



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 10:14 AM JST

PDB ID : 9K2N
Title : Crystal structure of Glutamine Synthetase-apo
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Deposited on : 2024-10-17
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

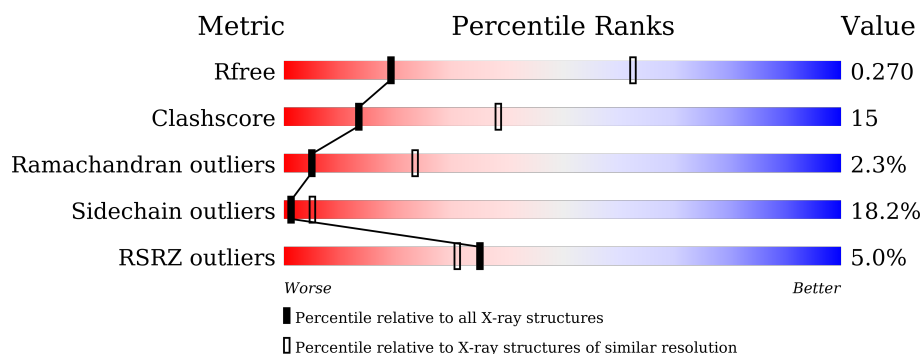
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	<div> <div>3%</div> <div>60%</div> <div>32%</div> <div>7%</div> </div>
1	B	468	<div> <div>4%</div> <div>60%</div> <div>29%</div> <div>9%</div> </div>
1	C	468	<div> <div>4%</div> <div>61%</div> <div>27%</div> <div>9%</div> </div>
1	D	468	<div> <div>6%</div> <div>65%</div> <div>27%</div> <div>6%</div> </div>
1	E	468	<div> <div>5%</div> <div>63%</div> <div>28%</div> <div>7%</div> </div>
1	F	468	<div> <div>7%</div> <div>63%</div> <div>29%</div> <div>7%</div> </div>

2 Entry composition [i](#)

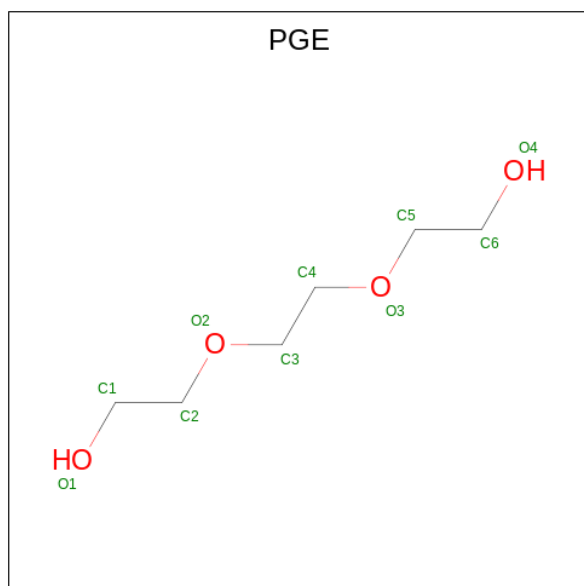
There are 5 unique types of molecules in this entry. The entry contains 43046 atoms, of which 21160 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

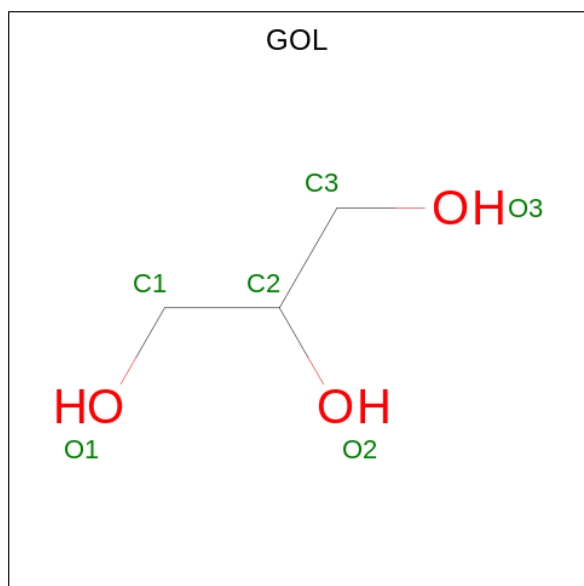
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	B	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	C	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	D	468	Total	C	H	N	O	S	111	0	0
			7155	2305	3517	613	699	21			
1	E	468	Total	C	H	N	O	S	113	0	0
			7142	2302	3508	612	699	21			
1	F	468	Total	C	H	N	O	S	110	0	0
			7149	2301	3514	613	700	21			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			24	6	14	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	C	1	Total	C	H	O	3	0
			14	3	8	3		
3	D	1	Total	C	H	O	3	0
			14	3	8	3		
3	E	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

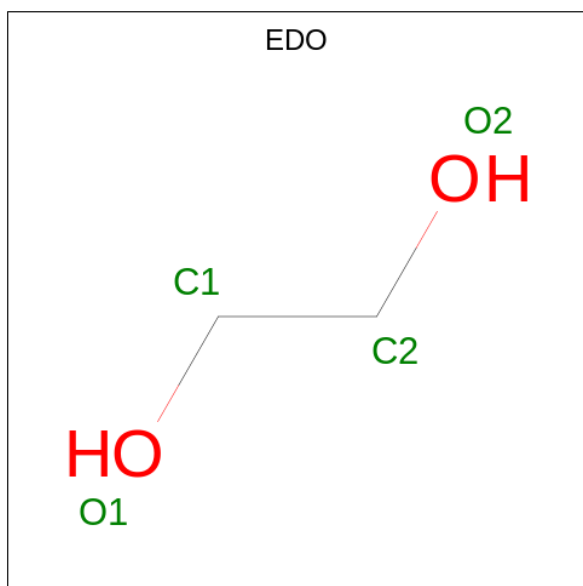
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0
4	D	2	Total 2	Mg 2	0	0
4	E	2	Total 2	Mg 2	0	0
4	F	2	Total 2	Mg 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

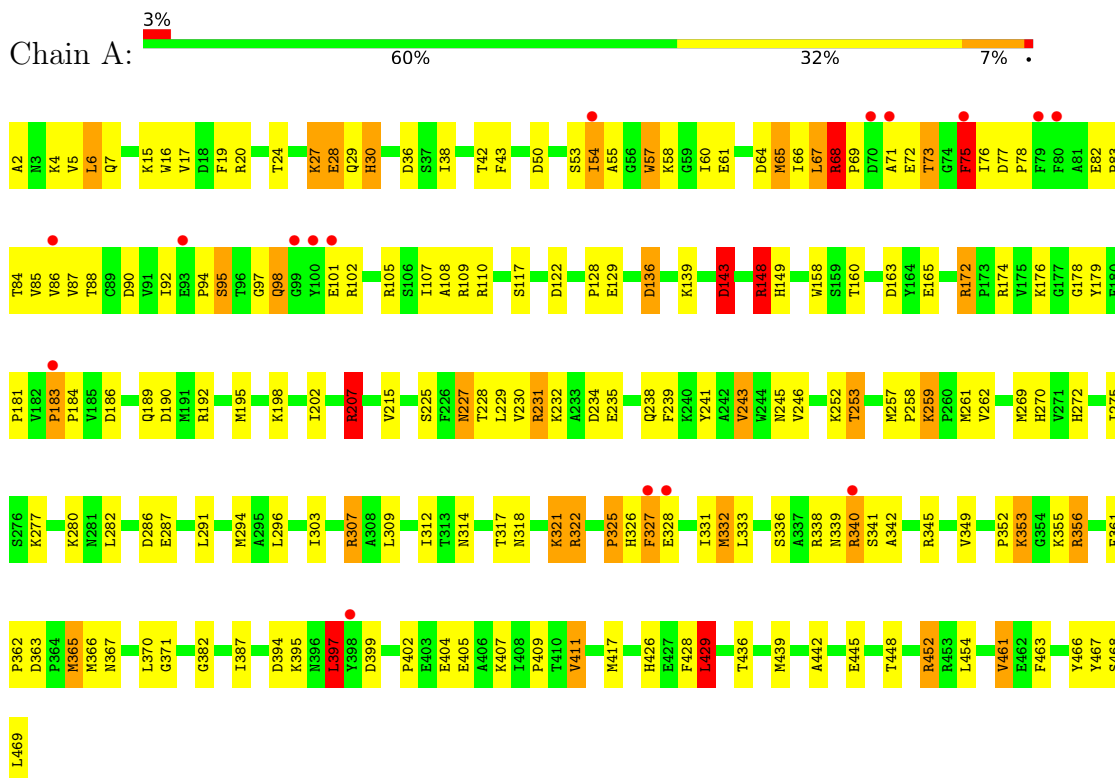


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total 10	C 2	H 6	O 2	2	0

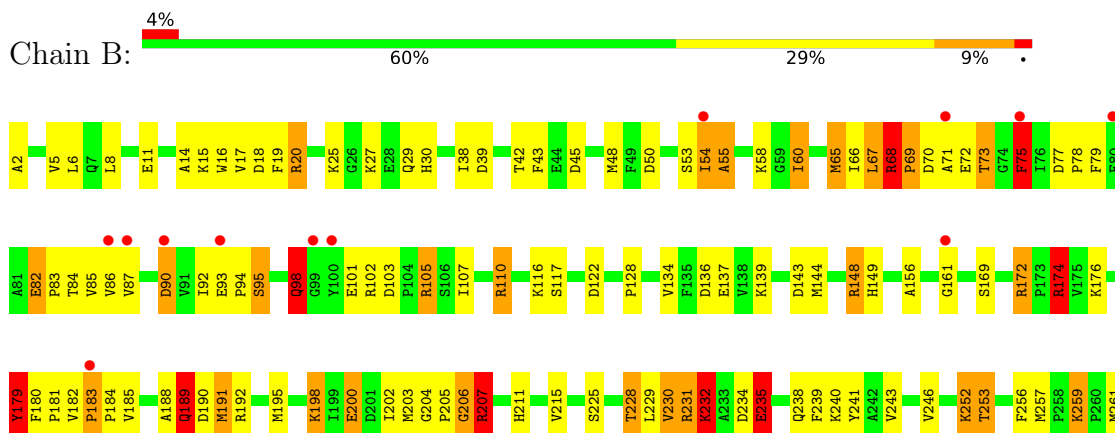
3 Residue-property plots

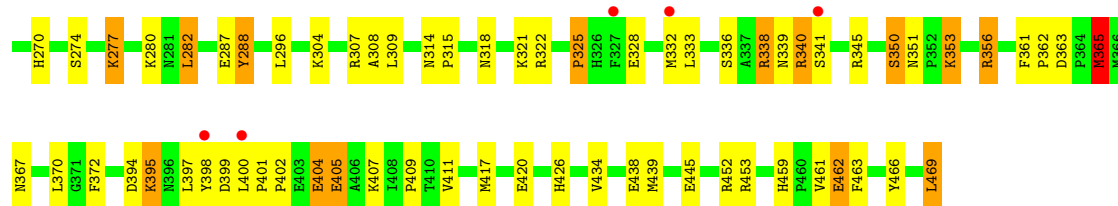
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutamine synthetase

