
1	I	104	GLY	2.7
1	H	180	ASN	2.7
1	F	215	VAL	2.7
1	G	64	ALA	2.7
1	G	96	THR	2.7
1	G	246	PHE	2.7
1	G	275	ALA	2.7
1	H	407	THR	2.7
1	I	57	ALA	2.7
1	J	103	PHE	2.7
1	B	11	PRO	2.7
1	H	396	ILE	2.6
1	G	415	HIS	2.6
1	G	144	GLU	2.6
1	J	43	GLU	2.6
1	I	36	THR	2.6
1	J	23	PHE	2.6
1	J	154	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	338	ASP	2.6
1	J	342	GLN	2.6
1	F	358	ILE	2.6
1	G	375	ILE	2.6
1	I	287	ILE	2.6
1	H	25	LEU	2.6
1	G	88	GLY	2.6
1	J	318	GLY	2.6
1	J	388	ASN	2.6
1	D	23	PHE	2.6
1	D	120	PRO	2.6
1	H	218	PHE	2.6
1	F	456	TYR	2.6
1	H	413	HIS	2.6
1	I	299	ARG	2.6
1	J	83	ARG	2.6
1	J	145	ARG	2.6
1	H	377	LYS	2.6
1	G	27	GLY	2.6
1	J	16	GLY	2.6
1	J	128	GLY	2.6
1	G	21	ALA	2.6
1	H	118	PHE	2.6
1	H	381	PRO	2.6
1	H	389	PRO	2.6
1	I	23	PHE	2.6
1	I	81	PRO	2.6
1	I	348	PRO	2.6
1	J	120	PRO	2.6
1	J	429	ALA	2.6
1	H	172	SER	2.6
1	I	150	SER	2.6
1	J	355	GLN	2.6
1	H	4	GLU	2.6
1	H	39	GLU	2.6
1	H	27	GLY	2.6
1	H	314	GLY	2.6
1	G	291	VAL	2.6
1	G	348	PRO	2.6
1	I	154	PRO	2.6
1	I	452	ALA	2.6
1	J	57	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	76	VAL	2.6
1	D	402	GLN	2.6
1	I	221	SER	2.5
1	F	1	MET	2.5
1	H	249	ASP	2.5
1	I	109	LYS	2.5
1	H	334	TYR	2.5
1	G	416	PRO	2.5
1	H	241	PRO	2.5
1	I	102	VAL	2.5
1	J	22	VAL	2.5
1	D	111	CYS	2.5
1	G	404	PHE	2.5
1	H	46	THR	2.5
1	I	419	THR	2.5
1	G	8	ILE	2.5
1	D	33	LEU	2.5
1	H	65	LEU	2.5
1	I	427	LEU	2.5
1	J	247	LEU	2.5
1	G	456	TYR	2.5
1	I	100	GLY	2.5
1	G	22	VAL	2.5
1	I	116	VAL	2.5
1	F	395	PHE	2.5
1	H	410	ALA	2.5
1	I	451	ALA	2.5
1	I	455	PHE	2.5
1	J	14	PHE	2.5
1	G	223	SER	2.5
1	G	152	ILE	2.5
1	H	171	TRP	2.5
1	I	133	ILE	2.5
1	I	156	ILE	2.5
1	G	270	LEU	2.5
1	H	274	ARG	2.5
1	H	370	LEU	2.5
1	I	33	LEU	2.5
1	I	126	TYR	2.5
1	J	30	GLY	2.5
1	G	381	PRO	2.5
1	G	116	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	408	MET	2.5
1	I	55	ALA	2.5
1	I	64	ALA	2.5
1	I	85	PHE	2.5
1	G	406	THR	2.5
1	D	3	LYS	2.5
1	H	12	ASN	2.5
1	G	6	ILE	2.5
1	H	140	LEU	2.5
1	I	358	ILE	2.5
1	J	368	SER	2.5
1	I	403	ASP	2.5
1	H	329	HIS	2.5
1	D	346	GLU	2.5
1	H	276	GLY	2.5
1	H	409	GLY	2.5
1	J	364	GLY	2.5
1	G	196	VAL	2.5
1	H	116	VAL	2.5
1	I	426	VAL	2.5
1	J	50	VAL	2.5
1	G	232	ALA	2.5
1	G	317	ALA	2.5
1	F	313	ILE	2.4
1	H	133	ILE	2.4
1	H	356	LEU	2.4
1	I	20	LEU	2.4
1	J	300	LEU	2.4
1	F	160	SER	2.4
1	J	346	GLU	2.4
1	I	16	GLY	2.4
1	B	225	TYR	2.4
1	H	117	TYR	2.4
1	J	456	TYR	2.4
1	D	34	VAL	2.4
1	G	40	VAL	2.4
1	I	108	VAL	2.4
1	J	121	GLN	2.4
1	H	326	ALA	2.4
1	J	269	PHE	2.4
1	I	310	THR	2.4
1	J	96	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	LEU	2.4
1	G	52	ILE	2.4
1	H	229	ILE	2.4
1	I	62	LEU	2.4
1	J	15	ASN	2.4
1	J	113	ILE	2.4
1	J	270	LEU	2.4
1	G	38	SER	2.4
1	H	188	ASP	2.4
1	H	136	MET	2.4
1	H	302	GLY	2.4
1	I	371	GLY	2.4
1	I	50	VAL	2.4
1	I	66	VAL	2.4
1	G	280	PHE	2.4
1	H	317	ALA	2.4
1	I	395	PHE	2.4
1	I	140	LEU	2.4
1	I	227	THR	2.4
1	J	152	ILE	2.4
1	J	453	ILE	2.4
1	I	219	ASN	2.4
1	J	10	ASN	2.4
1	I	365	GLU	2.4
1	D	1	MET	2.4
1	H	309	GLY	2.4
1	I	411	GLY	2.4
1	G	192	TYR	2.4
1	H	131	TYR	2.4
1	H	202	ALA	2.4
1	I	49	PHE	2.4
1	I	404	PHE	2.4
1	J	97	PHE	2.4
1	D	123	LEU	2.4
1	G	114	LEU	2.4
1	I	114	LEU	2.4
1	G	401	THR	2.4
1	I	375	ILE	2.4
1	I	396	ILE	2.4
1	G	48	SER	2.4
1	H	345	SER	2.4
1	I	414	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	95	MET	2.4
1	F	167	CYS	2.4
1	H	394	LYS	2.4
1	I	378	LYS	2.4
1	J	293	VAL	2.4
1	G	253	ALA	2.4
1	H	79	ALA	2.4
1	H	164	ALA	2.4
1	I	280	PHE	2.4
1	G	333	LEU	2.3
1	J	5	TYR	2.3
1	H	6	ILE	2.3
1	H	375	ILE	2.3
1	I	94	ILE	2.3
1	F	32	THR	2.3
1	H	159	THR	2.3
1	H	216	HIS	2.3
1	F	414	SER	2.3
1	H	194	LYS	2.3
1	J	457	ASP	2.3
1	I	344	TRP	2.3
1	F	309	GLY	2.3
1	H	100	GLY	2.3
1	H	400	GLY	2.3
1	G	108	VAL	2.3
1	G	324	VAL	2.3
1	H	340	PHE	2.3
1	I	269	PHE	2.3
1	J	166	LEU	2.3
1	J	326	ALA	2.3
1	I	383	ILE	2.3
1	H	67	TYR	2.3
1	I	456	TYR	2.3
1	F	295	THR	2.3
1	H	316	MET	2.3
1	G	243	SER	2.3
1	C	364	GLY	2.3
1	F	30	GLY	2.3
1	J	276	GLY	2.3
1	J	411	GLY	2.3
1	H	50	VAL	2.3
1	H	102	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	41	ALA	2.3
1	G	327	ALA	2.3
1	G	330	ALA	2.3
1	H	423	ALA	2.3
1	H	449	LEU	2.3
1	I	14	PHE	2.3
1	I	106	ALA	2.3
1	I	449	LEU	2.3
1	J	330	ALA	2.3
1	J	356	LEU	2.3
1	J	313	ILE	2.3
1	G	252	THR	2.3
1	G	310	THR	2.3
1	H	339	TYR	2.3
1	I	367	TYR	2.3
1	D	112	LYS	2.3
1	G	10	ASN	2.3
1	G	162	GLU	2.3
1	G	161	SER	2.3
1	F	154	PRO	2.3
1	H	127	ASP	2.3
1	J	86	ASP	2.3
1	J	345	SER	2.3
1	J	292	PRO	2.3
1	G	276	GLY	2.3
1	H	88	GLY	2.3
1	I	128	GLY	2.3
1	F	196	VAL	2.3
1	H	293	VAL	2.3
1	G	75	LEU	2.3
1	I	370	LEU	2.3
1	J	58	PHE	2.3
1	D	6	ILE	2.3
1	G	55	ALA	2.3
1	H	21	ALA	2.3
1	H	69	ILE	2.3
1	H	220	ILE	2.3
1	J	357	ALA	2.3
1	G	212	LYS	2.3
1	G	225	TYR	2.3
1	D	39	GLU	2.3
1	I	369	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	403	ASP	2.3
1	H	137	ARG	2.3
1	J	63	ASP	2.3
1	H	143	GLN	2.3
1	J	92	GLN	2.3
1	F	386	GLY	2.3
1	D	65	LEU	2.3
1	D	116	VAL	2.3
1	G	62	LEU	2.3
1	H	399	VAL	2.3
1	H	272	PHE	2.3
1	I	118	PHE	2.3
1	I	21	ALA	2.2
1	I	415	HIS	2.2
1	I	31	MET	2.2
1	J	3	LYS	2.2
1	J	230	LYS	2.2
1	A	372	TYR	2.2
1	D	126	TYR	2.2
1	I	430	TYR	2.2
1	D	348	PRO	2.2
1	G	183	PRO	2.2
1	J	381	PRO	2.2
1	G	384	SER	2.2
1	H	59	SER	2.2
1	G	174	GLY	2.2
1	G	400	GLY	2.2
1	J	309	GLY	2.2
1	D	102	VAL	2.2
1	J	248	VAL	2.2
1	G	153	LYS	2.2
1	H	269	PHE	2.2
1	I	6	ILE	2.2
1	I	311	ALA	2.2
1	J	42	ALA	2.2
1	J	377	LYS	2.2
1	J	136	MET	2.2
1	J	380	CYS	2.2
1	H	398	THR	2.2
1	H	200	ARG	2.2
1	I	180	ASN	2.2
1	J	146	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	454	GLN	2.2
1	I	2	GLN	2.2
1	G	100	GLY	2.2
1	G	414	SER	2.2
1	I	249	ASP	2.2
1	J	371	GLY	2.2
1	H	33	LEU	2.2
1	I	270	LEU	2.2
1	J	25	LEU	2.2
1	D	98	ILE	2.2
1	F	37	ALA	2.2
1	F	164	ALA	2.2
1	D	54	THR	2.2
1	I	292	PRO	2.2
1	H	26	GLN	2.2
1	D	30	GLY	2.2
1	G	173	GLY	2.2
1	G	172	SER	2.2
1	G	449	LEU	2.2
1	H	114	LEU	2.2
1	H	166	LEU	2.2
1	H	391	LEU	2.2
1	I	385	GLY	2.2
1	I	107	SER	2.2
1	I	222	SER	2.2
1	J	107	SER	2.2
1	G	195	MET	2.2
1	H	199	VAL	2.2
1	H	170	PHE	2.2
1	J	49	PHE	2.2
1	J	455	PHE	2.2
1	G	279	ALA	2.2
1	I	232	ALA	2.2
1	G	43	GLU	2.2
1	J	365	GLU	2.2
1	G	290	THR	2.2
1	J	252	THR	2.2
1	I	374	ARG	2.2
1	H	93	ASN	2.2
1	I	435	GLN	2.2
1	I	72	LYS	2.2
1	F	333	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	89	GLY	2.2
1	I	65	LEU	2.2
1	J	418	GLY	2.2
1	J	449	LEU	2.2
1	B	1	MET	2.2
1	F	95	MET	2.2
1	G	35	ASP	2.2
1	G	181	ASP	2.2
1	H	1	MET	2.2
1	I	228	MET	2.2
1	I	338	ASP	2.2
1	I	417	MET	2.2
1	G	34	VAL	2.2
1	H	271	HIS	2.2
1	I	392	ILE	2.2
1	J	69	ILE	2.2
1	J	306	ILE	2.2
1	D	85	PHE	2.2
1	H	85	PHE	2.2
1	J	189	PHE	2.2
1	J	344	TRP	2.1
1	J	362	ALA	2.1
1	I	322	GLU	2.1
1	F	419	THR	2.1
1	H	56	THR	2.1
1	I	407	THR	2.1
1	D	11	PRO	2.1
1	J	266	PRO	2.1
1	H	388	ASN	2.1
1	I	90	ASN	2.1
1	F	367	TYR	2.1
1	H	208	GLN	2.1
1	I	225	TYR	2.1
1	G	1	MET	2.1
1	G	379	MET	2.1
1	G	250	GLY	2.1
1	G	186	ASP	2.1
1	G	405	ILE	2.1
1	H	201	HIS	2.1
1	H	415	HIS	2.1
1	F	150	SER	2.1
1	H	160	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	384	SER	2.1
1	F	97	PHE	2.1
1	F	189	PHE	2.1
1	H	246	PHE	2.1
1	F	202	ALA	2.1
1	G	433	TRP	2.1
1	G	145	ARG	2.1
1	H	401	THR	2.1
1	H	191	PRO	2.1
1	E	7	GLN	2.1
1	G	228	MET	2.1
1	I	19	MET	2.1
1	H	139	TYR	2.1
1	J	334	TYR	2.1
1	H	305	GLY	2.1
1	J	393	GLY	2.1
1	D	13	VAL	2.1
1	F	34	VAL	2.1
1	G	151	ILE	2.1
1	G	198	ASP	2.1
1	G	347	ILE	2.1
1	H	178	VAL	2.1
1	I	457	ASP	2.1
1	J	188	ASP	2.1
1	D	44	SER	2.1
1	J	253	ALA	2.1
1	J	274	ARG	2.1
1	J	299	ARG	2.1
1	G	308	THR	2.1
1	H	120	PRO	2.1
1	C	1	MET	2.1
1	F	435	GLN	2.1
1	G	259	GLN	2.1
1	F	449	LEU	2.1
1	I	300	LEU	2.1
1	F	411	GLY	2.1
1	H	53	GLY	2.1
1	J	67	TYR	2.1
1	D	76	VAL	2.1
1	I	110	VAL	2.1
1	J	124	VAL	2.1
1	J	133	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	23	PHE	2.1
1	D	57	ALA	2.1
1	D	87	ARG	2.1
1	F	421	ALA	2.1
1	H	279	ALA	2.1
1	J	451	ALA	2.1
1	E	373	TRP	2.1
1	F	373	TRP	2.1
1	D	290	THR	2.1
1	F	381	PRO	2.1
1	G	154	PRO	2.1
1	I	389	PRO	2.1
1	D	256	MET	2.1
1	H	92	GLN	2.1
1	J	17	GLN	2.1
1	B	30	GLY	2.1
1	I	422	GLY	2.1
1	D	40	VAL	2.1
1	J	102	VAL	2.1
1	I	86	ASP	2.0
1	B	60	GLU	2.0
1	G	200	ARG	2.0
1	H	429	ALA	2.0
1	I	217	SER	2.0
1	F	444	LYS	2.0
1	G	51	LYS	2.0
1	H	350	LYS	2.0
1	D	82	TRP	2.0
1	F	310	THR	2.0
1	I	191	PRO	2.0
1	H	333	LEU	2.0
1	J	333	LEU	2.0
1	H	101	ASN	2.0
1	F	250	GLY	2.0
1	G	133	ILE	2.0
1	G	358	ILE	2.0
1	G	393	GLY	2.0
1	I	418	GLY	2.0
1	J	94	ILE	2.0
1	J	375	ILE	2.0
1	B	372	TYR	2.0
1	F	426	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	126	TYR	2.0
1	J	431	GLU	2.0
1	G	245	ALA	2.0
1	G	357	ALA	2.0
1	I	245	ALA	2.0
1	G	45	SER	2.0
1	G	335	SER	2.0
1	H	107	SER	2.0
1	H	203	MET	2.0
1	I	183	PRO	2.0
1	F	391	LEU	2.0
1	F	454	GLN	2.0
1	G	197	GLN	2.0
1	I	184	GLN	2.0
1	J	277	HIS	2.0
1	G	69	ILE	2.0
1	I	151	ILE	2.0
1	I	285	ASN	2.0
1	J	53	GLY	2.0
1	J	104	GLY	2.0
1	H	87	ARG	2.0
1	H	456	TYR	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 ⓘ