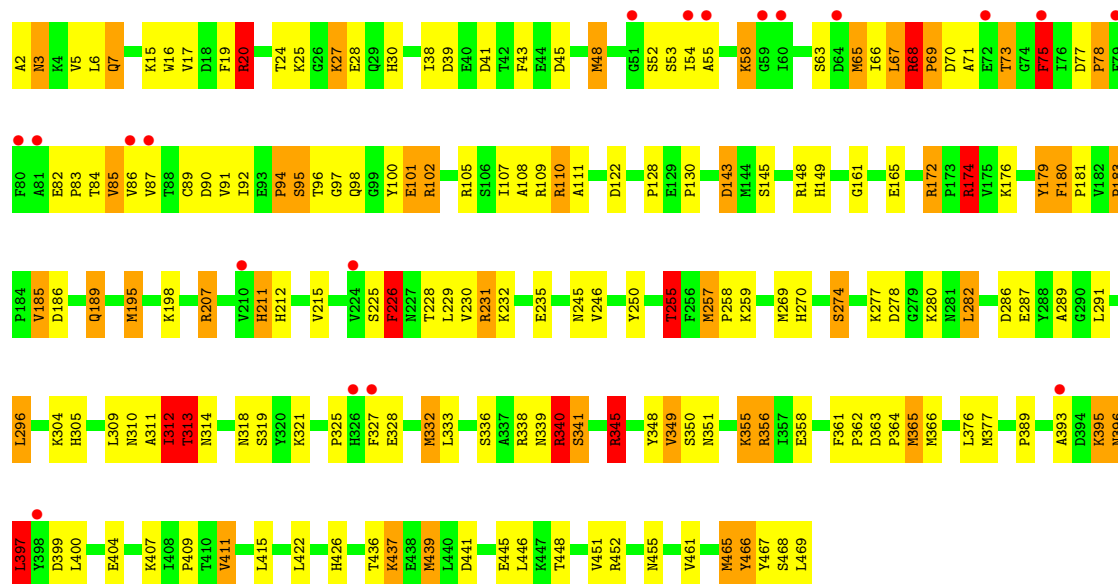


• Molecule 1: Glutamine synthetase

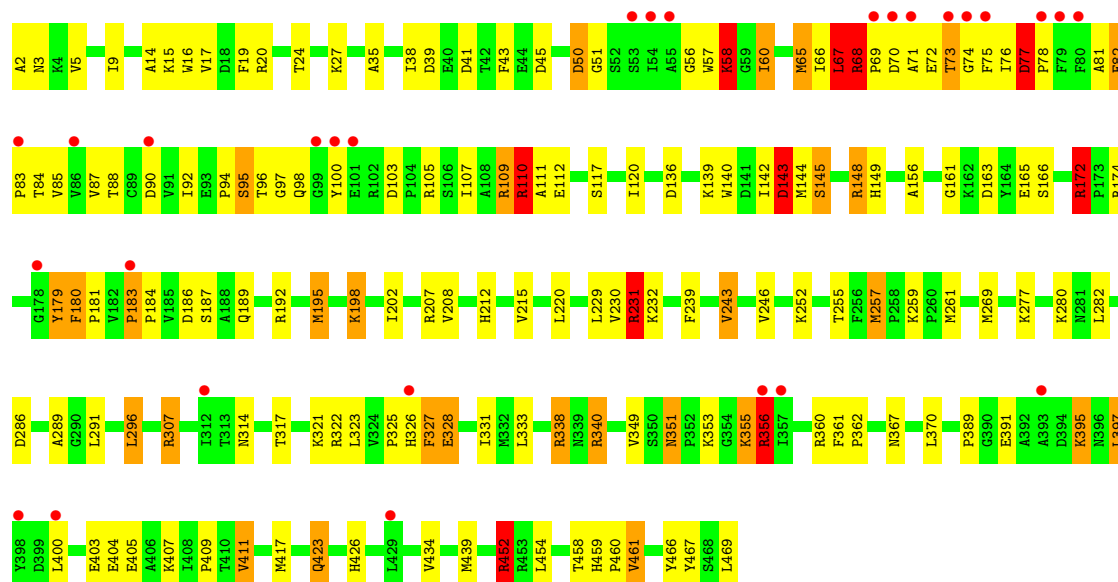




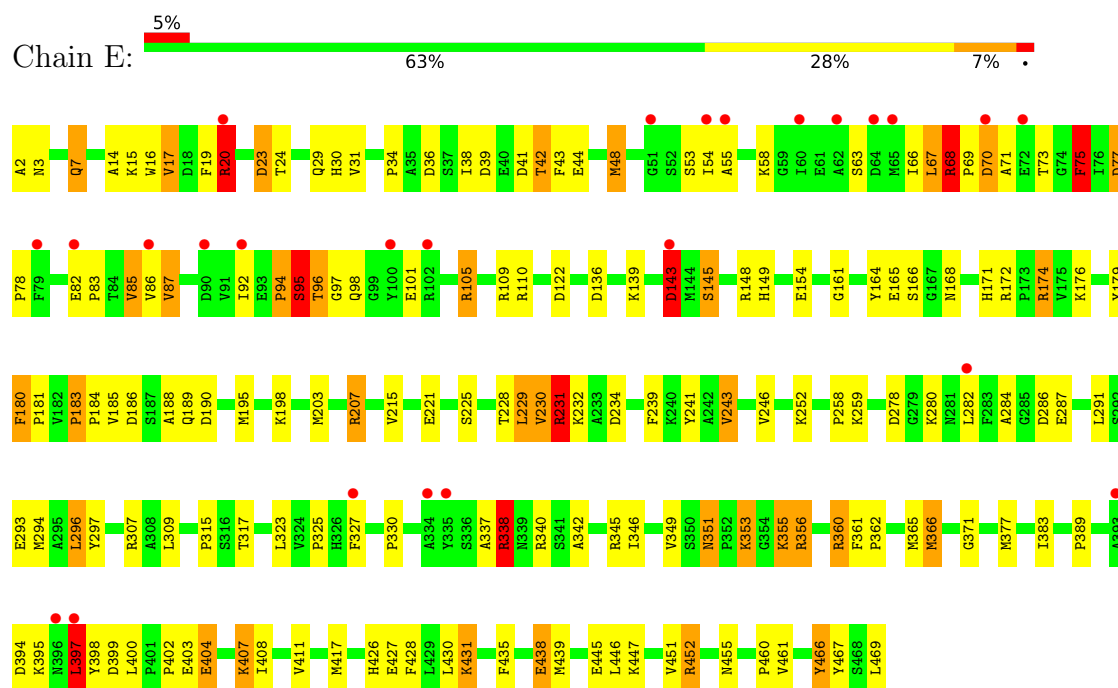
• Molecule 1: Glutamine synthetase



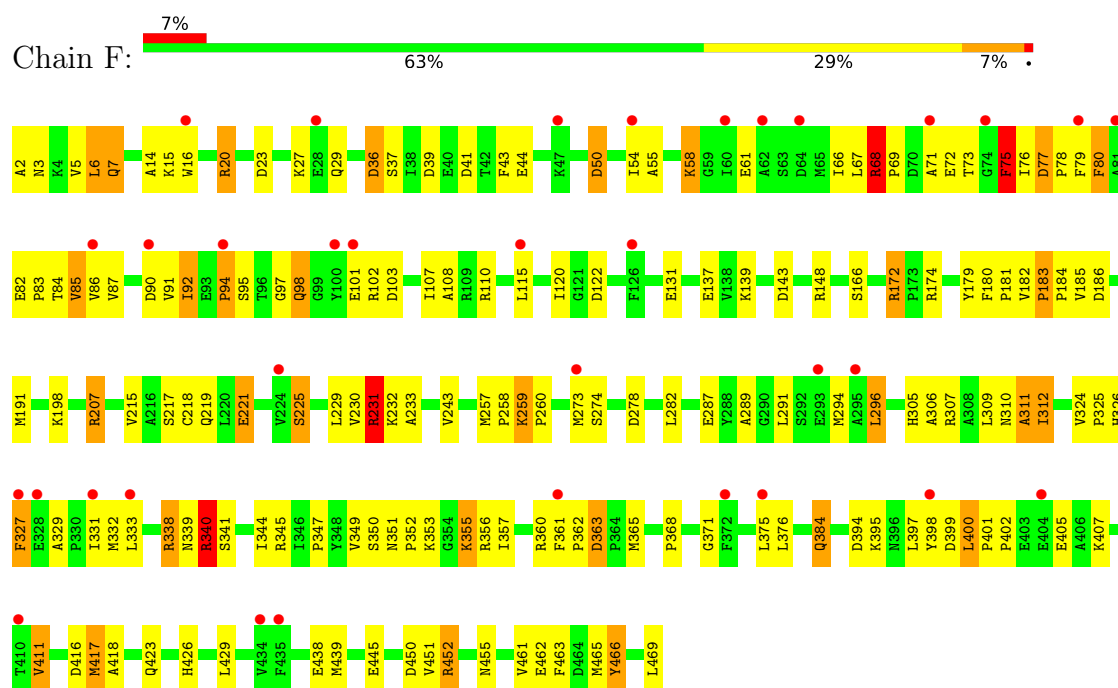
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	260.91Å 260.91Å 154.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.22 – 3.40 93.22 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (93.22-3.40) 98.0 (93.22-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.233 , 0.270 0.235 , 0.270	Depositor DCC
R_{free} test set	3606 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.961	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 129.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	43046	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, EDO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	1/3729 (0.0%)	1.26	31/5054 (0.6%)
1	B	0.65	1/3729 (0.0%)	1.22	32/5054 (0.6%)
1	C	0.61	1/3729 (0.0%)	1.21	38/5054 (0.8%)
1	D	0.58	2/3730 (0.1%)	1.17	21/5055 (0.4%)
1	E	0.52	1/3726 (0.0%)	1.08	15/5051 (0.3%)
1	F	0.53	0/3726	1.11	19/5049 (0.4%)
All	All	0.60	6/22369 (0.0%)	1.18	156/30317 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	11
1	C	0	8
1	D	0	13
1	E	0	11
1	F	0	6
All	All	0	56

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLU	CD-OE2	6.47	1.32	1.25
1	E	145	SER	CA-CB	-5.76	1.44	1.52
1	C	319	SER	CA-CB	-5.54	1.44	1.52
1	D	469	LEU	C-O	5.42	1.33	1.23
1	D	145	SER	CA-CB	-5.26	1.45	1.52
1	B	137	GLU	CD-OE2	5.10	1.31	1.25

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	20	ARG	NE-CZ-NH1	-15.81	112.39	120.30
1	A	322	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	D	322	ARG	NE-CZ-NH2	-11.87	114.37	120.30
1	B	75	PHE	N-CA-CB	11.34	131.01	110.60
1	E	148	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	B	75	PHE	CB-CA-C	-11.13	88.15	110.40
1	E	20	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	A	365	MET	CG-SD-CE	-10.53	83.36	100.20
1	C	110	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	B	77	ASP	CB-CA-C	10.13	130.66	110.40
1	B	365	MET	CG-SD-CE	-9.32	85.29	100.20
1	A	148	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	A	75	PHE	N-CA-CB	9.01	126.81	110.60
1	B	257	MET	CG-SD-CE	8.88	114.41	100.20
1	C	255	THR	OG1-CB-CG2	-8.84	89.66	110.00
1	C	48	MET	CG-SD-CE	8.79	114.26	100.20
1	F	257	MET	CG-SD-CE	8.78	114.25	100.20
1	A	77	ASP	CB-CA-C	8.49	127.38	110.40
1	F	340	ARG	CG-CD-NE	8.35	129.33	111.80
1	D	257	MET	CG-SD-CE	8.31	113.49	100.20
1	D	65	MET	CG-SD-CE	8.18	113.29	100.20
1	F	452	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	F	20	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	65	MET	CG-SD-CE	8.00	113.00	100.20
1	F	231	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	172	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	20	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	65	MET	CG-SD-CE	7.55	112.28	100.20
1	A	77	ASP	CB-CG-OD1	7.47	125.02	118.30
1	B	192	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	A	75	PHE	CB-CA-C	-7.34	95.71	110.40
1	C	185	VAL	N-CA-CB	7.21	127.36	111.50
1	F	148	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	77	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	340	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	58	LYS	CD-CE-NZ	7.07	127.97	111.70
1	E	174	ARG	CG-CD-NE	-7.04	97.01	111.80
1	E	469	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	B	148	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	261	MET	CB-CA-C	-6.95	96.50	110.40
1	C	148	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	218	CYS	CB-CA-C	6.90	124.19	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	65	MET	CG-SD-CE	6.82	111.11	100.20
1	C	439	MET	CG-SD-CE	6.74	110.98	100.20
1	C	441	ASP	CB-CA-C	6.74	123.88	110.40
1	F	231	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	D	231	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	C	377	MET	CG-SD-CE	-6.66	89.54	100.20
1	B	79	PHE	N-CA-CB	6.64	122.55	110.60
1	C	28	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	D	261	MET	CG-SD-CE	-6.60	89.64	100.20
1	A	353	LYS	N-CA-CB	6.60	122.48	110.60
1	F	143	ASP	CB-CA-C	-6.43	97.53	110.40
1	C	68	ARG	N-CA-CB	-6.41	99.07	110.60
1	B	232	LYS	N-CA-CB	6.38	122.08	110.60
1	C	340	ARG	CD-NE-CZ	6.32	132.45	123.60
1	C	143	ASP	CB-CA-C	-6.29	97.81	110.40
1	D	143	ASP	CB-CA-C	-6.28	97.84	110.40
1	A	136	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	332	MET	CG-SD-CE	6.25	110.21	100.20
1	A	122	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	4	LYS	CB-CA-C	6.20	122.81	110.40
1	E	452	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	C	345	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	E	143	ASP	CB-CA-C	-6.17	98.06	110.40
1	E	466	TYR	N-CA-CB	-6.16	99.52	110.60
1	D	3	ASN	CB-CA-C	6.15	122.70	110.40
1	C	465	MET	CG-SD-CE	-6.14	90.37	100.20
1	A	259	LYS	CD-CE-NZ	-6.12	97.62	111.70
1	F	466	TYR	N-CA-CB	-6.12	99.59	110.60
1	A	307	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	269	MET	CG-SD-CE	6.01	109.81	100.20
1	A	143	ASP	CB-CA-C	-5.98	98.44	110.40
1	B	174	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	102	ARG	CB-CA-C	-5.97	98.46	110.40
1	B	77	ASP	OD1-CG-OD2	-5.97	111.96	123.30
1	C	466	TYR	N-CA-CB	-5.96	99.87	110.60
1	E	366	MET	CG-SD-CE	-5.95	90.67	100.20
1	E	469	LEU	CB-CG-CD1	5.95	121.11	111.00
1	A	257	MET	CG-SD-CE	5.92	109.67	100.20
1	B	143	ASP	CB-CA-C	-5.91	98.59	110.40
1	C	340	ARG	CG-CD-NE	5.85	124.09	111.80
1	F	148	ARG	NE-CZ-NH1	5.85	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	OD1-CG-OD2	-5.84	112.21	123.30
1	B	105	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	429	LEU	CB-CG-CD1	5.83	120.91	111.00
1	A	231	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	415	LEU	CB-CG-CD2	5.81	120.88	111.00
1	F	75	PHE	N-CA-CB	5.79	121.02	110.60
1	B	453	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	F	20	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	F	363	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	77	ASP	CB-CA-C	5.75	121.90	110.40
1	A	207	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	313	THR	N-CA-CB	5.69	121.11	110.30
1	D	73	THR	OG1-CB-CG2	-5.69	96.91	110.00
1	A	160	THR	OG1-CB-CG2	5.69	123.09	110.00
1	D	82	GLU	CG-CD-OE2	5.68	129.67	118.30
1	C	174	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	462	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	C	185	VAL	CG1-CB-CG2	-5.65	101.85	110.90
1	A	466	TYR	N-CA-CB	-5.65	100.44	110.60
1	C	250	TYR	CB-CG-CD1	5.63	124.38	121.00
1	B	82	GLU	CB-CG-CD	5.61	129.35	114.20
1	B	73	THR	CA-CB-OG1	5.61	120.78	109.00
1	C	73	THR	OG1-CB-CG2	-5.56	97.22	110.00
1	D	82	GLU	CG-CD-OE1	-5.51	107.28	118.30
1	F	77	ASP	CB-CA-C	5.48	121.36	110.40
1	B	82	GLU	OE1-CD-OE2	-5.47	116.74	123.30
1	C	226	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	C	358	GLU	CG-CD-OE1	5.45	129.19	118.30
1	E	23	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	332	MET	CG-SD-CE	5.40	108.83	100.20
1	D	195	MET	CG-SD-CE	-5.39	91.57	100.20
1	B	77	ASP	CB-CG-OD1	5.39	123.15	118.30
1	E	377	MET	CG-SD-CE	-5.39	91.58	100.20
1	C	20	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	348	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	68	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	148	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	F	218	CYS	N-CA-C	-5.33	96.61	111.00
1	F	191	MET	CG-SD-CE	5.32	108.71	100.20
1	A	192	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	E	403	GLU	CG-CD-OE1	5.31	128.93	118.30
1	D	172	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	E	77	ASP	CB-CA-C	5.29	120.98	110.40
1	A	445	GLU	CB-CG-CD	-5.28	99.95	114.20
1	B	356	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	98	GLN	N-CA-CB	5.26	120.07	110.60
1	C	226	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	469	LEU	CB-CG-CD2	5.25	119.93	111.00
1	F	172	ARG	CB-CG-CD	5.25	125.26	111.60
1	D	110	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	353	LYS	CD-CE-NZ	5.23	123.73	111.70
1	B	235	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	144	MET	CG-SD-CE	5.19	108.51	100.20
1	D	144	MET	CG-SD-CE	-5.19	91.90	100.20
1	B	452	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	B	191	MET	CG-SD-CE	-5.14	91.97	100.20
1	C	448	THR	CA-CB-CG2	-5.12	105.23	112.40
1	B	179	TYR	C-N-CA	-5.11	108.92	121.70
1	C	75	PHE	CB-CA-C	-5.11	100.18	110.40
1	D	67	LEU	CB-CG-CD1	5.10	119.67	111.00
1	D	269	MET	CG-SD-CE	5.09	108.35	100.20
1	B	8	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	466	TYR	N-CA-CB	-5.06	101.50	110.60
1	F	417	MET	CG-SD-CE	5.05	108.28	100.20
1	C	110	ARG	NH1-CZ-NH2	5.05	124.95	119.40
1	C	195	MET	CG-SD-CE	-5.04	92.13	100.20
1	D	77	ASP	CA-CB-CG	5.03	124.47	113.40
1	D	90	ASP	CB-CG-OD1	5.03	122.83	118.30
1	E	221	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	D	50	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	452	ARG	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	452	ARG	Sidechain
1	A	68	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	110	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	20	ARG	Sidechain
1	B	308	ALA	Mainchain
1	B	322	ARG	Sidechain
1	B	338	ARG	Sidechain
1	B	356	ARG	Sidechain
1	B	68	ARG	Sidechain
1	B	69	PRO	Peptide
1	B	75	PHE	Peptide
1	C	109	ARG	Sidechain
1	C	20	ARG	Sidechain
1	C	231	ARG	Sidechain
1	C	340	ARG	Sidechain
1	C	345	ARG	Sidechain
1	C	356	ARG	Sidechain
1	C	422	LEU	Mainchain
1	C	68	ARG	Sidechain
1	D	105	ARG	Sidechain
1	D	110	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	20	ARG	Sidechain
1	D	207	ARG	Sidechain
1	D	231	ARG	Sidechain
1	D	307	ARG	Sidechain
1	D	338	ARG	Sidechain
1	D	340	ARG	Sidechain
1	D	356	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	452	ARG	Sidechain
1	D	68	ARG	Sidechain
1	E	105	ARG	Sidechain
1	E	109	ARG	Sidechain
1	E	110	ARG	Sidechain
1	E	174	ARG	Sidechain
1	E	20	ARG	Sidechain
1	E	231	ARG	Sidechain
1	E	338	ARG	Sidechain
1	E	345	ARG	Sidechain
1	E	356	ARG	Sidechain
1	E	360	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	68	ARG	Sidechain
1	F	110	ARG	Sidechain
1	F	231	ARG	Sidechain
1	F	340	ARG	Sidechain
1	F	356	ARG	Sidechain
1	F	360	ARG	Sidechain
1	F	68	ARG	Sidechain