There are no oligosaccharides in this entry.

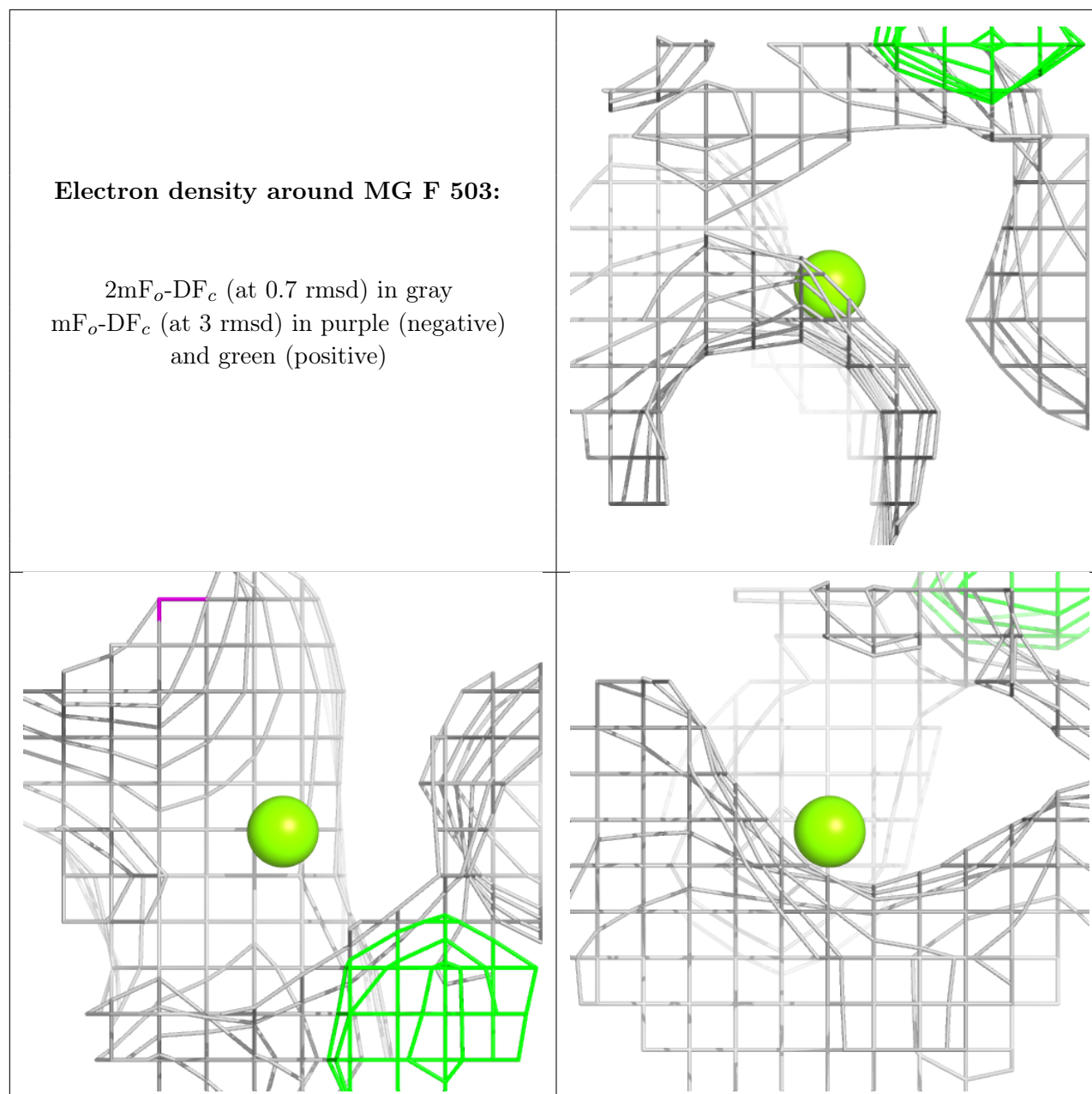
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	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

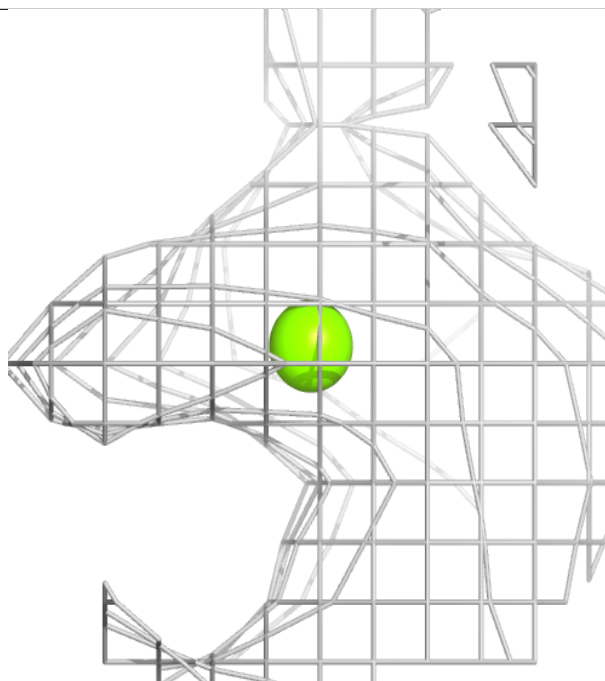
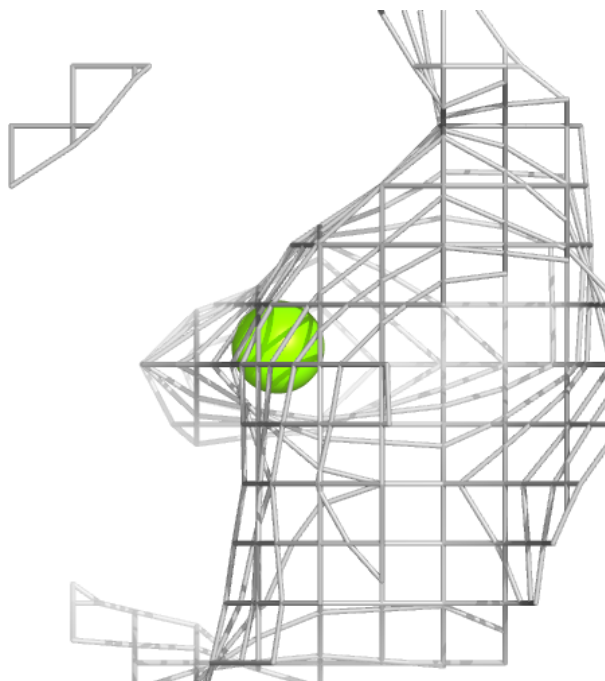
The following is a graphical depiction of the model fit to experimental electron density of all

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.