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	3637	3515	3485	137	1
1	B	3637	3515	3485	127	0
1	C	3637	3515	3485	118	0
1	D	3638	3517	3487	113	1
1	E	3634	3508	3476	102	0
1	F	3635	3514	3484	92	0
2	A	10	14	14	0	0
3	A	12	16	16	0	0
3	B	12	16	16	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	6	8	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	F	4	6	6	0	0
All	All	21886	21160	20978	622	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 15.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PHE:CE2	1:B:78:PRO:HG2	1.94	1.03
1:C:2:ALA:HB1	1:C:69:PRO:HB3	1.40	1.01
1:E:67:LEU:HB3	1:E:87:VAL:HB	1.42	0.99
1:C:207:ARG:HH21	1:C:225:SER:HB2	1.30	0.96
1:A:253:THR:OG1	1:D:467:TYR:OH	1.86	0.94
1:A:75:PHE:CE2	1:A:78:PRO:HG2	2.03	0.92
1:A:75:PHE:HE1	1:A:241:TYR:HH	1.15	0.92
1:A:67:LEU:HD12	1:A:105:ARG:HH21	1.35	0.91
1:C:100:TYR:O	1:C:102:ARG:N	2.04	0.90
1:B:253:THR:HG1	1:E:467:TYR:HH	1.02	0.89
1:B:206:GLY:O	1:B:207:ARG:HB2	1.72	0.88
1:C:469:LEU:HD23	1:F:365:MET:HE3	1.53	0.87
1:B:207:ARG:HH21	1:B:225:SER:HB2	1.41	0.85
1:B:206:GLY:O	1:B:207:ARG:CB	2.25	0.85
1:A:452:ARG:HH12	1:D:325:PRO:HD2	1.41	0.83
1:B:5:VAL:HG23	1:B:68:ARG:HD2	1.62	0.82
1:C:68:ARG:HG3	1:C:70:ASP:HB3	1.61	0.82
1:A:55:ALA:HB2	1:A:101:GLU:HG2	1.61	0.82
1:A:92:ILE:HG12	1:A:94:PRO:HD2	1.64	0.79
1:F:310:ASN:O	1:F:418:ALA:HB1	1.81	0.79
1:B:94:PRO:O	1:B:95:SER:HB3	1.83	0.78
1:E:16:TRP:HB2	1:E:82:GLU:HG2	1.66	0.78
1:A:5:VAL:HG23	1:A:68:ARG:HD2	1.66	0.77
1:D:74:GLY:O	1:D:76:ILE:HG12	1.85	0.76
1:B:67:LEU:HD12	1:B:105:ARG:HH21	1.51	0.76
1:C:75:PHE:CE2	1:C:78:PRO:HG2	2.21	0.75
1:A:189:GLN:O	1:A:190:ASP:HB2	1.87	0.75
1:C:189:GLN:HE21	1:C:211:HIS:HE1	1.35	0.75
1:F:71:ALA:HB2	1:F:87:VAL:HG22	1.69	0.74
1:D:92:ILE:HG12	1:D:94:PRO:HD2	1.70	0.74
1:E:404:GLU:OE2	1:E:407:LYS:HD2	1.87	0.74
1:B:75:PHE:CE1	1:B:241:TYR:OH	2.39	0.74
1:F:36:ASP:O	1:F:37:SER:OG	2.03	0.73
1:E:66:ILE:HD11	1:E:85:VAL:HB	1.68	0.73
1:F:67:LEU:HB3	1:F:69:PRO:HD2	1.71	0.73
1:A:69:PRO:HG3	1:A:87:VAL:HG22	1.69	0.73
1:C:66:ILE:HD11	1:C:85:VAL:HB	1.71	0.72
1:D:459:HIS:ND1	1:D:461:VAL:HG22	2.02	0.72
1:E:85:VAL:HG12	1:E:87:VAL:HG23	1.71	0.72
1:B:66:ILE:HD11	1:B:85:VAL:HB	1.71	0.72
1:D:459:HIS:CE1	1:D:461:VAL:HG22	2.25	0.71
1:A:336:SER:OG	1:A:394:ASP:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:MET:CE	1:E:466:TYR:HB3	2.18	0.71
1:F:75:PHE:CD2	1:F:78:PRO:HB2	2.25	0.71
1:F:349:VAL:HG21	1:F:355:LYS:HA	1.73	0.71
1:A:98:GLN:HB2	1:A:102:ARG:HA	1.72	0.71
1:F:401:PRO:HB3	1:F:405:GLU:HB2	1.72	0.71
1:C:183:PRO:HA	1:C:186:ASP:HB3	1.73	0.70
1:F:312:ILE:CG2	1:F:371:GLY:HA2	2.20	0.70
1:C:52:SER:HA	1:C:55:ALA:HB2	1.72	0.70
1:C:313:THR:HA	1:C:366:MET:HB2	1.71	0.70
1:C:451:VAL:HG12	1:C:455:ASN:OD1	1.91	0.70
1:D:16:TRP:HB2	1:D:82:GLU:HG2	1.73	0.70
1:B:2:ALA:HB1	1:B:68:ARG:HG2	1.73	0.70
1:A:66:ILE:HD11	1:A:85:VAL:HB	1.72	0.69
1:B:98:GLN:HB2	1:B:102:ARG:HA	1.73	0.69
1:F:312:ILE:HG23	1:F:371:GLY:HA2	1.74	0.69
1:D:183:PRO:HA	1:D:186:ASP:HB3	1.73	0.69
1:C:92:ILE:HG12	1:C:94:PRO:HD2	1.74	0.69
1:B:75:PHE:CD2	1:B:78:PRO:HG2	2.28	0.69
1:E:92:ILE:HG22	1:E:95:SER:O	1.93	0.69
1:B:14:ALA:HB1	1:B:83:PRO:HD2	1.75	0.68
1:B:67:LEU:HD12	1:B:105:ARG:NH2	2.07	0.68
1:F:183:PRO:HA	1:F:186:ASP:HB3	1.75	0.68
1:A:336:SER:HG	1:A:394:ASP:HB3	1.57	0.68
1:F:68:ARG:N	1:F:69:PRO:HD2	2.08	0.68
1:A:452:ARG:NH1	1:D:325:PRO:HD2	2.08	0.68
1:A:183:PRO:HA	1:A:186:ASP:HB3	1.73	0.68
1:E:404:GLU:OE2	1:E:407:LYS:CD	2.42	0.68
1:F:90:ASP:HB3	1:F:103:ASP:HB2	1.74	0.68
1:D:180:PHE:O	1:E:29:GLN:HA	1.94	0.67
1:B:136:ASP:HA	1:B:252:LYS:HG2	1.75	0.67
1:A:16:TRP:HB2	1:A:82:GLU:HG2	1.77	0.66
1:A:75:PHE:HE1	1:A:241:TYR:OH	1.78	0.66
1:E:183:PRO:HA	1:E:186:ASP:HB3	1.75	0.66
1:B:17:VAL:HG21	1:B:38:ILE:HG13	1.76	0.66
1:D:17:VAL:HG21	1:D:38:ILE:HG13	1.78	0.65
1:E:17:VAL:HG21	1:E:38:ILE:HG13	1.77	0.65
1:C:17:VAL:HG21	1:C:38:ILE:HG13	1.79	0.64
1:E:338:ARG:HE	1:E:394:ASP:HB3	1.62	0.64
1:A:402:PRO:HD2	1:A:405:GLU:HB2	1.79	0.64
1:A:2:ALA:HB3	1:A:5:VAL:HB	1.79	0.64
1:B:139:LYS:HB3	1:C:161:GLY:HA2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HB3	1:A:341:SER:O	1.98	0.63
1:A:463:PHE:CE1	1:D:149:HIS:CE1	2.86	0.63
1:F:75:PHE:CZ	1:F:78:PRO:HG2	2.33	0.63
1:A:69:PRO:HD3	1:A:85:VAL:HG13	1.80	0.63
1:C:3:ASN:O	1:C:7:GLN:HB3	1.97	0.63
1:F:3:ASN:O	1:F:7:GLN:HB3	1.98	0.63
1:A:69:PRO:HG2	1:A:72:GLU:HA	1.79	0.63
1:C:98:GLN:HG2	1:C:110:ARG:HH22	1.63	0.63
1:A:17:VAL:HG21	1:A:38:ILE:HG13	1.81	0.63
1:B:206:GLY:O	1:B:207:ARG:CG	2.47	0.63
1:C:100:TYR:O	1:C:101:GLU:C	2.36	0.63
1:A:333:LEU:HD12	1:A:409:PRO:HB2	1.81	0.63
1:A:66:ILE:HD11	1:A:85:VAL:CB	2.28	0.63
1:F:2:ALA:HB3	1:F:6:LEU:HB2	1.81	0.63
1:C:274:SER:HB3	1:C:356:ARG:HG2	1.81	0.62
1:D:109:ARG:C	1:D:110:ARG:O	2.35	0.62
1:A:428:PHE:CE2	1:A:429:LEU:HD13	2.34	0.62
1:C:68:ARG:O	1:C:70:ASP:N	2.32	0.62
1:D:75:PHE:CD1	1:D:81:ALA:HA	2.34	0.62
1:F:66:ILE:HD11	1:F:85:VAL:HB	1.80	0.62
1:B:69:PRO:HG2	1:B:72:GLU:HA	1.82	0.62
1:C:311:ALA:C	1:C:312:ILE:HG13	2.20	0.62
1:C:20:ARG:HB2	1:C:86:VAL:HA	1.82	0.61
1:F:16:TRP:HB2	1:F:82:GLU:HG2	1.82	0.61
1:B:231:ARG:O	1:B:235:GLU:HB2	1.99	0.61
1:F:345:ARG:HH22	1:F:347:PRO:HA	1.64	0.61
1:D:75:PHE:HB2	1:D:78:PRO:HD2	1.81	0.61
1:D:349:VAL:HG21	1:D:355:LYS:HA	1.82	0.61
1:C:67:LEU:O	1:C:68:ARG:C	2.38	0.61
1:A:55:ALA:O	1:A:60:ILE:HD11	2.01	0.61
1:D:2:ALA:HB3	1:D:5:VAL:HB	1.82	0.61
1:B:66:ILE:HD11	1:B:85:VAL:CB	2.30	0.61
1:B:69:PRO:HG3	1:B:87:VAL:HG22	1.81	0.61
1:B:230:VAL:C	1:B:232:LYS:N	2.54	0.60
1:C:207:ARG:NH1	1:C:235:GLU:OE2	2.34	0.60
1:D:331:ILE:HG13	1:D:411:VAL:HG12	1.83	0.60
1:E:3:ASN:O	1:E:7:GLN:HB3	2.00	0.60
1:C:16:TRP:HB2	1:C:82:GLU:HG2	1.83	0.60
1:E:66:ILE:HD11	1:E:85:VAL:CB	2.30	0.60
1:C:349:VAL:HG21	1:C:355:LYS:HA	1.83	0.60
1:B:230:VAL:C	1:B:232:LYS:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLY:HA2	1:E:139:LYS:HB3	1.84	0.60
1:B:16:TRP:HB2	1:B:82:GLU:HG2	1.84	0.60
1:F:229:LEU:O	1:F:230:VAL:HB	2.02	0.60
1:B:18:ASP:OD1	1:B:30:HIS:HB2	2.02	0.59
1:B:20:ARG:NH2	1:B:75:PHE:CZ	2.70	0.59
1:F:2:ALA:HB1	1:F:68:ARG:HD2	1.83	0.59
1:C:94:PRO:O	1:C:95:SER:C	2.41	0.59
1:E:71:ALA:HB3	1:E:87:VAL:HG22	1.83	0.59
1:D:111:ALA:HB2	1:D:434:VAL:HG11	1.84	0.59
1:A:312:ILE:CG2	1:A:371:GLY:HA2	2.33	0.59
1:B:55:ALA:HB2	1:B:101:GLU:HG2	1.85	0.59
1:C:467:TYR:CE2	1:E:171:HIS:CE1	2.91	0.59
1:C:66:ILE:HD11	1:C:85:VAL:CG2	2.32	0.59
1:F:352:PRO:HA	1:F:355:LYS:HG2	1.85	0.58
1:C:229:LEU:O	1:C:230:VAL:HB	2.02	0.58
1:A:68:ARG:NH2	1:A:69:PRO:O	2.36	0.58
1:F:289:ALA:O	1:F:355:LYS:NZ	2.35	0.58
1:A:349:VAL:HG11	1:A:355:LYS:HA	1.86	0.58
1:B:188:ALA:O	1:B:189:GLN:C	2.41	0.58
1:D:66:ILE:HD11	1:D:85:VAL:HB	1.85	0.58
1:B:69:PRO:HD3	1:B:85:VAL:HG13	1.84	0.57
1:B:207:ARG:HH21	1:B:225:SER:CB	2.15	0.57
1:B:229:LEU:O	1:B:230:VAL:HB	2.03	0.57
1:C:365:MET:CE	1:F:466:TYR:HB3	2.33	0.57
1:E:188:ALA:O	1:E:190:ASP:N	2.37	0.57
1:A:67:LEU:O	1:A:68:ARG:C	2.41	0.57
1:B:75:PHE:CE2	1:B:78:PRO:CG	2.81	0.57
1:B:94:PRO:O	1:B:95:SER:CB	2.53	0.57
1:C:149:HIS:CE1	1:F:463:PHE:CE1	2.93	0.57
1:F:310:ASN:O	1:F:311:ALA:HB2	2.05	0.57
1:A:57:TRP:HA	1:A:57:TRP:CE3	2.40	0.57
1:B:69:PRO:HB3	1:B:87:VAL:HG13	1.85	0.57
1:B:75:PHE:HE1	1:B:241:TYR:OH	1.83	0.57
1:E:229:LEU:C	1:E:231:ARG:H	2.06	0.57
1:F:229:LEU:HD23	1:F:230:VAL:H	1.69	0.57
1:C:289:ALA:O	1:C:355:LYS:NZ	2.36	0.56
1:C:255:THR:OG1	1:C:257:MET:HB2	2.05	0.56
1:A:139:LYS:HB3	1:B:161:GLY:HA2	1.87	0.56
1:C:68:ARG:O	1:C:87:VAL:HG21	2.04	0.56
1:E:75:PHE:HB3	1:E:78:PRO:HD2	1.88	0.56
1:C:287:GLU:HB2	1:C:291:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PHE:HE1	1:B:241:TYR:CZ	2.23	0.56
1:D:180:PHE:N	1:D:181:PRO:HD3	2.21	0.56
1:B:287:GLU:O	1:B:288:TYR:HB2	2.04	0.56
1:A:75:PHE:CE1	1:A:241:TYR:OH	2.52	0.56
1:E:143:ASP:HB2	1:E:145:SER:H	1.71	0.56
1:A:86:VAL:HG13	1:A:87:VAL:HG13	1.87	0.55
1:C:207:ARG:HH21	1:C:225:SER:CB	2.12	0.55
1:A:229:LEU:O	1:A:230:VAL:HB	2.04	0.55
1:C:66:ILE:HD11	1:C:85:VAL:CB	2.36	0.55
1:D:66:ILE:HD11	1:D:85:VAL:CB	2.36	0.55
1:F:180:PHE:N	1:F:181:PRO:HD3	2.22	0.55
1:A:382:GLY:HA2	1:A:387:ILE:HG13	1.89	0.55
1:E:2:ALA:HB2	1:E:68:ARG:HB3	1.88	0.55
1:D:367:ASN:O	1:D:370:LEU:O	2.25	0.55
1:A:317:THR:HB	1:A:454:LEU:HD22	1.88	0.55
1:C:130:PRO:HB3	1:C:269:MET:HG3	1.87	0.55
1:C:312:ILE:O	1:C:313:THR:HG23	2.07	0.55
1:C:98:GLN:CD	1:C:102:ARG:HA	2.27	0.55
1:C:467:TYR:HE2	1:E:171:HIS:CE1	2.26	0.54
1:E:338:ARG:NE	1:E:394:ASP:HB3	2.22	0.54
1:C:466:TYR:OH	1:F:450:ASP:HB3	2.08	0.54
1:B:43:PHE:CD2	1:B:66:ILE:HG23	2.43	0.54
1:D:69:PRO:HD3	1:D:87:VAL:HG22	1.89	0.54
1:A:86:VAL:HG21	1:A:238:GLN:HG3	1.90	0.54
1:B:259:LYS:HG2	1:B:321:LYS:HB3	1.88	0.54
1:C:85:VAL:HG12	1:C:87:VAL:HG23	1.89	0.54
1:F:98:GLN:NE2	1:F:101:GLU:O	2.41	0.54
1:C:229:LEU:HD23	1:C:230:VAL:H	1.74	0.53
1:D:66:ILE:HD11	1:D:85:VAL:HG21	1.90	0.53
1:D:289:ALA:O	1:D:355:LYS:NZ	2.41	0.53
1:A:69:PRO:HD2	1:A:72:GLU:CB	2.38	0.53
1:A:136:ASP:HA	1:A:252:LYS:HG2	1.90	0.53
1:A:331:ILE:HG13	1:A:411:VAL:HG12	1.89	0.53
1:E:75:PHE:CD2	1:E:78:PRO:HG2	2.43	0.53
1:E:180:PHE:N	1:E:181:PRO:HD3	2.23	0.53
1:E:340:ARG:O	1:E:397:LEU:HB3	2.09	0.53
1:A:29:GLN:HB3	1:B:180:PHE:HB2	1.90	0.53
1:C:27:LYS:HG2	1:F:469:LEU:HD12	1.89	0.53
1:C:350:SER:OG	1:C:351:ASN:N	2.39	0.52
1:A:245:ASN:HD21	1:B:184:PRO:HD3	1.74	0.52
1:A:43:PHE:CD2	1:A:66:ILE:HG23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:TYR:CE1	1:D:255:THR:HB	2.45	0.52
1:A:66:ILE:HD11	1:A:85:VAL:CG2	2.39	0.52
1:C:277:LYS:HB2	1:C:282:LEU:HD21	1.91	0.52
1:D:56:GLY:HA2	1:D:100:TYR:CB	2.39	0.52
1:E:340:ARG:NH2	1:F:50:ASP:OD1	2.42	0.52
1:C:180:PHE:N	1:C:181:PRO:HD3	2.25	0.52
1:C:365:MET:HE2	1:F:466:TYR:HB3	1.90	0.52
1:F:66:ILE:HG13	1:F:85:VAL:HG11	1.90	0.52
1:B:188:ALA:O	1:B:190:ASP:N	2.42	0.52
1:D:229:LEU:O	1:D:230:VAL:HB	2.09	0.52
1:E:20:ARG:HB2	1:E:86:VAL:HA	1.92	0.52
1:F:338:ARG:CZ	1:F:394:ASP:HB3	2.40	0.52
1:D:69:PRO:HD3	1:D:85:VAL:HG13	1.92	0.51
1:E:258:PRO:O	1:E:259:LYS:C	2.48	0.51
1:A:66:ILE:HD11	1:A:85:VAL:HG21	1.93	0.51
1:F:327:PHE:C	1:F:329:ALA:H	2.13	0.51
1:B:68:ARG:NH2	1:B:68:ARG:HG3	2.26	0.51
1:F:451:VAL:HG12	1:F:455:ASN:OD1	2.10	0.51
1:A:258:PRO:HD3	1:A:365:MET:HG2	1.93	0.51
1:E:330:PRO:HB3	1:E:360:ARG:HB2	1.92	0.51
1:A:207:ARG:NH1	1:A:235:GLU:OE2	2.44	0.51
1:F:326:HIS:CE1	1:F:327:PHE:HD1	2.28	0.51
1:A:75:PHE:CZ	1:A:78:PRO:HG2	2.43	0.51
1:B:14:ALA:CB	1:B:83:PRO:HD2	2.41	0.51
1:D:67:LEU:HB3	1:D:87:VAL:HG23	1.93	0.51
1:D:98:GLN:HB2	1:D:103:ASP:H	1.76	0.51
1:A:20:ARG:HD3	1:A:30:HIS:HB3	1.93	0.51
1:E:43:PHE:CD2	1:E:66:ILE:HG23	2.45	0.51
1:A:69:PRO:HD3	1:A:85:VAL:CG1	2.40	0.51
1:A:331:ILE:O	1:A:331:ILE:HG12	2.11	0.51
1:E:349:VAL:HG11	1:E:355:LYS:N	2.26	0.51
1:D:66:ILE:HD11	1:D:85:VAL:CG2	2.41	0.51
1:E:54:ILE:HG22	1:E:101:GLU:HB2	1.92	0.51
1:E:404:GLU:OE1	1:E:408:ILE:HD11	2.10	0.51
1:F:68:ARG:N	1:F:69:PRO:CD	2.74	0.51
1:A:69:PRO:CG	1:A:87:VAL:HG22	2.40	0.51
1:C:313:THR:N	1:C:366:MET:HG3	2.25	0.51
1:E:94:PRO:O	1:E:95:SER:C	2.50	0.50
1:E:287:GLU:HB2	1:E:291:LEU:O	2.10	0.50
1:A:402:PRO:HG2	1:A:404:GLU:HB2	1.91	0.50
1:C:2:ALA:CB	1:C:69:PRO:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PHE:CD2	1:D:66:ILE:HG23	2.47	0.50
1:D:68:ARG:O	1:D:68:ARG:NE	2.44	0.50
1:F:20:ARG:HB2	1:F:86:VAL:HA	1.93	0.50
1:F:287:GLU:HB2	1:F:291:LEU:O	2.11	0.50
1:D:16:TRP:O	1:D:83:PRO:HD2	2.12	0.50
1:E:428:PHE:HA	1:E:431:LYS:HD3	1.94	0.50
1:A:75:PHE:HD2	1:A:82:GLU:HB2	1.77	0.50
1:D:69:PRO:CD	1:D:87:VAL:HG22	2.41	0.50
1:D:180:PHE:HB2	1:E:29:GLN:HB3	1.92	0.50
1:F:131:GLU:HG2	1:F:221:GLU:HG3	1.94	0.50
1:B:54:ILE:HG22	1:B:101:GLU:HB2	1.94	0.50
1:B:277:LYS:HB2	1:B:282:LEU:HD21	1.93	0.50
1:C:333:LEU:HB2	1:C:409:PRO:HG2	1.94	0.50
1:D:69:PRO:HD3	1:D:85:VAL:CG1	2.42	0.50
1:A:402:PRO:C	1:A:404:GLU:H	2.14	0.49
1:B:180:PHE:N	1:B:181:PRO:HD3	2.27	0.49
1:B:463:PHE:CE1	1:E:149:HIS:CE1	3.00	0.49
1:B:469:LEU:HB3	1:E:365:MET:CE	2.42	0.49
1:C:259:LYS:HG2	1:C:321:LYS:HB3	1.93	0.49
1:E:351:ASN:OD1	1:E:353:LYS:HB2	2.12	0.49
1:B:66:ILE:HD11	1:B:85:VAL:CG2	2.42	0.49
1:C:75:PHE:CD2	1:C:78:PRO:HB2	2.46	0.49
1:F:310:ASN:O	1:F:311:ALA:CB	2.58	0.49
1:C:195:MET:HA	1:C:246:VAL:HG21	1.95	0.49
1:B:203:MET:HE1	1:B:235:GLU:HG3	1.94	0.49
1:D:58:LYS:NZ	1:D:58:LYS:HA	2.26	0.49
1:F:98:GLN:CD	1:F:102:ARG:HA	2.33	0.49
1:A:327:PHE:O	1:A:328:GLU:HB2	2.12	0.49
1:C:19:PHE:CD1	1:C:66:ILE:HD13	2.47	0.49
1:E:161:GLY:HA2	1:F:139:LYS:HB3	1.94	0.49
1:A:195:MET:HA	1:A:246:VAL:HG21	1.94	0.49
1:A:229:LEU:HD23	1:A:230:VAL:N	2.27	0.49
1:A:397:LEU:HD12	1:A:399:ASP:H	1.78	0.49
1:C:304:LYS:HD3	1:C:305:HIS:CE1	2.47	0.49
1:E:48:MET:HA	1:E:63:SER:HA	1.94	0.49
1:C:75:PHE:CG	1:C:78:PRO:HD2	2.48	0.49
1:D:66:ILE:HA	1:D:88:THR:HG23	1.95	0.49
1:F:98:GLN:CG	1:F:102:ARG:HA	2.42	0.49
1:D:94:PRO:O	1:D:95:SER:CB	2.60	0.49
1:D:183:PRO:HD2	1:E:241:TYR:HE1	1.78	0.49
1:A:2:ALA:O	1:A:6:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:HG21	1:B:191:MET:HE3	1.95	0.49
1:B:189:GLN:HE21	1:B:211:HIS:HE1	1.61	0.49
1:C:2:ALA:HB1	1:C:69:PRO:CB	2.28	0.49
1:E:451:VAL:HG12	1:E:455:ASN:OD1	2.13	0.49
1:B:307:ARG:NH2	1:B:417:MET:SD	2.86	0.48
1:C:172:ARG:O	1:C:174:ARG:NH1	2.46	0.48
1:A:143:ASP:OD1	1:A:148:ARG:NH2	2.46	0.48
1:A:365:MET:HE2	1:D:466:TYR:HB3	1.94	0.48
1:D:73:THR:CG2	1:D:202:ILE:HG23	2.43	0.48
1:E:16:TRP:O	1:E:83:PRO:HD2	2.13	0.48
1:F:55:ALA:HB3	1:F:58:LYS:HG2	1.95	0.48
1:B:402:PRO:C	1:B:404:GLU:H	2.17	0.48
1:C:66:ILE:HD11	1:C:85:VAL:HG21	1.95	0.48
1:C:75:PHE:CZ	1:C:78:PRO:HG2	2.49	0.48
1:D:307:ARG:NH2	1:D:417:MET:SD	2.86	0.48
1:E:71:ALA:HB1	1:E:86:VAL:HB	1.95	0.48
1:B:65:MET:CE	1:B:67:LEU:HD21	2.44	0.48
1:D:192:ARG:HD3	1:D:220:LEU:HD22	1.95	0.48
1:A:2:ALA:HB2	1:A:43:PHE:CE2	2.48	0.48
1:A:30:HIS:H	1:B:180:PHE:HB3	1.78	0.48
1:B:183:PRO:O	1:B:184:PRO:C	2.52	0.48
1:B:463:PHE:HE1	1:E:149:HIS:CE1	2.32	0.48
1:C:16:TRP:O	1:C:83:PRO:HD2	2.14	0.48
1:E:95:SER:O	1:E:97:GLY:N	2.47	0.48
1:D:314:ASN:HD21	1:D:362:PRO:HA	1.79	0.48
1:E:75:PHE:HB2	1:E:82:GLU:O	2.14	0.48
1:A:272:HIS:HB3	1:A:356:ARG:HD2	1.95	0.48
1:C:258:PRO:O	1:C:259:LYS:C	2.52	0.48
1:D:69:PRO:HG3	1:D:87:VAL:HG22	1.96	0.48
1:D:183:PRO:O	1:D:184:PRO:C	2.52	0.48
1:E:337:ALA:HA	1:E:346:ILE:H	1.77	0.48
1:F:349:VAL:C	1:F:351:ASN:H	2.17	0.48
1:A:463:PHE:HE1	1:D:149:HIS:CE1	2.30	0.48
1:B:107:ILE:HA	1:B:110:ARG:HD2	1.95	0.48
1:B:367:ASN:HB3	1:B:370:LEU:HB2	1.95	0.48
1:C:55:ALA:O	1:C:58:LYS:HB2	2.14	0.48
1:C:95:SER:O	1:C:97:GLY:N	2.47	0.48
1:D:76:ILE:O	1:D:77:ASP:CB	2.62	0.48
1:D:208:VAL:O	1:E:34:PRO:HG2	2.14	0.48
1:A:67:LEU:CD1	1:A:105:ARG:HH21	2.17	0.47
1:A:73:THR:CG2	1:A:202:ILE:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:O	1:A:328:GLU:CB	2.60	0.47
1:B:230:VAL:O	1:B:232:LYS:N	2.47	0.47
1:D:71:ALA:O	1:D:72:GLU:C	2.52	0.47
1:E:351:ASN:HD21	1:E:353:LYS:HD2	1.79	0.47
1:F:36:ASP:O	1:F:37:SER:CB	2.61	0.47
1:C:189:GLN:HE21	1:C:211:HIS:CE1	2.24	0.47
1:E:427:GLU:HA	1:E:430:LEU:HD12	1.96	0.47
1:A:16:TRP:O	1:A:83:PRO:HD2	2.14	0.47
1:B:203:MET:CE	1:B:235:GLU:HG3	2.44	0.47
1:F:16:TRP:O	1:F:83:PRO:HD2	2.14	0.47
1:F:207:ARG:HH22	1:F:225:SER:HB2	1.79	0.47
1:B:68:ARG:NH1	1:B:69:PRO:O	2.48	0.47
1:B:401:PRO:HA	1:B:405:GLU:HB2	1.96	0.47
1:C:2:ALA:HB3	1:C:5:VAL:HB	1.97	0.47
1:C:310:ASN:HD21	1:C:411:VAL:HG22	1.78	0.47
1:E:307:ARG:NH2	1:E:417:MET:SD	2.87	0.47
1:A:262:VAL:HG21	1:D:458:THR:H	1.78	0.47
1:D:326:HIS:CD2	1:D:328:GLU:HB3	2.49	0.47
1:F:183:PRO:O	1:F:184:PRO:C	2.53	0.47
1:A:57:TRP:HA	1:A:57:TRP:HE3	1.79	0.47
1:B:333:LEU:HB2	1:B:409:PRO:HG2	1.95	0.47
1:B:92:ILE:HG12	1:B:94:PRO:HD2	1.95	0.47
1:B:228:THR:O	1:B:230:VAL:O	2.33	0.47
1:C:469:LEU:HB3	1:F:365:MET:CE	2.44	0.47
1:D:403:GLU:O	1:D:405:GLU:N	2.48	0.47
1:F:43:PHE:CD2	1:F:66:ILE:HG23	2.50	0.47
1:A:58:LYS:CE	1:B:395:LYS:HA	2.45	0.47
1:A:229:LEU:HD23	1:A:230:VAL:H	1.79	0.47
1:C:52:SER:O	1:C:53:SER:OG	2.24	0.47
1:C:71:ALA:HB1	1:C:86:VAL:HB	1.97	0.47
1:E:296:LEU:HD13	1:E:296:LEU:HA	1.81	0.47
1:A:92:ILE:HG22	1:A:97:GLY:H	1.80	0.46
1:B:336:SER:O	1:B:345:ARG:HA	2.15	0.46
1:C:43:PHE:CD2	1:C:66:ILE:HG23	2.50	0.46
1:D:229:LEU:HD23	1:D:230:VAL:H	1.79	0.46
1:E:297:TYR:HB3	1:E:383:ILE:HA	1.98	0.46
1:F:76:ILE:HG23	1:F:77:ASP:H	1.80	0.46
1:A:366:MET:SD	1:A:371:GLY:HA3	2.56	0.46
1:B:69:PRO:HD2	1:B:72:GLU:CB	2.46	0.46
1:C:20:ARG:HD3	1:C:30:HIS:HB3	1.97	0.46
1:E:70:ASP:OD1	1:E:71:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLU:HA	1:E:164:TYR:OH	2.15	0.46
1:F:90:ASP:H	1:F:103:ASP:CG	2.18	0.46
1:F:92:ILE:HG23	1:F:94:PRO:HD2	1.97	0.46
1:C:75:PHE:CD2	1:C:78:PRO:HG2	2.49	0.46
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.59	0.46
1:F:91:VAL:HA	1:F:97:GLY:O	2.15	0.46
1:B:232:LYS:HB3	1:B:372:PHE:CE2	2.51	0.46
1:F:258:PRO:O	1:F:259:LYS:C	2.54	0.46
1:A:367:ASN:HB3	1:A:370:LEU:HB2	1.98	0.46
1:E:402:PRO:C	1:E:404:GLU:H	2.17	0.46
1:D:397:LEU:H	1:D:397:LEU:HG	1.62	0.46
1:A:85:VAL:C	1:A:87:VAL:N	2.70	0.46
1:A:158:TRP:CZ2	1:D:145:SER:HA	2.51	0.46
1:B:365:MET:HE2	1:E:466:TYR:HB3	1.98	0.46
1:D:19:PHE:CD1	1:D:66:ILE:HD13	2.51	0.46
1:D:195:MET:HA	1:D:246:VAL:HG21	1.97	0.46
1:D:333:LEU:HB2	1:D:409:PRO:HG2	1.98	0.46
1:E:94:PRO:O	1:E:96:THR:N	2.49	0.46
1:A:58:LYS:HE3	1:B:394:ASP:O	2.16	0.46
1:A:336:SER:O	1:A:345:ARG:HA	2.16	0.46
1:B:207:ARG:NH2	1:B:225:SER:O	2.49	0.46
1:B:287:GLU:O	1:B:288:TYR:CB	2.63	0.46
1:C:108:ALA:HB1	1:C:229:LEU:HD22	1.97	0.46
1:C:111:ALA:HB1	1:C:376:LEU:HD22	1.97	0.46
1:E:24:THR:OG1	1:E:54:ILE:HG23	2.16	0.46
1:E:430:LEU:HD23	1:E:435:PHE:O	2.16	0.46
1:A:183:PRO:O	1:A:184:PRO:C	2.53	0.45
1:E:67:LEU:HD13	1:E:69:PRO:HD2	1.99	0.45
1:A:259:LYS:HG2	1:A:321:LYS:HB3	1.98	0.45
1:C:67:LEU:HB2	1:C:89:CYS:H	1.82	0.45
1:F:331:ILE:HD12	1:F:411:VAL:HG12	1.98	0.45
1:A:94:PRO:O	1:A:95:SER:CB	2.65	0.45
1:A:101:GLU:HG3	1:A:442:ALA:CB	2.46	0.45
1:A:307:ARG:NH2	1:A:417:MET:SD	2.89	0.45
1:D:317:THR:HB	1:D:454:LEU:HD22	1.98	0.45
1:D:9:ILE:HG21	1:D:35:ALA:HB1	1.97	0.45
1:A:29:GLN:HA	1:B:180:PHE:O	2.16	0.45
1:A:253:THR:CG2	1:B:169:SER:HA	2.47	0.45
1:B:469:LEU:HD22	1:E:365:MET:HE3	1.98	0.45
1:C:180:PHE:HE1	1:C:212:HIS:CD2	2.34	0.45
1:D:95:SER:OG	1:D:96:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:HD23	1:D:230:VAL:N	2.31	0.45
1:D:239:PHE:O	1:D:243:VAL:HG13	2.15	0.45
1:E:183:PRO:O	1:E:184:PRO:C	2.52	0.45
1:A:105:ARG:NH1	1:A:234:ASP:OD1	2.50	0.45
1:F:3:ASN:OD1	1:F:68:ARG:NH2	2.50	0.45
1:A:58:LYS:HA	1:A:58:LYS:HD2	1.70	0.45
1:B:243:VAL:HG11	1:B:256:PHE:HZ	1.81	0.45
1:C:71:ALA:HB3	1:C:87:VAL:HG22	1.97	0.45
1:C:365:MET:SD	1:F:469:LEU:HD23	2.56	0.45
1:C:207:ARG:HE	1:C:207:ARG:HA	1.82	0.45
1:D:259:LYS:HG2	1:D:321:LYS:HB3	1.99	0.45
1:E:338:ARG:HE	1:E:394:ASP:CB	2.30	0.45
1:F:312:ILE:HG21	1:F:371:GLY:HA2	1.98	0.45
1:F:307:ARG:NH2	1:F:417:MET:SD	2.90	0.44
1:C:339:ASN:ND2	1:C:340:ARG:O	2.50	0.44
1:D:19:PHE:CG	1:D:66:ILE:HD13	2.52	0.44
1:D:296:LEU:HD12	1:D:389:PRO:HG3	2.00	0.44
1:D:307:ARG:NH1	1:D:411:VAL:O	2.49	0.44
1:D:68:ARG:O	1:D:68:ARG:CZ	2.64	0.44
1:D:72:GLU:O	1:D:73:THR:C	2.55	0.44
1:F:400:LEU:H	1:F:400:LEU:HG	1.68	0.44
1:A:333:LEU:HB2	1:A:409:PRO:HG2	1.98	0.44
1:D:136:ASP:HA	1:D:252:LYS:HG2	2.00	0.44
1:E:180:PHE:HB2	1:F:29:GLN:HB3	2.00	0.44
1:B:189:GLN:O	1:B:190:ASP:C	2.55	0.44
1:D:85:VAL:C	1:D:87:VAL:N	2.71	0.44
1:E:85:VAL:C	1:E:87:VAL:N	2.71	0.44
1:F:108:ALA:HB1	1:F:229:LEU:HD22	2.00	0.44
1:A:108:ALA:HB1	1:A:229:LEU:CD2	2.48	0.44
1:B:179:TYR:HD1	1:B:179:TYR:HA	1.68	0.44
1:B:206:GLY:C	1:B:207:ARG:HG2	2.38	0.44
1:D:180:PHE:O	1:E:29:GLN:CA	2.63	0.44
1:F:85:VAL:C	1:F:87:VAL:N	2.70	0.44
1:B:66:ILE:HD11	1:B:85:VAL:HG21	1.99	0.44
1:C:19:PHE:CG	1:C:66:ILE:HD13	2.53	0.44
1:C:91:VAL:HA	1:C:97:GLY:O	2.18	0.44
1:E:136:ASP:HA	1:E:252:LYS:HG2	1.98	0.44
1:A:325:PRO:HD2	1:D:452:ARG:HH12	1.82	0.44
1:B:29:GLN:HB3	1:C:180:PHE:HB2	2.00	0.44
1:C:336:SER:O	1:C:345:ARG:HA	2.18	0.44
1:F:338:ARG:NE	1:F:394:ASP:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:HE2	1:B:395:LYS:HA	2.00	0.43
1:C:310:ASN:O	1:C:313:THR:O	2.36	0.43
1:E:230:VAL:HG12	1:E:230:VAL:O	2.17	0.43
1:A:149:HIS:HD2	1:D:460:PRO:HG3	1.83	0.43
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.86	0.43
1:B:75:PHE:HE1	1:B:241:TYR:CE2	2.37	0.43
1:A:340:ARG:O	1:A:341:SER:CB	2.65	0.43
1:D:14:ALA:CB	1:D:83:PRO:HD3	2.48	0.43
1:D:67:LEU:HB3	1:D:87:VAL:CG2	2.48	0.43
1:D:110:ARG:O	1:D:112:GLU:N	2.49	0.43
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.83	0.43
1:D:353:LYS:HD2	1:D:353:LYS:HA	1.85	0.43
1:E:85:VAL:C	1:E:87:VAL:H	2.22	0.43
1:B:332:MET:HB2	1:B:341:SER:O	2.19	0.43
1:C:296:LEU:HD12	1:C:389:PRO:HG3	1.99	0.43
1:D:423:GLN:HE21	1:D:423:GLN:HB2	1.65	0.43
1:B:198:LYS:HD3	1:B:198:LYS:HA	1.76	0.43
1:B:206:GLY:C	1:B:207:ARG:CG	2.86	0.43
1:B:230:VAL:HG12	1:B:231:ARG:HG3	2.01	0.43
1:C:318:ASN:ND2	1:F:462:GLU:OE1	2.52	0.43
1:E:207:ARG:NH2	1:E:225:SER:O	2.52	0.43
1:B:182:VAL:HB	1:B:183:PRO:HD2	2.00	0.43
1:E:55:ALA:HB1	1:E:58:LYS:HD3	2.01	0.43
1:E:284:ALA:HA	1:E:355:LYS:HG2	1.99	0.43
1:F:2:ALA:HB2	1:F:6:LEU:HD22	2.01	0.43
1:A:5:VAL:HG11	1:A:43:PHE:HZ	1.84	0.43
1:C:2:ALA:HB2	1:C:43:PHE:CE2	2.53	0.43
1:C:296:LEU:HD13	1:C:296:LEU:HA	1.86	0.43
1:A:69:PRO:HB3	1:A:87:VAL:HG13	2.01	0.43
1:A:314:ASN:HD21	1:A:362:PRO:HA	1.84	0.43
1:A:463:PHE:HA	1:D:257:MET:CE	2.48	0.43
1:B:200:GLU:O	1:B:204:GLY:N	2.49	0.43
1:B:325:PRO:HD2	1:E:452:ARG:HH12	1.84	0.43
1:B:459:HIS:HB3	1:B:462:GLU:HG3	2.00	0.43
1:C:321:LYS:HE3	1:F:455:ASN:O	2.18	0.43
1:D:351:ASN:HD21	1:D:353:LYS:HB3	1.83	0.43
1:E:183:PRO:N	1:E:184:PRO:HD2	2.34	0.43
1:A:57:TRP:HB2	1:A:60:ILE:HG12	2.00	0.43
1:D:67:LEU:CB	1:D:87:VAL:HG23	2.49	0.43
1:E:340:ARG:C	1:E:342:ALA:H	2.22	0.43
1:A:28:GLU:OE2	1:A:86:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PHE:CD2	1:A:429:LEU:HD13	2.54	0.42
1:C:85:VAL:C	1:C:87:VAL:N	2.71	0.42
1:C:361:PHE:N	1:C:362:PRO:CD	2.82	0.42
1:F:183:PRO:N	1:F:184:PRO:HD2	2.34	0.42
1:A:340:ARG:C	1:A:342:ALA:H	2.22	0.42
1:B:232:LYS:HD2	1:B:232:LYS:HA	1.43	0.42
1:A:50:ASP:HA	1:A:60:ILE:O	2.20	0.42
1:A:461:VAL:HG23	1:D:142:ILE:HD13	2.02	0.42
1:C:128:PRO:O	1:C:270:HIS:O	2.37	0.42
1:C:310:ASN:HD21	1:C:411:VAL:CG2	2.33	0.42
1:D:179:TYR:HD1	1:D:179:TYR:HA	1.70	0.42
1:C:311:ALA:O	1:C:312:ILE:HG13	2.20	0.42
1:A:352:PRO:O	1:A:353:LYS:HB2	2.19	0.42
1:B:195:MET:HA	1:B:246:VAL:HG21	2.02	0.42
1:C:226:PHE:O	1:C:226:PHE:CD1	2.73	0.42
1:E:42:THR:HG23	1:E:66:ILE:HG21	2.02	0.42
1:E:168:ASN:H	1:F:137:GLU:HG3	1.84	0.42
1:F:43:PHE:HA	1:F:66:ILE:HG22	2.00	0.42
1:F:75:PHE:CE2	1:F:78:PRO:HG2	2.54	0.42
1:B:50:ASP:HB3	1:C:179:TYR:OH	2.20	0.42
1:B:183:PRO:N	1:B:184:PRO:HD2	2.34	0.42
1:C:66:ILE:CD1	1:C:85:VAL:HB	2.45	0.42
1:D:183:PRO:N	1:D:184:PRO:HD2	2.35	0.42
1:D:212:HIS:HB3	1:E:31:VAL:HG13	2.01	0.42
1:E:19:PHE:CG	1:E:66:ILE:HD13	2.55	0.42
1:E:361:PHE:N	1:E:362:PRO:CD	2.83	0.42
1:F:339:ASN:ND2	1:F:340:ARG:O	2.53	0.42
1:B:66:ILE:HD12	1:B:66:ILE:HA	1.94	0.42
1:B:149:HIS:HD2	1:E:460:PRO:HG3	1.83	0.42
1:C:309:LEU:O	1:C:311:ALA:O	2.38	0.42
1:D:361:PHE:N	1:D:362:PRO:CD	2.83	0.42
1:A:75:PHE:HB2	1:A:82:GLU:O	2.20	0.42
1:C:332:MET:HB2	1:C:341:SER:O	2.19	0.42
1:C:393:ALA:HA	1:C:395:LYS:HE2	2.02	0.42
1:A:85:VAL:C	1:A:87:VAL:H	2.22	0.42
1:C:63:SER:HB3	1:C:91:VAL:HG23	2.02	0.42
1:E:2:ALA:CB	1:E:68:ARG:HB3	2.49	0.42
1:A:19:PHE:CD1	1:A:66:ILE:HD13	2.55	0.41
1:A:178:GLY:HA2	1:A:181:PRO:HG3	2.02	0.41
1:C:310:ASN:OD1	1:C:411:VAL:HG22	2.20	0.41
1:D:57:TRP:O	1:D:58:LYS:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:LEU:HD23	1:E:291:LEU:HA	1.85	0.41
1:A:19:PHE:CG	1:A:66:ILE:HD13	2.55	0.41
1:A:27:LYS:HE2	1:B:182:VAL:HG22	2.02	0.41
1:B:128:PRO:HA	1:B:270:HIS:O	2.20	0.41
1:D:73:THR:HG22	1:D:202:ILE:HG23	2.01	0.41
1:D:143:ASP:HB2	1:D:145:SER:H	1.85	0.41
1:D:180:PHE:O	1:E:30:HIS:N	2.52	0.41
1:D:395:LYS:H	1:D:395:LYS:HG2	1.60	0.41
1:F:327:PHE:O	1:F:329:ALA:N	2.50	0.41
1:A:66:ILE:HA	1:A:88:THR:HG23	2.01	0.41
1:A:339:ASN:ND2	1:A:340:ARG:O	2.53	0.41
1:B:85:VAL:C	1:B:87:VAL:N	2.71	0.41
1:B:462:GLU:OE2	1:E:317:THR:OG1	2.29	0.41
1:E:195:MET:HA	1:E:246:VAL:HG21	2.00	0.41
1:F:233:ALA:HA	1:F:368:PRO:HB2	2.01	0.41
1:B:60:ILE:H	1:B:60:ILE:HG13	1.64	0.41
1:B:182:VAL:C	1:B:184:PRO:HD2	2.40	0.41
1:B:314:ASN:ND2	1:B:362:PRO:HA	2.35	0.41
1:B:315:PRO:HG2	1:B:365:MET:HB3	2.02	0.41
1:B:365:MET:HE1	1:E:466:TYR:HB3	2.00	0.41
1:C:149:HIS:CE1	1:F:463:PHE:HE1	2.38	0.41
1:C:437:LYS:HA	1:C:437:LYS:HD3	1.82	0.41
1:E:366:MET:SD	1:E:371:GLY:HA3	2.60	0.41
1:A:55:ALA:HB2	1:A:101:GLU:H	1.86	0.41
1:A:207:ARG:NH2	1:A:225:SER:O	2.53	0.41
1:A:365:MET:CE	1:D:466:TYR:HB3	2.50	0.41
1:A:463:PHE:CE1	1:D:149:HIS:ND1	2.89	0.41
1:D:327:PHE:HD2	1:D:397:LEU:HD13	1.86	0.41
1:E:239:PHE:O	1:E:243:VAL:HG13	2.21	0.41
1:E:315:PRO:HB2	1:E:447:LYS:HE3	2.03	0.41
1:A:239:PHE:O	1:A:243:VAL:HG13	2.20	0.41
1:A:397:LEU:H	1:A:397:LEU:HG	1.72	0.41
1:A:463:PHE:HB3	1:D:140:TRP:CE3	2.56	0.41
1:B:19:PHE:CG	1:B:66:ILE:HD13	2.55	0.41
1:B:20:ARG:HA	1:B:29:GLN:O	2.21	0.41
1:A:128:PRO:HA	1:A:270:HIS:O	2.21	0.41
1:B:85:VAL:C	1:B:87:VAL:H	2.23	0.41
1:C:2:ALA:O	1:C:6:LEU:HB2	2.20	0.41
1:C:149:HIS:ND1	1:F:463:PHE:CE1	2.89	0.41
1:A:227:ASN:HD22	1:A:227:ASN:HA	1.58	0.41
1:A:303:ILE:HG23	1:A:333:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:HIS:ND1	1:A:327:PHE:O	2.53	0.41
1:C:207:ARG:NH2	1:C:225:SER:O	2.54	0.41
1:C:341:SER:HB3	1:C:397:LEU:HB3	2.03	0.41
1:D:67:LEU:HD22	1:D:67:LEU:HA	1.84	0.41
1:F:20:ARG:HH21	1:F:75:PHE:HE1	1.67	0.41
1:F:120:ILE:HD11	1:F:384:GLN:HE22	1.84	0.41
1:F:357:ILE:HG13	1:F:357:ILE:O	2.21	0.41
1:A:54:ILE:O	1:A:55:ALA:HB3	2.21	0.41
1:B:69:PRO:HB3	1:B:87:VAL:CG1	2.49	0.41
1:B:339:ASN:ND2	1:B:340:ARG:O	2.54	0.41
1:D:51:GLY:H	1:D:60:ILE:HG13	1.85	0.41
1:D:356:ARG:CZ	1:D:356:ARG:HB2	2.50	0.41
1:E:438:GLU:H	1:E:438:GLU:HG3	1.74	0.41
1:F:332:MET:HB2	1:F:341:SER:O	2.21	0.41
1:F:361:PHE:N	1:F:362:PRO:CD	2.84	0.41
1:A:69:PRO:HG2	1:A:72:GLU:CA	2.48	0.41
1:B:110:ARG:HB3	1:B:434:VAL:HA	2.03	0.41
1:C:269:MET:SD	1:C:364:PRO:HA	2.61	0.41
1:E:71:ALA:HB3	1:E:87:VAL:CG2	2.51	0.41
1:F:85:VAL:C	1:F:87:VAL:H	2.24	0.41
1:F:182:VAL:C	1:F:184:PRO:HD2	2.41	0.41
1:F:296:LEU:HD13	1:F:296:LEU:HA	1.87	0.41
1:A:336:SER:CB	1:A:394:ASP:HB3	2.51	0.40
1:B:361:PHE:N	1:B:362:PRO:CD	2.84	0.40
1:B:463:PHE:CE1	1:E:149:HIS:ND1	2.89	0.40
1:C:85:VAL:C	1:C:87:VAL:H	2.24	0.40
1:D:69:PRO:CG	1:D:87:VAL:HG22	2.51	0.40
1:D:156:ALA:O	1:D:172:ARG:HD3	2.21	0.40
1:E:296:LEU:HD12	1:E:389:PRO:HG3	2.02	0.40
1:A:143:ASP:OD1	1:A:143:ASP:N	2.55	0.40
1:B:230:VAL:HG12	1:B:231:ARG:N	2.36	0.40
1:B:239:PHE:O	1:B:240:LYS:C	2.59	0.40
1:C:143:ASP:HB2	1:C:145:SER:H	1.87	0.40
1:C:396:ASN:HD22	1:C:396:ASN:HA	1.71	0.40
1:B:86:VAL:HG11	1:B:238:GLN:HG3	2.02	0.40
1:D:111:ALA:HB2	1:D:434:VAL:CG1	2.50	0.40
1:E:14:ALA:CB	1:E:83:PRO:HD3	2.51	0.40
1:B:156:ALA:O	1:B:172:ARG:HD3	2.21	0.40
1:D:143:ASP:OD1	1:D:148:ARG:NH2	2.54	0.40
1:A:361:PHE:N	1:A:362:PRO:CD	2.84	0.40
1:B:90:ASP:OD2	1:B:103:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LYS:HD2	1:C:58:LYS:HA	1.64	0.40
1:D:107:ILE:HA	1:D:110:ARG:HD2	2.03	0.40
1:D:143:ASP:OD1	1:D:143:ASP:N	2.54	0.40
1:F:229:LEU:HD23	1:F:230:VAL:N	2.34	0.40
1:F:305:HIS:O	1:F:307:ARG:N	2.54	0.40
1:F:400:LEU:HA	1:F:401:PRO:HD3	1.93	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:A:163:ASP:OD1	1:D:139:LYS:HZ2[8_554]	1.57	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/468 (100%)	421 (90%)	39 (8%)	6 (1%)	10	33
1	B	466/468 (100%)	412 (88%)	36 (8%)	18 (4%)	2	15
1	C	466/468 (100%)	410 (88%)	43 (9%)	13 (3%)	4	20
1	D	466/468 (100%)	423 (91%)	37 (8%)	6 (1%)	10	33
1	E	466/468 (100%)	417 (90%)	36 (8%)	13 (3%)	4	20
1	F	466/468 (100%)	422 (91%)	35 (8%)	9 (2%)	6	26
All	All	2796/2808 (100%)	2505 (90%)	226 (8%)	65 (2%)	5	23