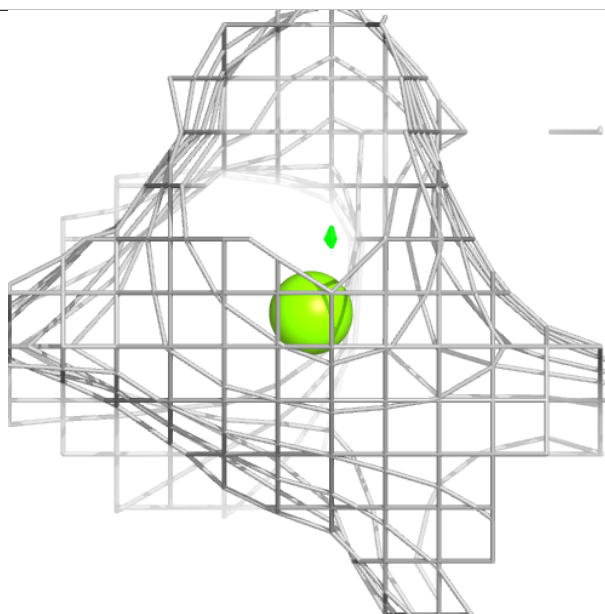
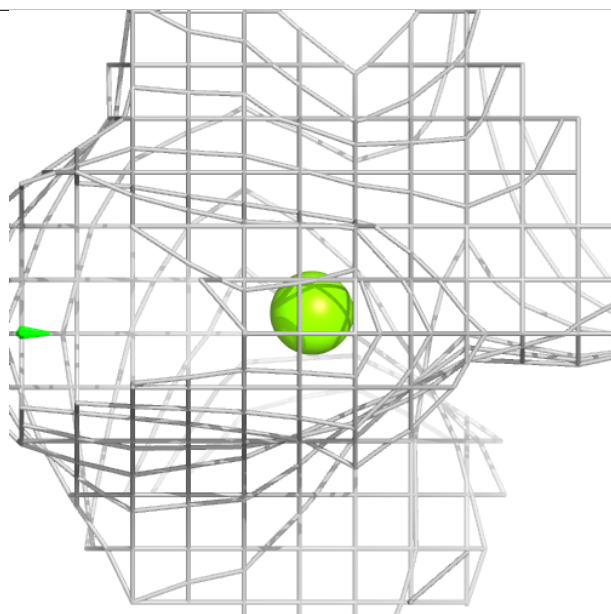
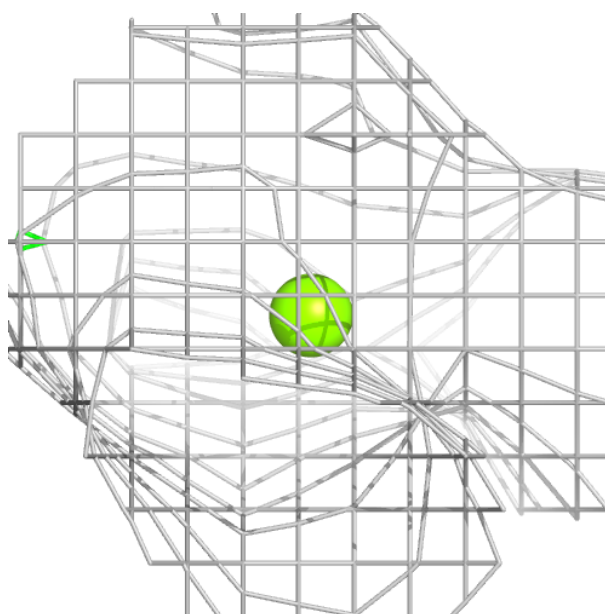
Electron density around MG E 503:

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



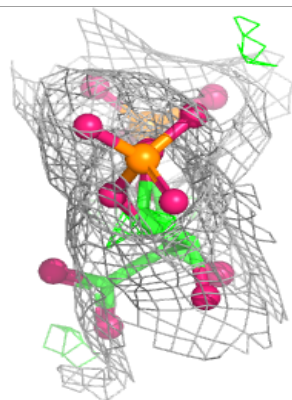
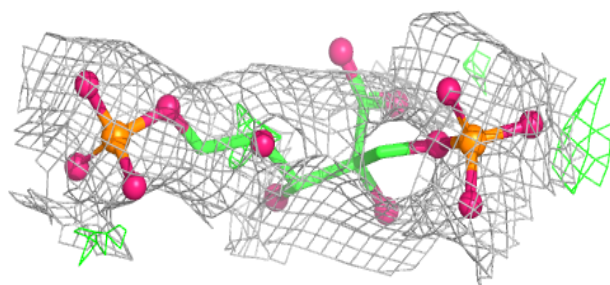
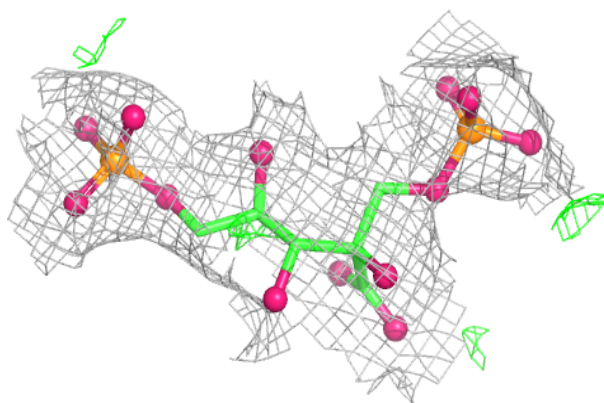
Electron density around MG H 503:

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and green (positive)

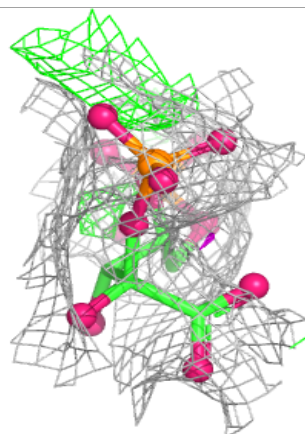
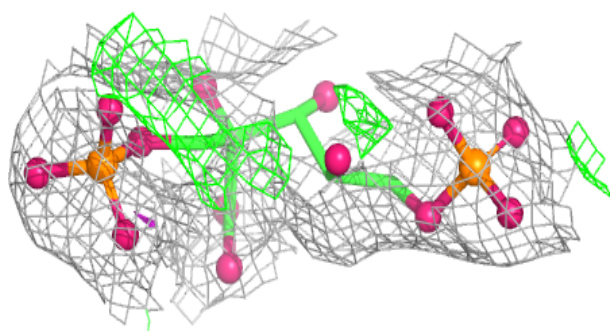
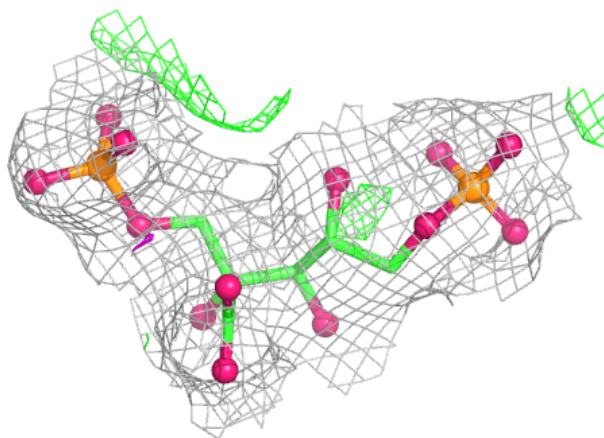


Electron density around CAP G 501:

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and green (positive)

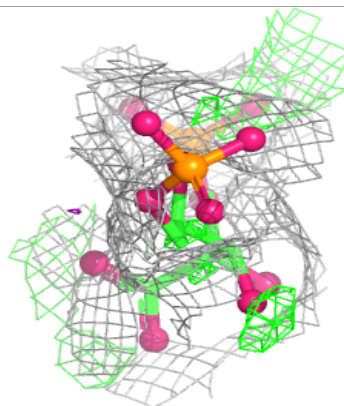
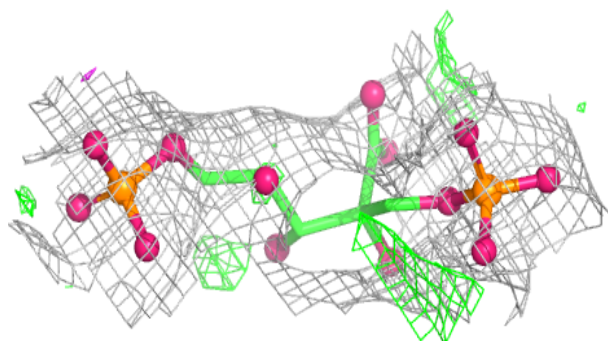
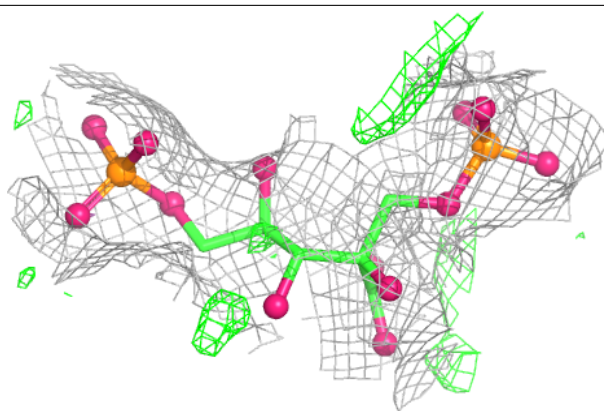
**Electron density around CAP H 501:**

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and green (positive)

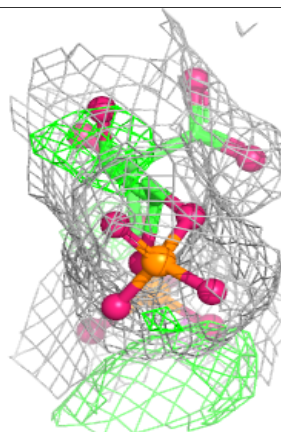
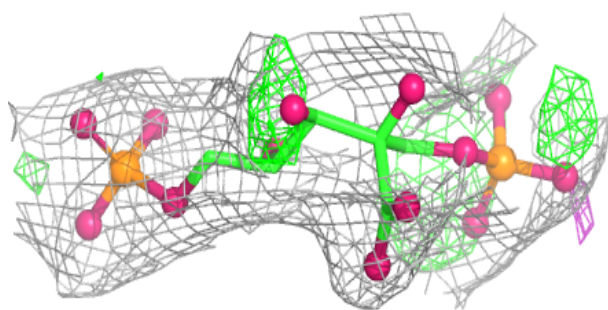
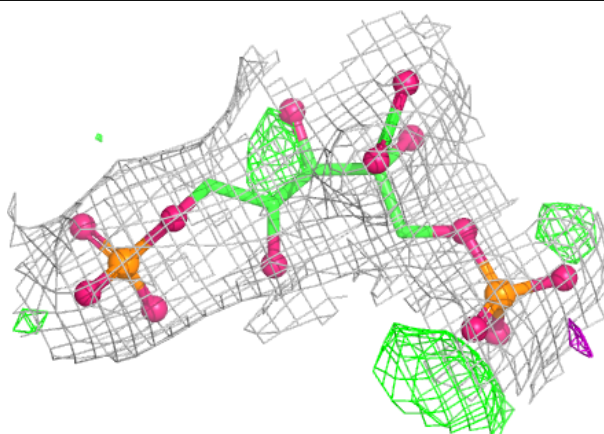


Electron density around CAP J 502:

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and green (positive)

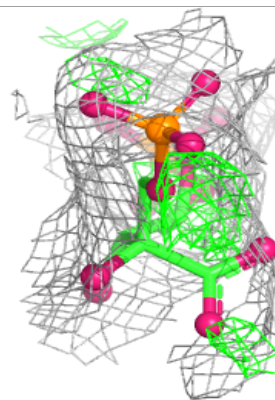
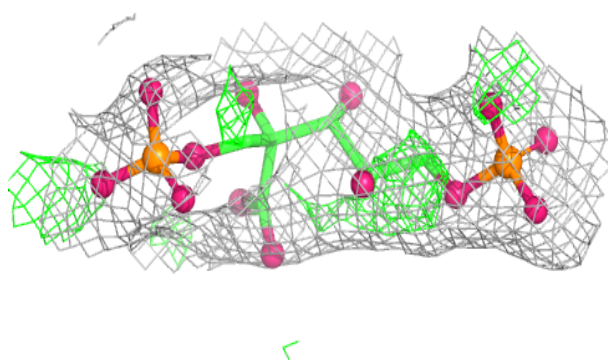
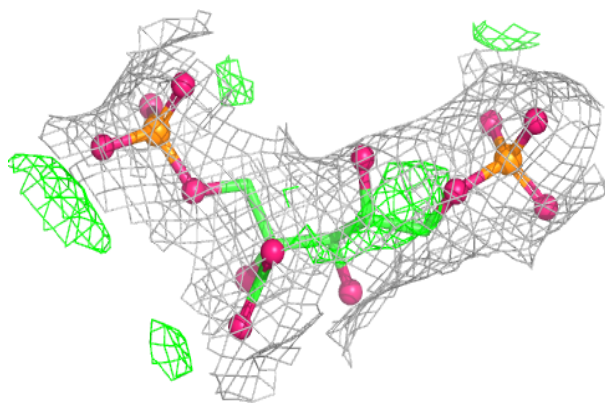
**Electron density around CAP F 501:**