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	SER
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	288	TYR
1	C	96	THR
1	C	101	GLU
1	C	180	PHE
1	C	185	VAL
1	D	77	ASP
1	D	95	SER
1	D	404	GLU
1	D	411	VAL
1	E	95	SER
1	E	96	THR
1	E	230	VAL
1	F	402	PRO
1	A	95	SER
1	A	397	LEU
1	B	55	ALA
1	B	70	ASP
1	B	207	ARG
1	B	230	VAL
1	C	95	SER
1	C	397	LEU
1	E	53	SER
1	E	94	PRO
1	E	180	PHE
1	E	189	GLN
1	E	351	ASN
1	F	14	ALA
1	F	219	GLN
1	F	306	ALA
1	F	311	ALA
1	A	325	PRO
1	B	231	ARG
1	B	325	PRO
1	B	350	SER
1	C	69	PRO
1	C	75	PHE
1	A	71	ALA
1	B	71	ALA
1	B	202	ILE
1	B	205	PRO
1	C	68	ARG
1	C	313	THR

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Mol	Chain	Res	Type
1	E	68	ARG
1	E	325	PRO
1	E	399	ASP
1	B	75	PHE
1	B	179	TYR
1	B	206	GLY
1	C	94	PRO
1	C	312	ILE
1	C	325	PRO
1	D	180	PHE
1	E	75	PHE
1	E	397	LEU
1	F	80	PHE
1	F	325	PRO
1	A	68	ARG
1	B	68	ARG
1	B	259	LYS
1	A	76	ILE
1	D	97	GLY
1	F	94	PRO
1	F	259	LYS