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and green (positive)



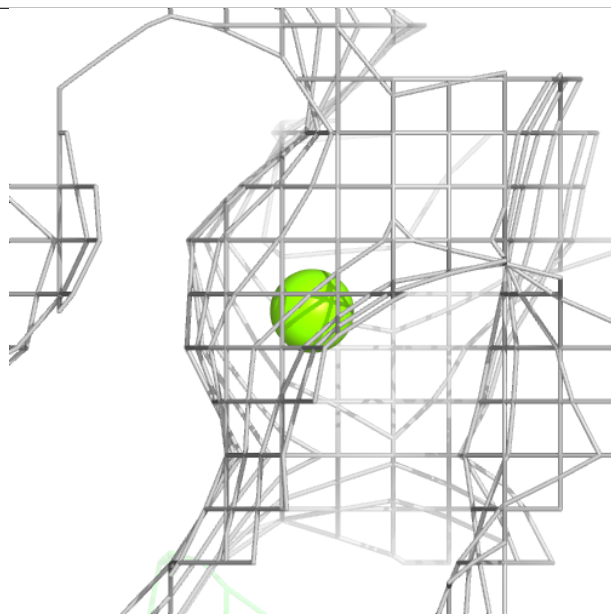
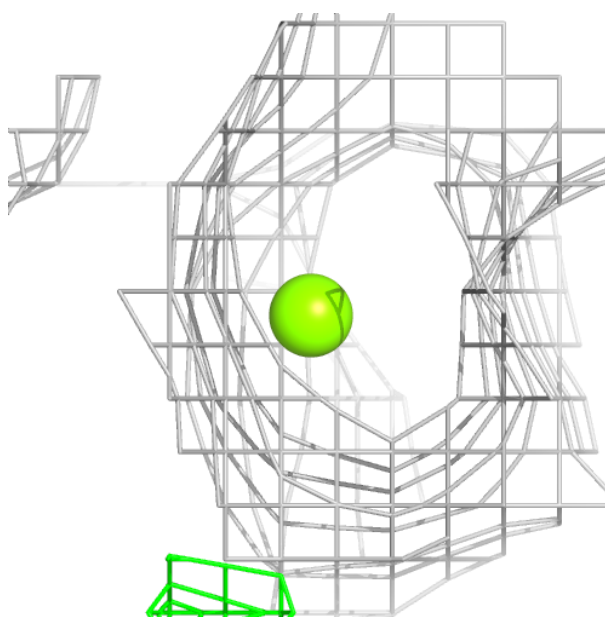
Electron density around CAP I 502:

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



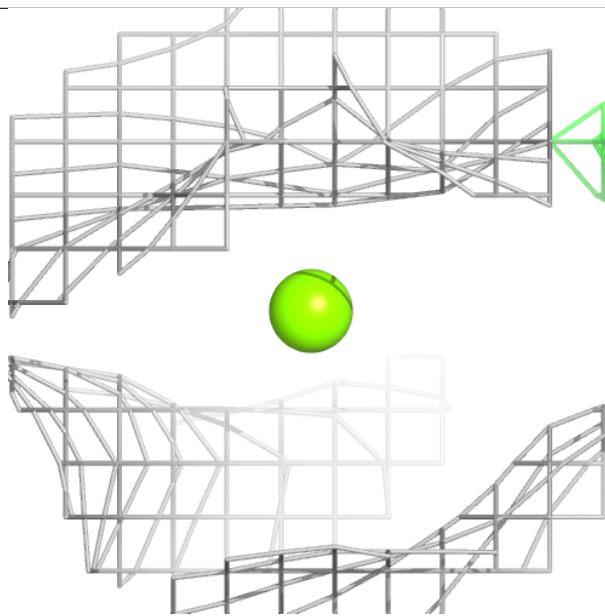
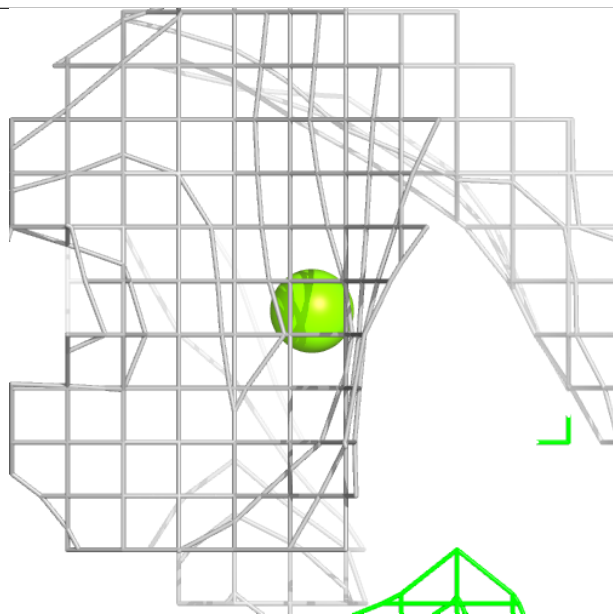
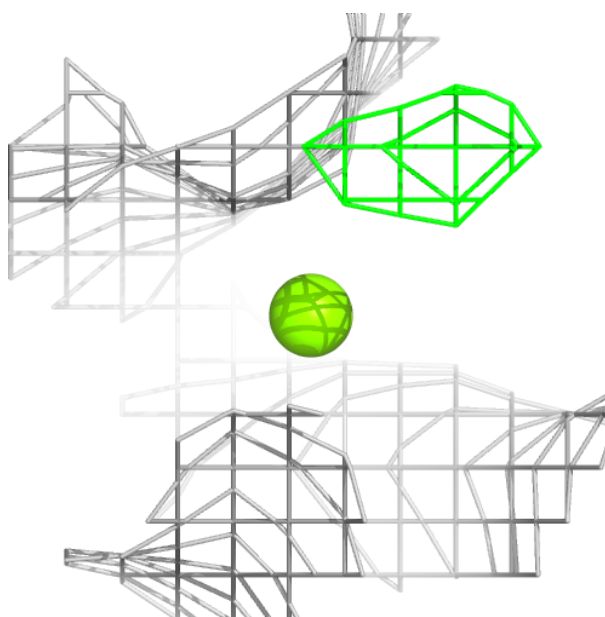
Electron density around MG A 504:

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and green (positive)



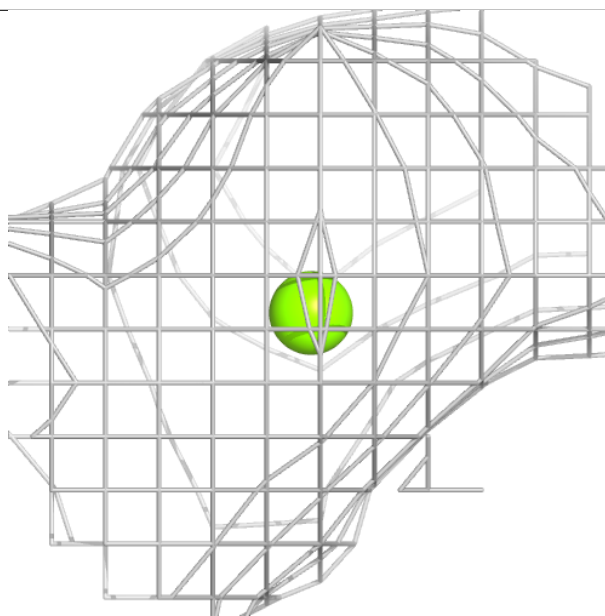
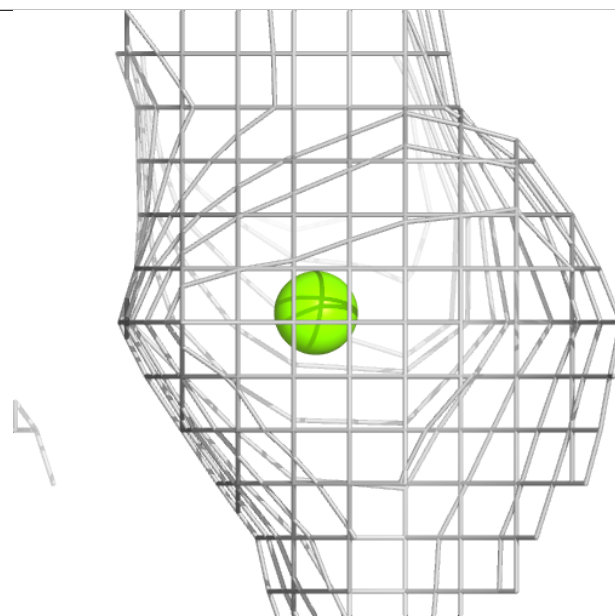
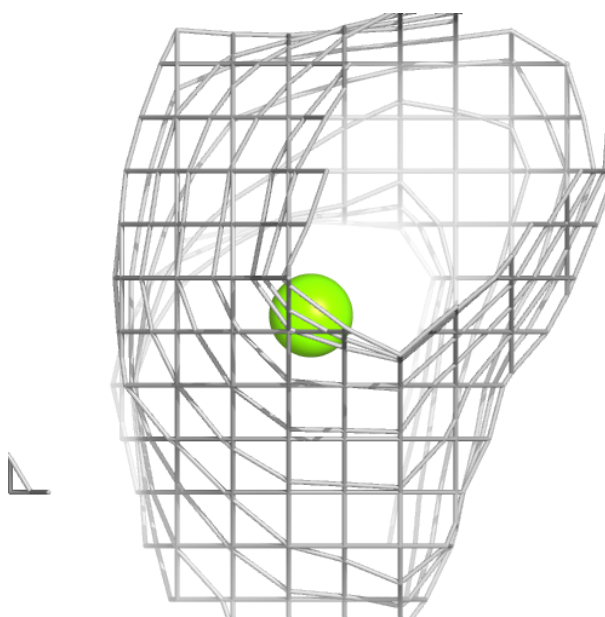
Electron density around MG J 503:

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



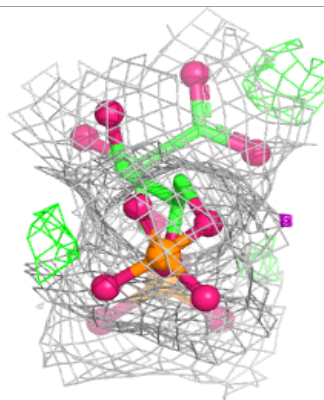
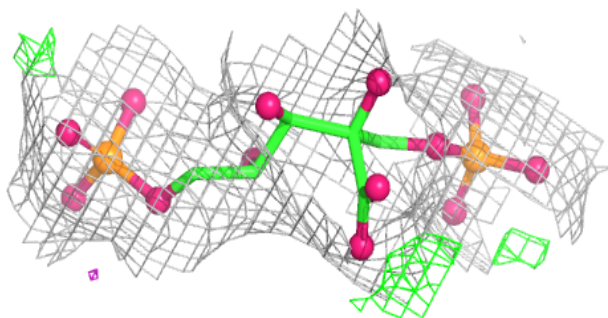
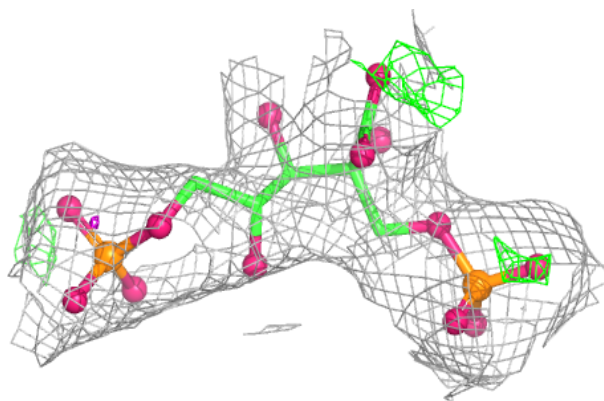
Electron density around MG G 503:

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



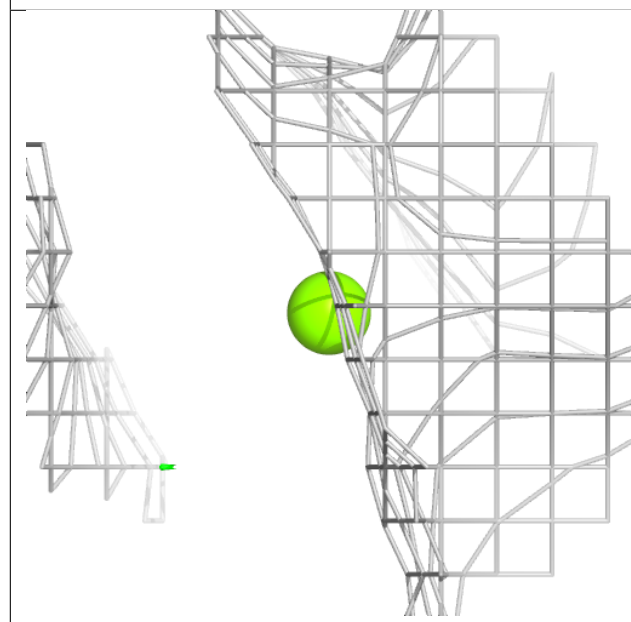
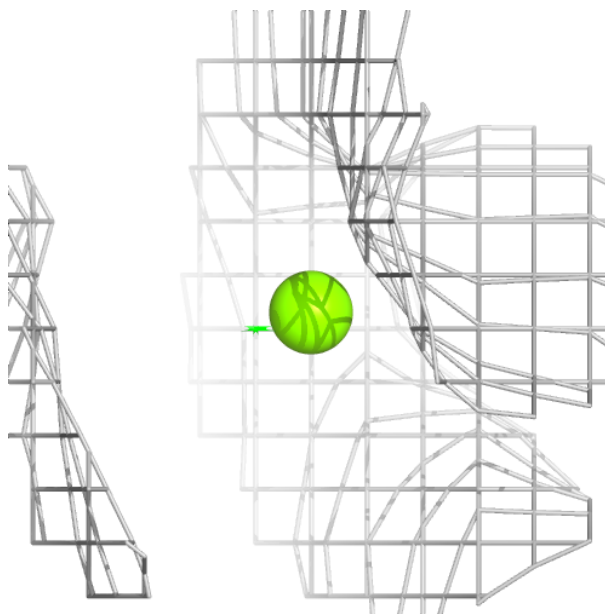
Electron density around CAP D 502:

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



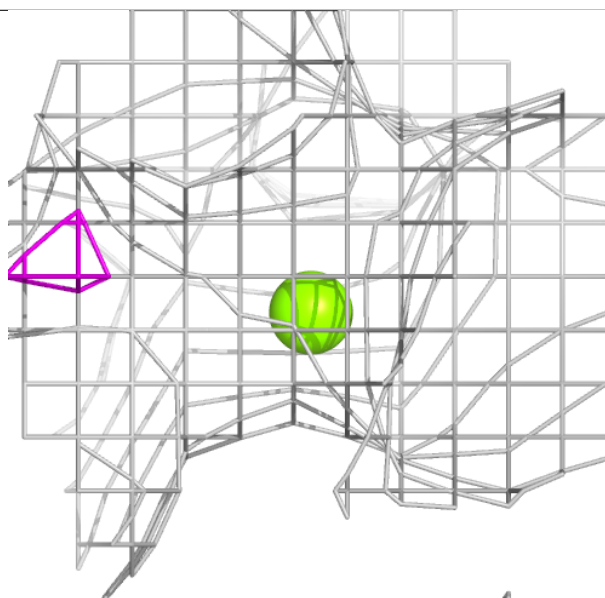
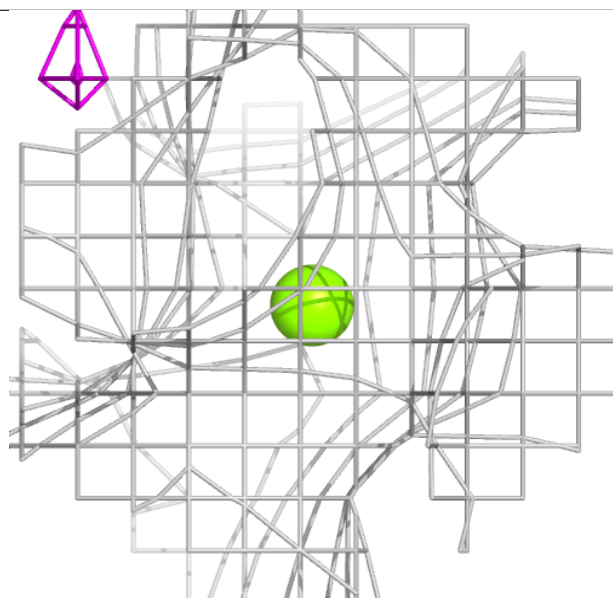
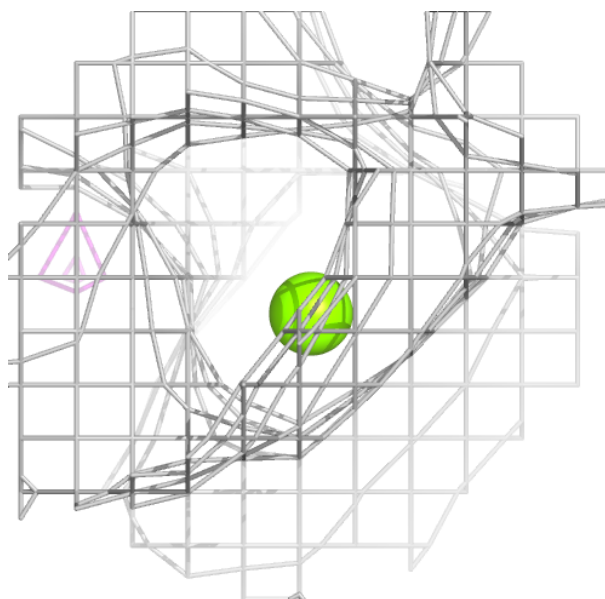
Electron density around MG I 503:

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



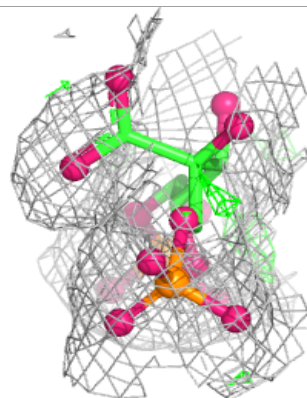
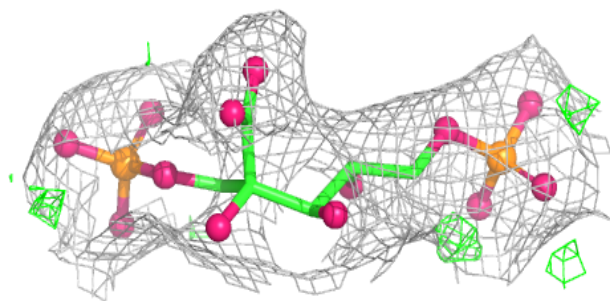
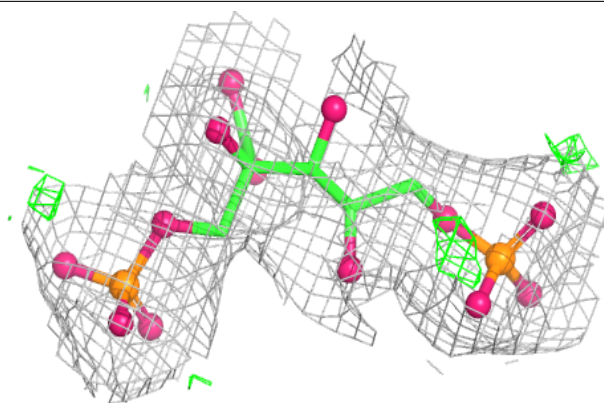
Electron density around MG B 503:

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and green (positive)

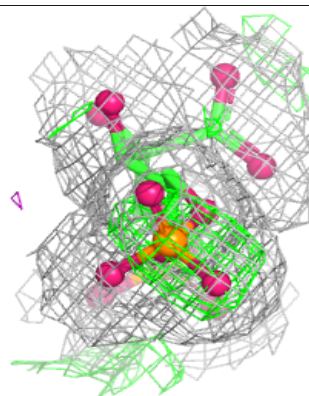
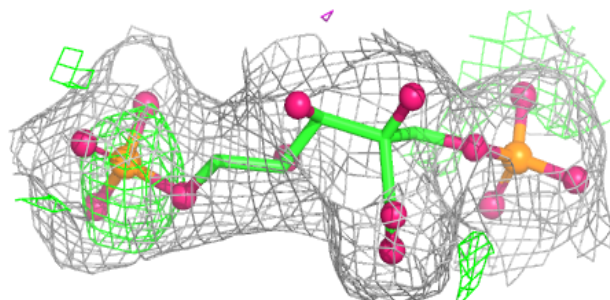
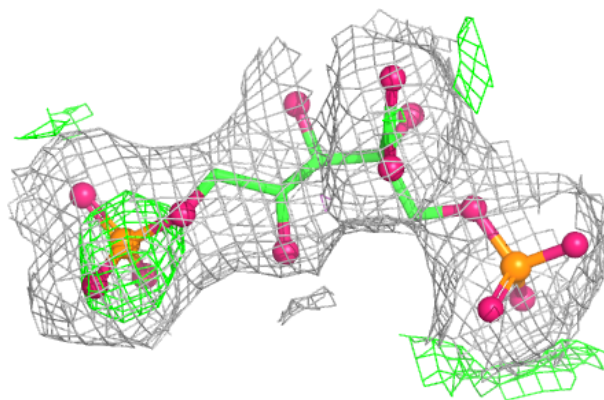


Electron density around CAP E 501:

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

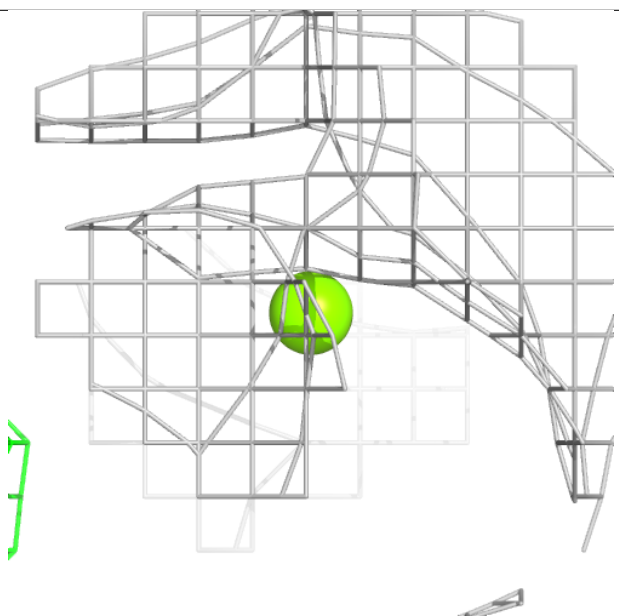
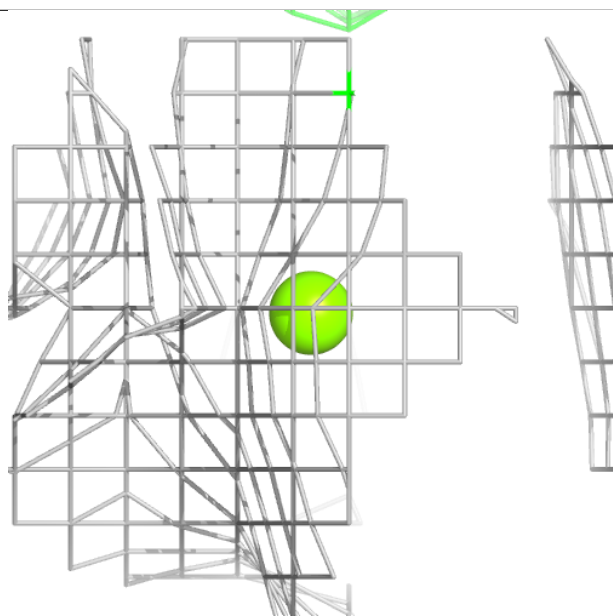
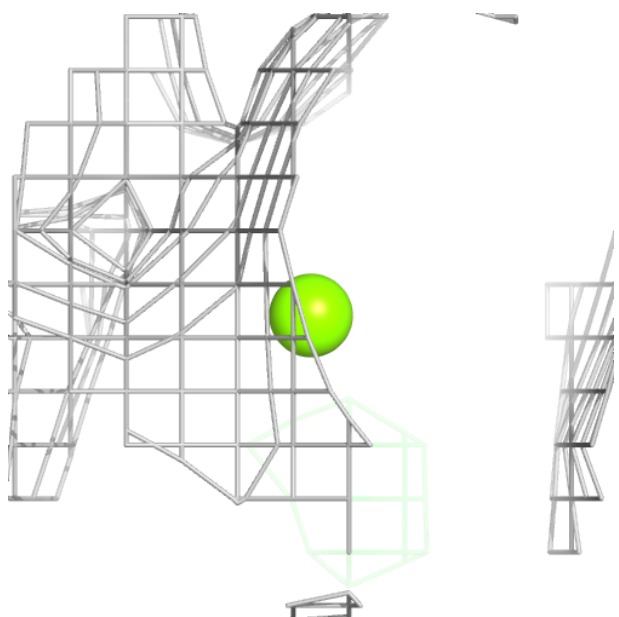
**Electron density around CAP A 501:**