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	381/387 (98%)	316 (83%)	65 (17%)	1	6
1	B	381/387 (98%)	308 (81%)	73 (19%)	1	3
1	C	381/387 (98%)	306 (80%)	75 (20%)	1	3
1	D	381/387 (98%)	327 (86%)	54 (14%)	2	11
1	E	380/387 (98%)	312 (82%)	68 (18%)	1	5
1	F	381/387 (98%)	300 (79%)	81 (21%)	1	2
All	All	2285/2322 (98%)	1869 (82%)	416 (18%)	1	5

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	GLN
1	A	15	LYS
1	A	24	THR
1	A	27	LYS
1	A	30	HIS
1	A	36	ASP
1	A	42	THR
1	A	53	SER
1	A	54	ILE
1	A	57	TRP
1	A	61	GLU
1	A	64	ASP
1	A	65	MET
1	A	67	LEU
1	A	73	THR
1	A	75	PHE
1	A	84	THR
1	A	90	ASP
1	A	98	GLN
1	A	107	ILE
1	A	109	ARG
1	A	117	SER
1	A	143	ASP
1	A	165	GLU
1	A	172	ARG
1	A	174	ARG
1	A	176	LYS
1	A	179	TYR
1	A	183	PRO
1	A	198	LYS
1	A	215	VAL
1	A	227	ASN
1	A	228	THR
1	A	231	ARG
1	A	232	LYS
1	A	243	VAL
1	A	253	THR
1	A	261	MET
1	A	275	ILE
1	A	277	LYS
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	286	ASP
1	A	287	GLU
1	A	294	MET
1	A	296	LEU
1	A	309	LEU
1	A	318	ASN
1	A	321	LYS
1	A	327	PHE
1	A	338	ARG
1	A	340	ARG
1	A	363	ASP
1	A	395	LYS
1	A	397	LEU
1	A	407	LYS
1	A	411	VAL
1	A	426	HIS
1	A	429	LEU
1	A	436	THR
1	A	439	MET
1	A	448	THR
1	A	461	VAL
1	A	468	SER
1	B	6	LEU
1	B	11	GLU
1	B	15	LYS
1	B	25	LYS
1	B	27	LYS
1	B	39	ASP
1	B	42	THR
1	B	45	ASP
1	B	48	MET
1	B	53	SER
1	B	54	ILE
1	B	58	LYS
1	B	60	ILE
1	B	67	LEU
1	B	68	ARG
1	B	73	THR
1	B	75	PHE
1	B	84	THR
1	B	90	ASP

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Mol	Chain	Res	Type
1	B	93	GLU
1	B	98	GLN
1	B	116	LYS
1	B	117	SER
1	B	122	ASP
1	B	172	ARG
1	B	174	ARG
1	B	176	LYS
1	B	179	TYR
1	B	183	PRO
1	B	185	VAL
1	B	189	GLN
1	B	198	LYS
1	B	200	GLU
1	B	207	ARG
1	B	215	VAL
1	B	228	THR
1	B	232	LYS
1	B	234	ASP
1	B	235	GLU
1	B	252	LYS
1	B	253	THR
1	B	274	SER
1	B	277	LYS
1	B	280	LYS
1	B	282	LEU
1	B	296	LEU
1	B	304	LYS
1	B	309	LEU
1	B	318	ASN
1	B	328	GLU
1	B	338	ARG
1	B	340	ARG
1	B	350	SER
1	B	351	ASN
1	B	353	LYS
1	B	363	ASP
1	B	365	MET
1	B	395	LYS
1	B	397	LEU
1	B	398	TYR
1	B	399	ASP