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



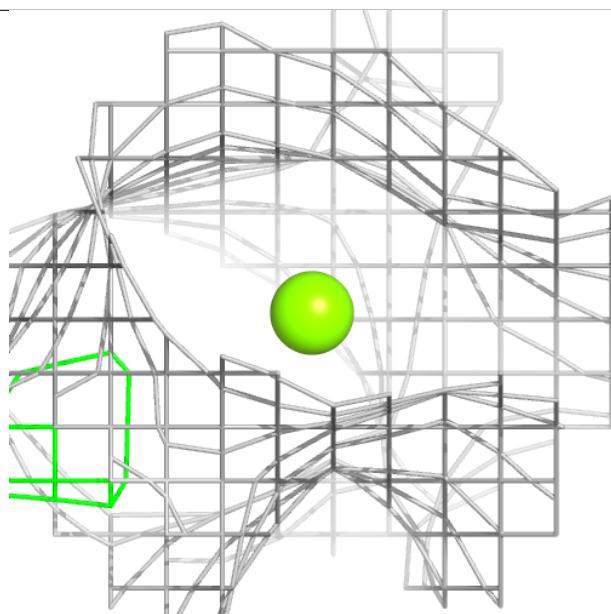
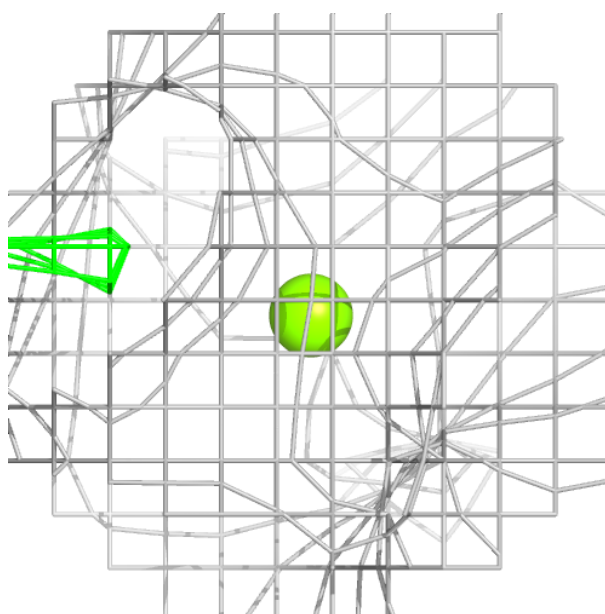
Electron density around MG G 502:

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and green (positive)



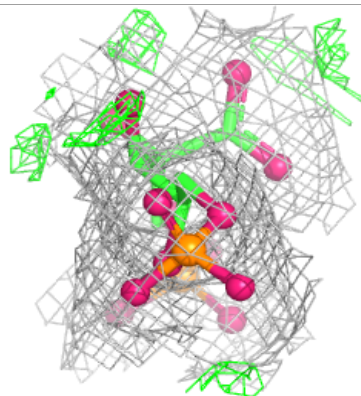
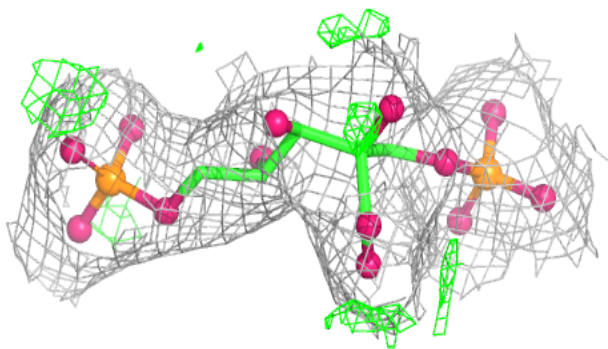
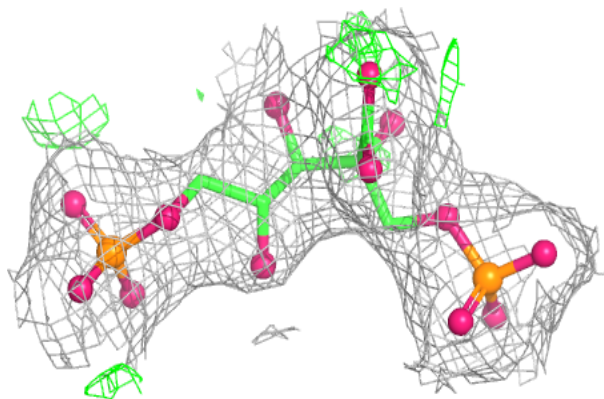
Electron density around MG A 503:

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and green (positive)



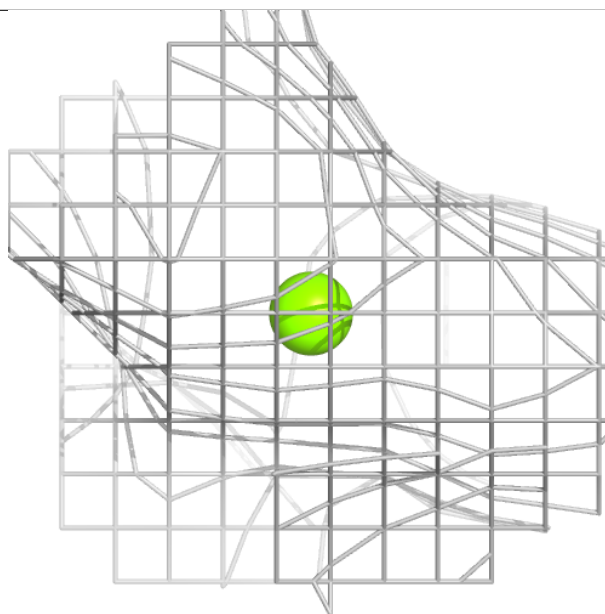
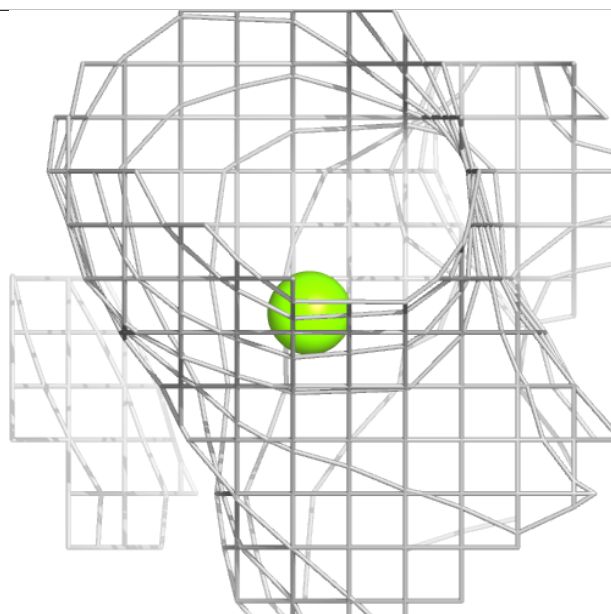
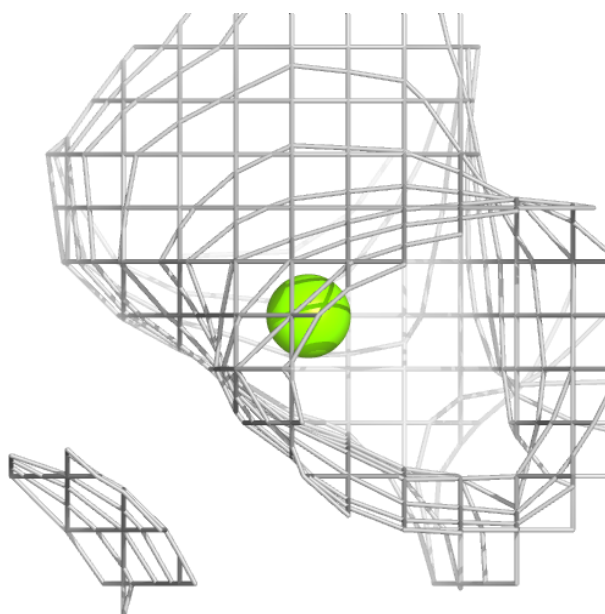
Electron density around CAP B 501:

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and green (positive)



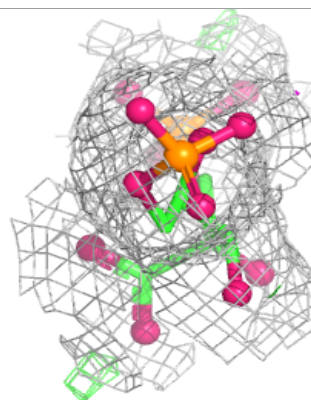
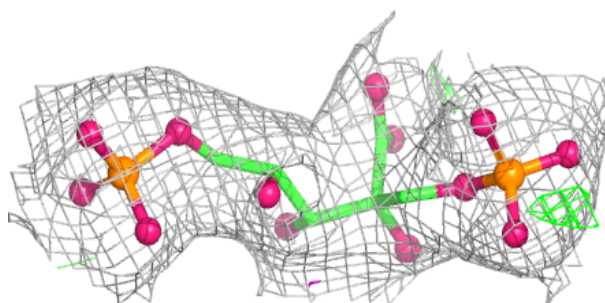
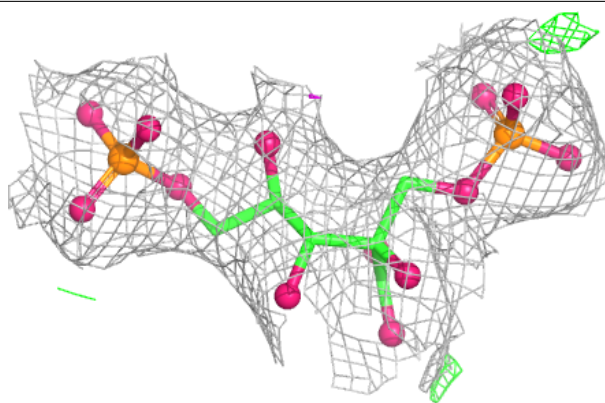
Electron density around MG J 501:

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



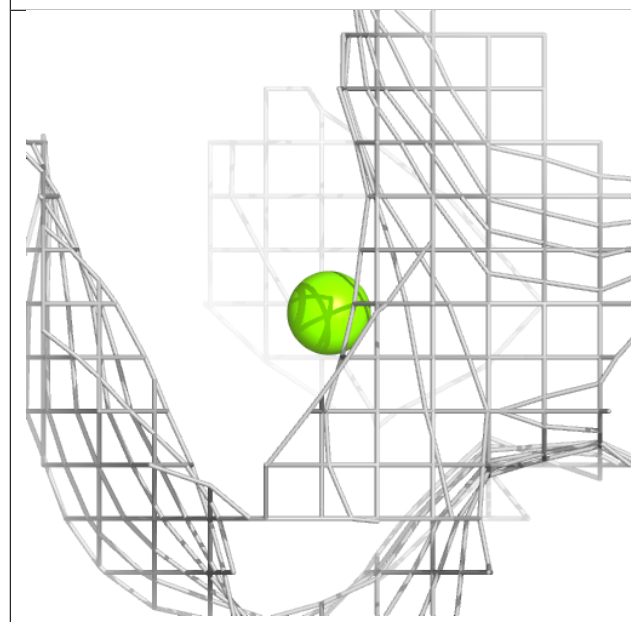
Electron density around CAP C 501:

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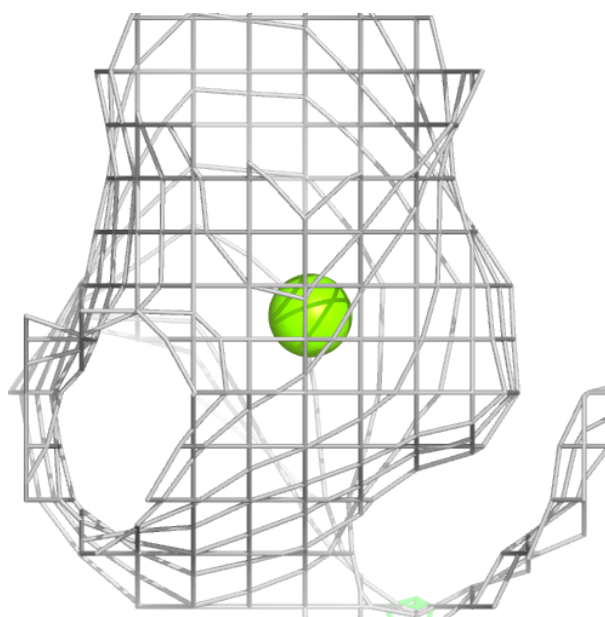
Electron density around MG H 502:

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and green (positive)



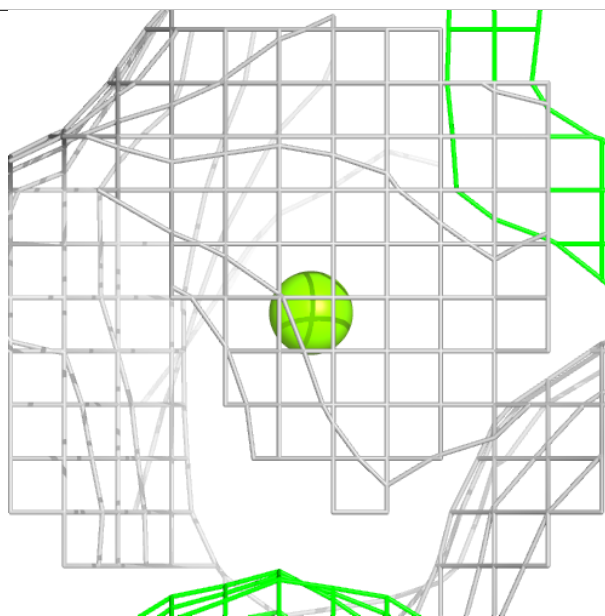
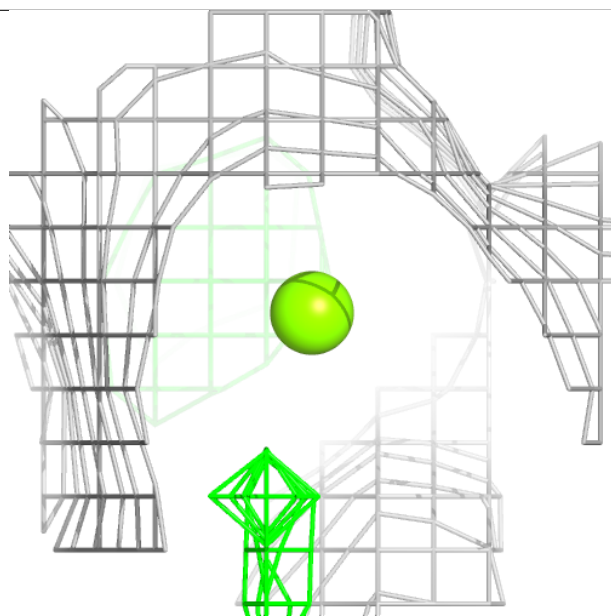
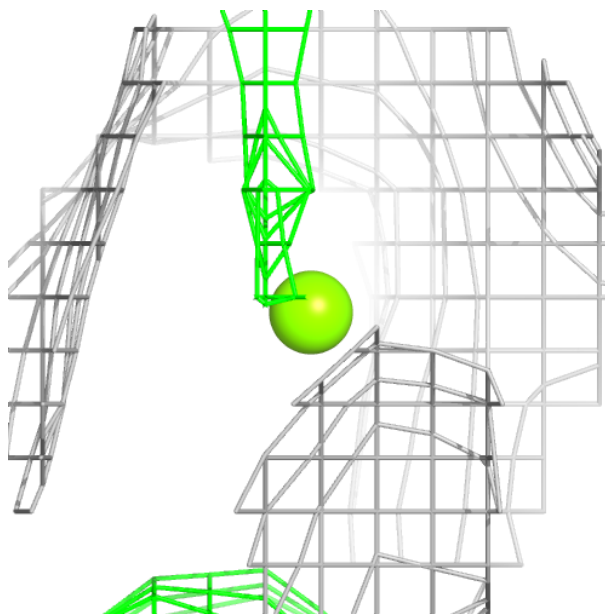
Electron density around MG I 501:

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and green (positive)



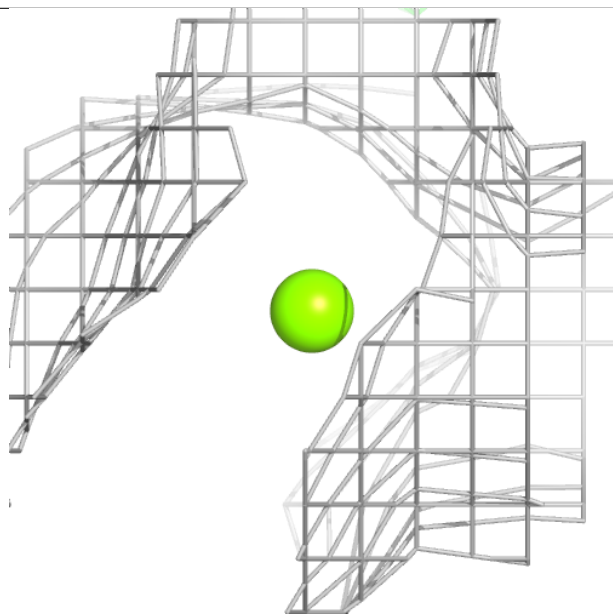
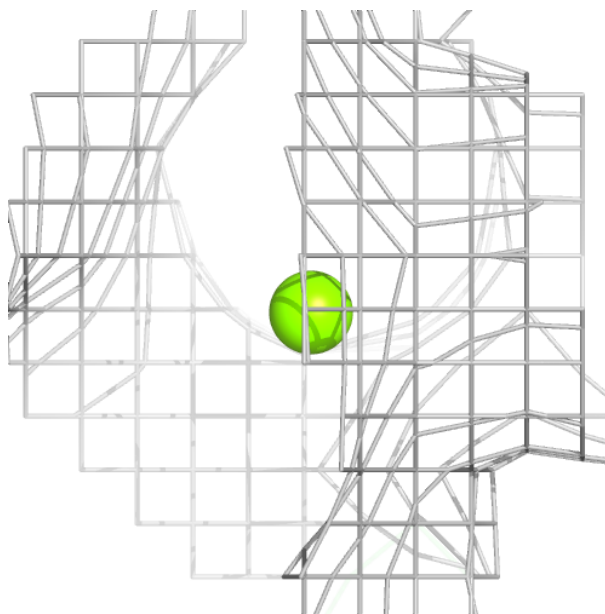
Electron density around MG F 502:

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



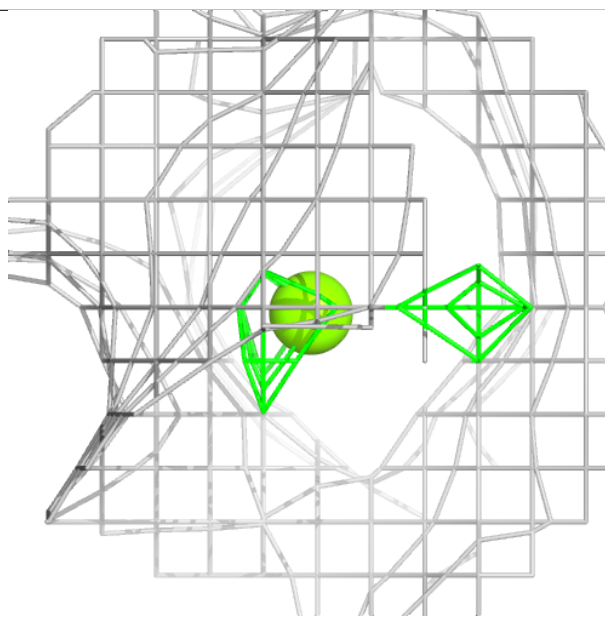
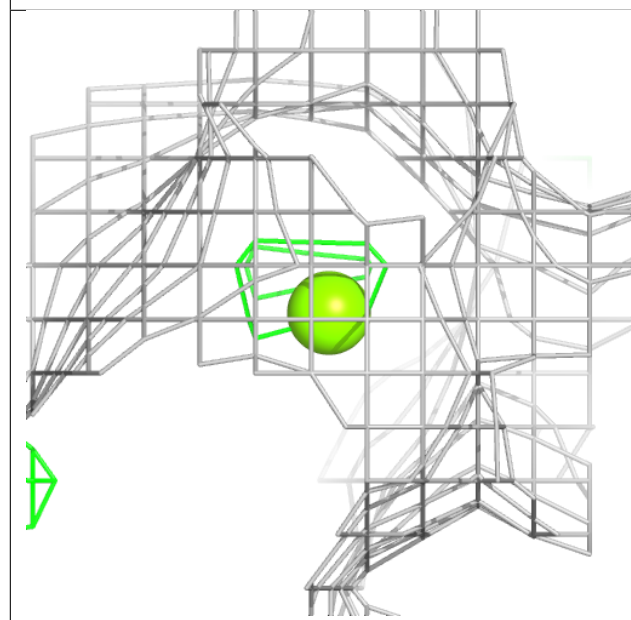
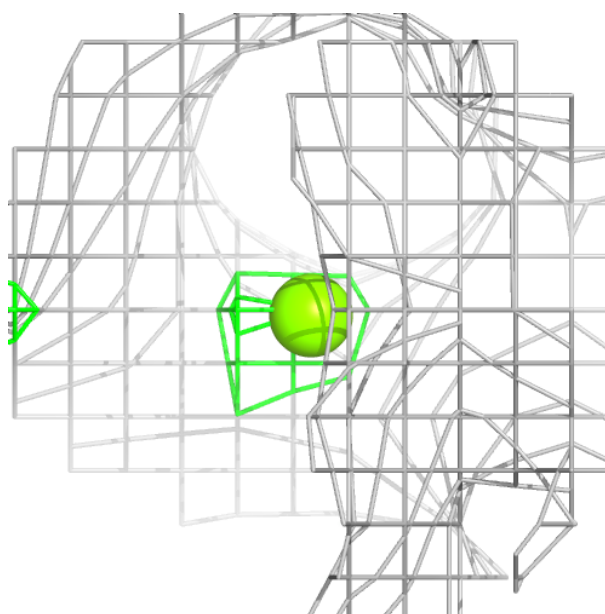
Electron density around MG A 502:

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



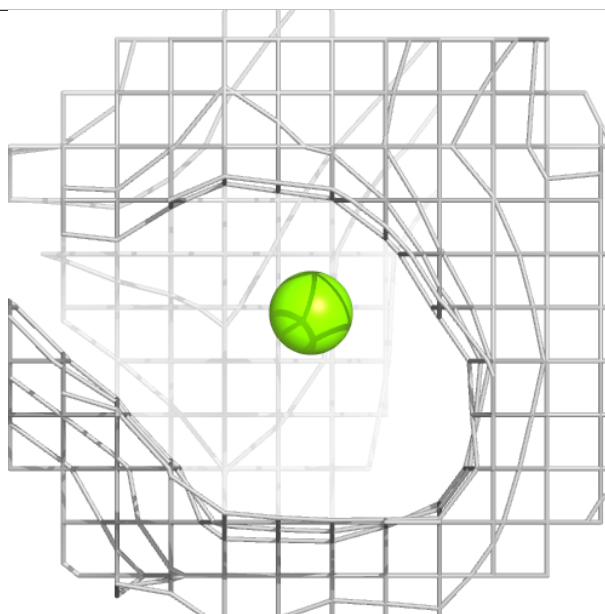
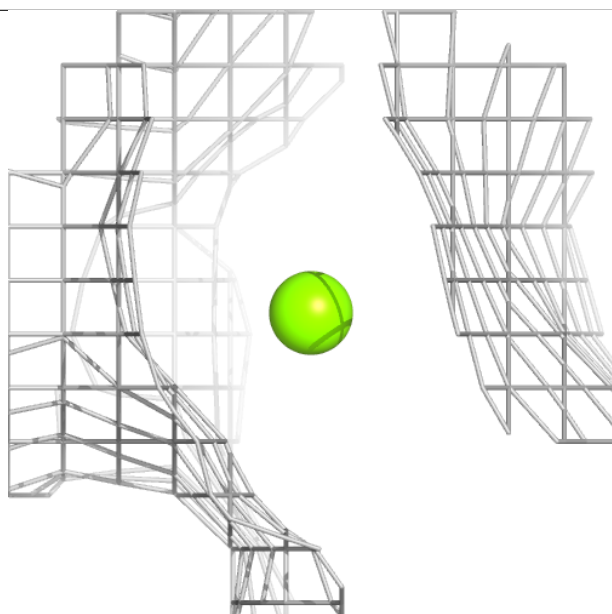
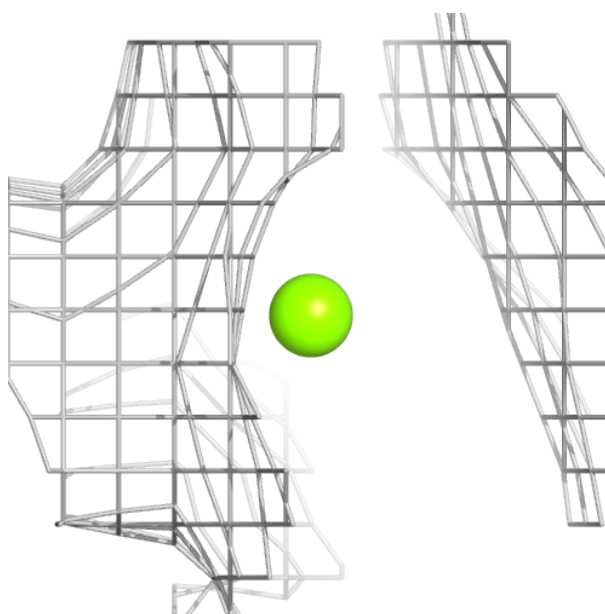
Electron density around MG B 502:

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and green (positive)



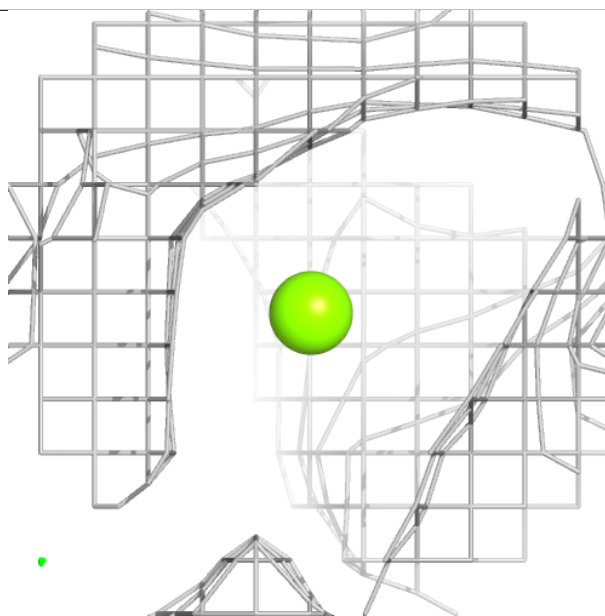
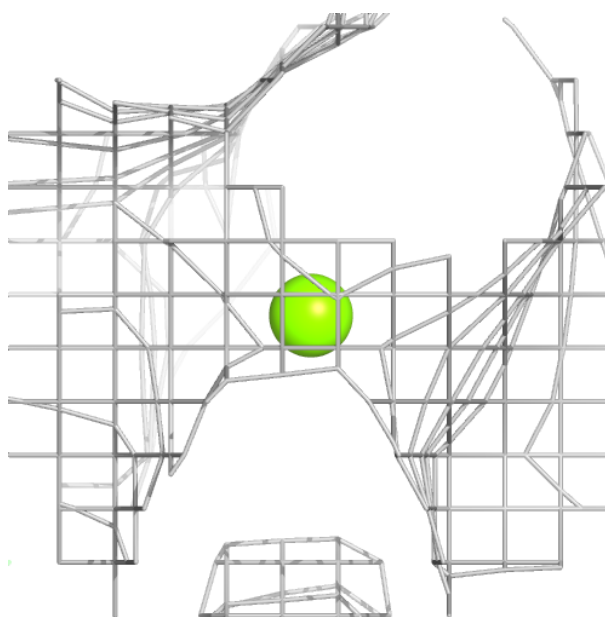
Electron density around MG E 502:

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and green (positive)



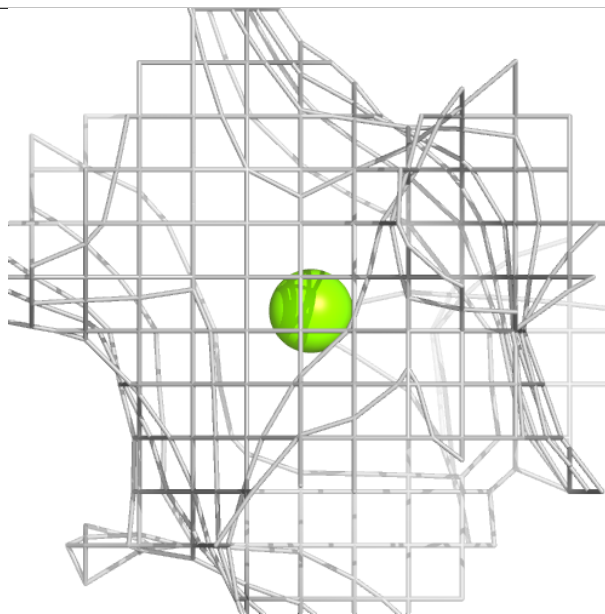
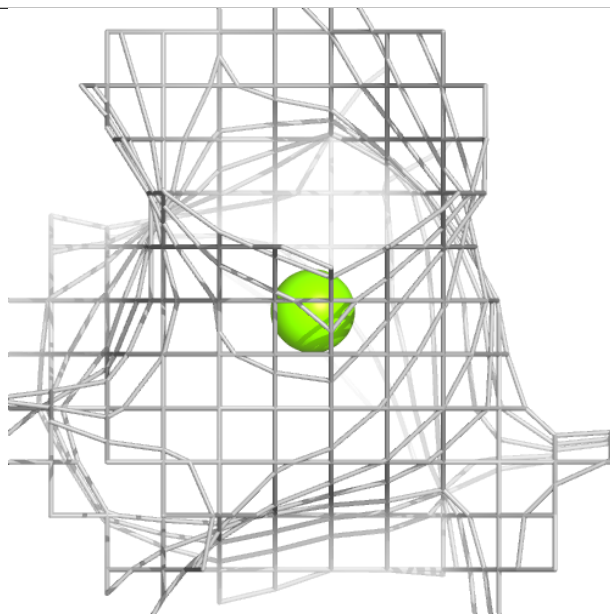
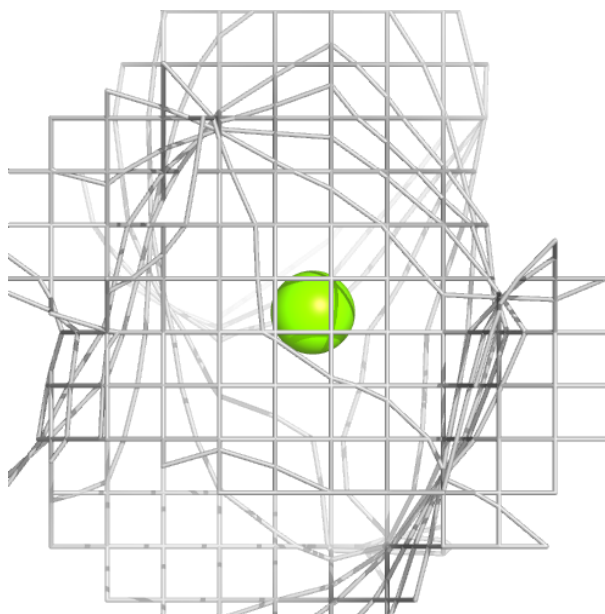
Electron density around MG C 502:

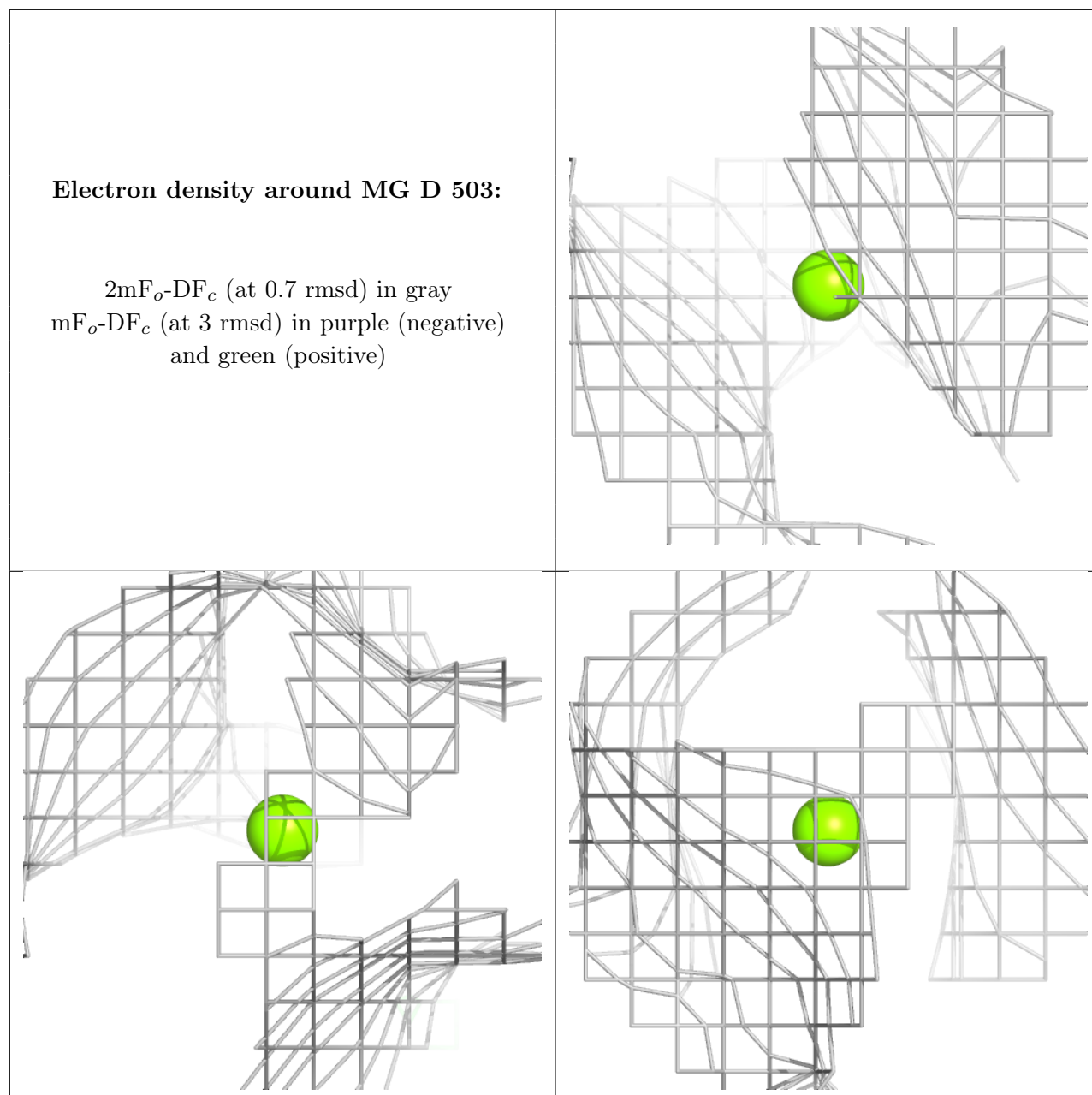
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.