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Mol	Chain	Res	Type
1	B	400	LEU
1	B	404	GLU
1	B	405	GLU
1	B	407	LYS
1	B	411	VAL
1	B	420	GLU
1	B	426	HIS
1	B	438	GLU
1	B	439	MET
1	B	445	GLU
1	B	461	VAL
1	B	469	LEU
1	C	3	ASN
1	C	7	GLN
1	C	15	LYS
1	C	24	THR
1	C	25	LYS
1	C	27	LYS
1	C	39	ASP
1	C	41	ASP
1	C	45	ASP
1	C	48	MET
1	C	54	ILE
1	C	58	LYS
1	C	65	MET
1	C	67	LEU
1	C	73	THR
1	C	75	PHE
1	C	78	PRO
1	C	84	THR
1	C	85	VAL
1	C	90	ASP
1	C	105	ARG
1	C	107	ILE
1	C	122	ASP
1	C	165	GLU
1	C	172	ARG
1	C	174	ARG
1	C	176	LYS
1	C	179	TYR
1	C	183	PRO
1	C	189	GLN

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Mol	Chain	Res	Type
1	C	198	LYS
1	C	207	ARG
1	C	211	HIS
1	C	215	VAL
1	C	226	PHE
1	C	228	THR
1	C	231	ARG
1	C	232	LYS
1	C	245	ASN
1	C	255	THR
1	C	257	MET
1	C	274	SER
1	C	278	ASP
1	C	280	LYS
1	C	282	LEU
1	C	286	ASP
1	C	296	LEU
1	C	312	ILE
1	C	314	ASN
1	C	327	PHE
1	C	328	GLU
1	C	338	ARG
1	C	341	SER
1	C	345	ARG
1	C	349	VAL
1	C	355	LYS
1	C	363	ASP
1	C	365	MET
1	C	395	LYS
1	C	396	ASN
1	C	397	LEU
1	C	399	ASP
1	C	400	LEU
1	C	404	GLU
1	C	407	LYS
1	C	411	VAL
1	C	426	HIS
1	C	436	THR
1	C	437	LYS
1	C	439	MET
1	C	445	GLU
1	C	446	LEU

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Mol	Chain	Res	Type
1	C	461	VAL
1	C	465	MET
1	C	468	SER
1	D	15	LYS
1	D	24	THR
1	D	27	LYS
1	D	39	ASP
1	D	41	ASP
1	D	45	ASP
1	D	50	ASP
1	D	58	LYS
1	D	60	ILE
1	D	65	MET
1	D	67	LEU
1	D	68	ARG
1	D	84	THR
1	D	109	ARG
1	D	117	SER
1	D	120	ILE
1	D	143	ASP
1	D	163	ASP
1	D	165	GLU
1	D	166	SER
1	D	172	ARG
1	D	174	ARG
1	D	179	TYR
1	D	183	PRO
1	D	187	SER
1	D	189	GLN
1	D	198	LYS
1	D	215	VAL
1	D	231	ARG
1	D	232	LYS
1	D	243	VAL
1	D	277	LYS
1	D	280	LYS
1	D	282	LEU
1	D	286	ASP
1	D	296	LEU
1	D	323	LEU
1	D	327	PHE
1	D	328	GLU

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Mol	Chain	Res	Type
1	D	338	ARG
1	D	340	ARG
1	D	351	ASN
1	D	355	LYS
1	D	356	ARG
1	D	391	GLU
1	D	395	LYS
1	D	397	LEU
1	D	400	LEU
1	D	407	LYS
1	D	423	GLN
1	D	426	HIS
1	D	439	MET
1	D	452	ARG
1	D	461	VAL
1	E	7	GLN
1	E	15	LYS
1	E	17	VAL
1	E	23	ASP
1	E	36	ASP
1	E	39	ASP
1	E	41	ASP
1	E	42	THR
1	E	44	GLU
1	E	48	MET
1	E	67	LEU
1	E	68	ARG
1	E	70	ASP
1	E	73	THR
1	E	75	PHE
1	E	77	ASP
1	E	85	VAL
1	E	87	VAL
1	E	95	SER
1	E	98	GLN
1	E	105	ARG
1	E	122	ASP
1	E	143	ASP
1	E	165	GLU
1	E	166	SER
1	E	172	ARG
1	E	176	LYS

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Mol	Chain	Res	Type
1	E	179	TYR
1	E	183	PRO
1	E	185	VAL
1	E	198	LYS
1	E	203	MET
1	E	207	ARG
1	E	215	VAL
1	E	228	THR
1	E	229	LEU
1	E	231	ARG
1	E	232	LYS
1	E	234	ASP
1	E	243	VAL
1	E	278	ASP
1	E	280	LYS
1	E	282	LEU
1	E	286	ASP
1	E	293	GLU
1	E	294	MET
1	E	296	LEU
1	E	309	LEU
1	E	323	LEU
1	E	327	PHE
1	E	338	ARG
1	E	353	LYS
1	E	355	LYS
1	E	356	ARG
1	E	395	LYS
1	E	397	LEU
1	E	398	TYR
1	E	400	LEU
1	E	404	GLU
1	E	407	LYS
1	E	411	VAL
1	E	426	HIS
1	E	431	LYS
1	E	438	GLU
1	E	439	MET
1	E	445	GLU
1	E	446	LEU
1	E	461	VAL
1	F	5	VAL

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Mol	Chain	Res	Type
1	F	6	LEU
1	F	7	GLN
1	F	15	LYS
1	F	23	ASP
1	F	27	LYS
1	F	36	ASP
1	F	39	ASP
1	F	41	ASP
1	F	44	GLU
1	F	50	ASP
1	F	54	ILE
1	F	58	LYS
1	F	61	GLU
1	F	68	ARG
1	F	72	GLU
1	F	73	THR
1	F	75	PHE
1	F	79	PHE
1	F	80	PHE
1	F	84	THR
1	F	85	VAL
1	F	92	ILE
1	F	95	SER
1	F	98	GLN
1	F	107	ILE
1	F	115	LEU
1	F	122	ASP
1	F	166	SER
1	F	172	ARG
1	F	174	ARG
1	F	179	TYR
1	F	183	PRO
1	F	185	VAL
1	F	198	LYS
1	F	207	ARG
1	F	215	VAL
1	F	217	SER
1	F	221	GLU
1	F	225	SER
1	F	231	ARG
1	F	232	LYS
1	F	243	VAL

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Mol	Chain	Res	Type
1	F	260	PRO
1	F	273	MET
1	F	274	SER
1	F	278	ASP
1	F	282	LEU
1	F	294	MET
1	F	296	LEU
1	F	309	LEU
1	F	312	ILE
1	F	324	VAL
1	F	327	PHE
1	F	333	LEU
1	F	338	ARG
1	F	344	ILE
1	F	350	SER
1	F	353	LYS
1	F	355	LYS
1	F	363	ASP
1	F	375	LEU
1	F	376	LEU
1	F	384	GLN
1	F	395	LYS
1	F	397	LEU
1	F	398	TYR
1	F	399	ASP
1	F	400	LEU
1	F	407	LYS
1	F	411	VAL
1	F	416	ASP
1	F	423	GLN
1	F	426	HIS
1	F	429	LEU
1	F	438	GLU
1	F	439	MET
1	F	445	GLU
1	F	452	ARG
1	F	461	VAL
1	F	465	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	227	ASN
1	A	339	ASN
1	A	455	ASN
1	B	7	GLN
1	B	149	HIS
1	B	189	GLN
1	B	249	GLN
1	B	272	HIS
1	B	396	ASN
1	C	3	ASN
1	C	189	GLN
1	C	212	HIS
1	C	249	GLN
1	C	318	ASN
1	C	339	ASN
1	C	396	ASN
1	D	270	HIS
1	D	326	HIS
1	D	339	ASN
1	D	384	GLN
1	D	423	GLN
1	E	10	GLN
1	E	30	HIS
1	E	149	HIS
1	F	326	HIS
1	F	339	ASN
1	F	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	501	-	5,5,5	0.19	0	5,5,5	0.66	0
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.36	0
5	EDO	F	501	-	3,3,3	0.42	0	2,2,2	0.54	0
3	GOL	C	501	-	5,5,5	0.25	0	5,5,5	0.47	0
2	PGE	A	501	-	9,9,9	0.26	0	8,8,8	0.21	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.31	0
3	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.41	0
3	GOL	B	501	-	5,5,5	0.21	0	5,5,5	0.65	0
3	GOL	E	501	-	5,5,5	0.16	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
5	EDO	F	501	-	-	1/1/1/1	-
3	GOL	C	501	-	-	2/4/4/4	-
2	PGE	A	501	-	-	4/7/7/7	-
3	GOL	B	502	-	-	3/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	B	501	-	-	2/4/4/4	-
3	GOL	E	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

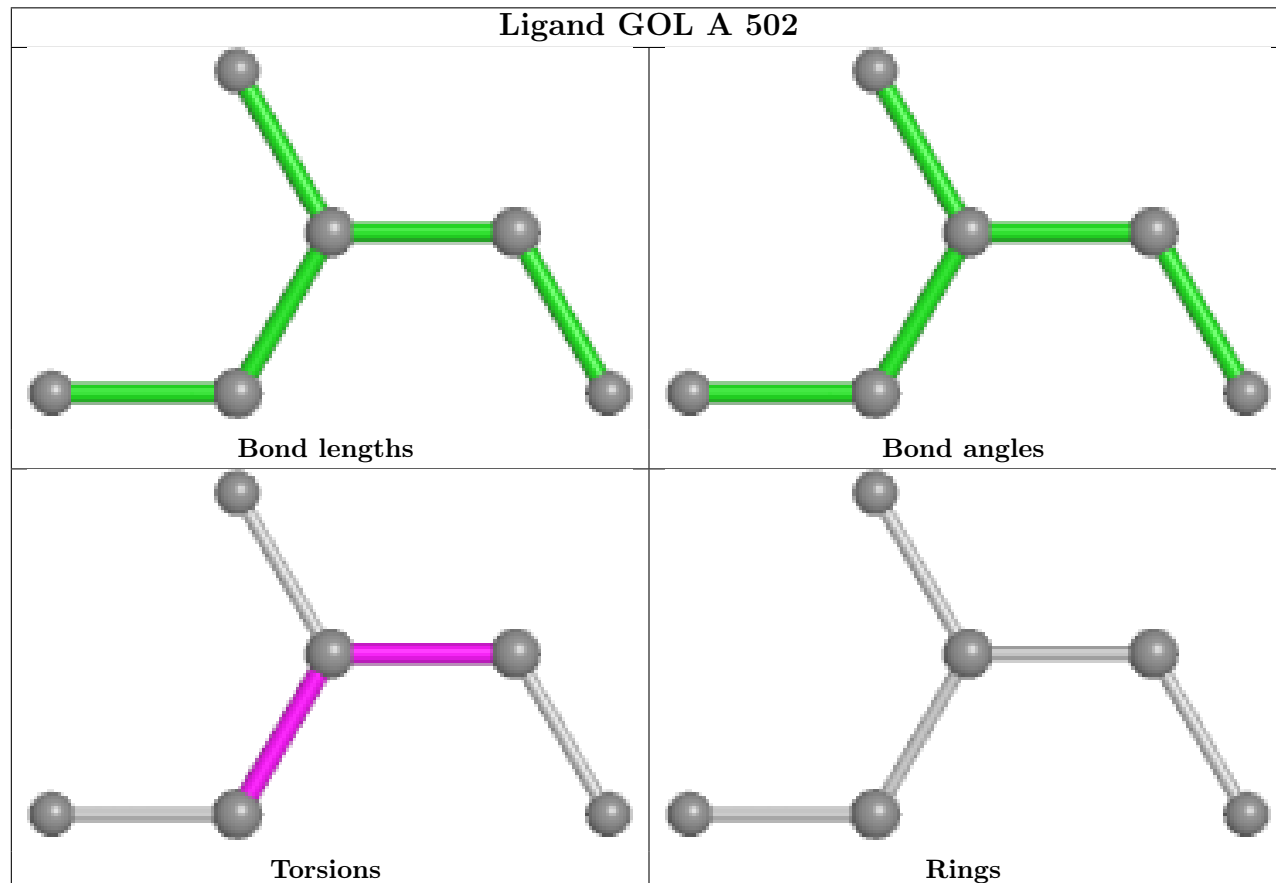
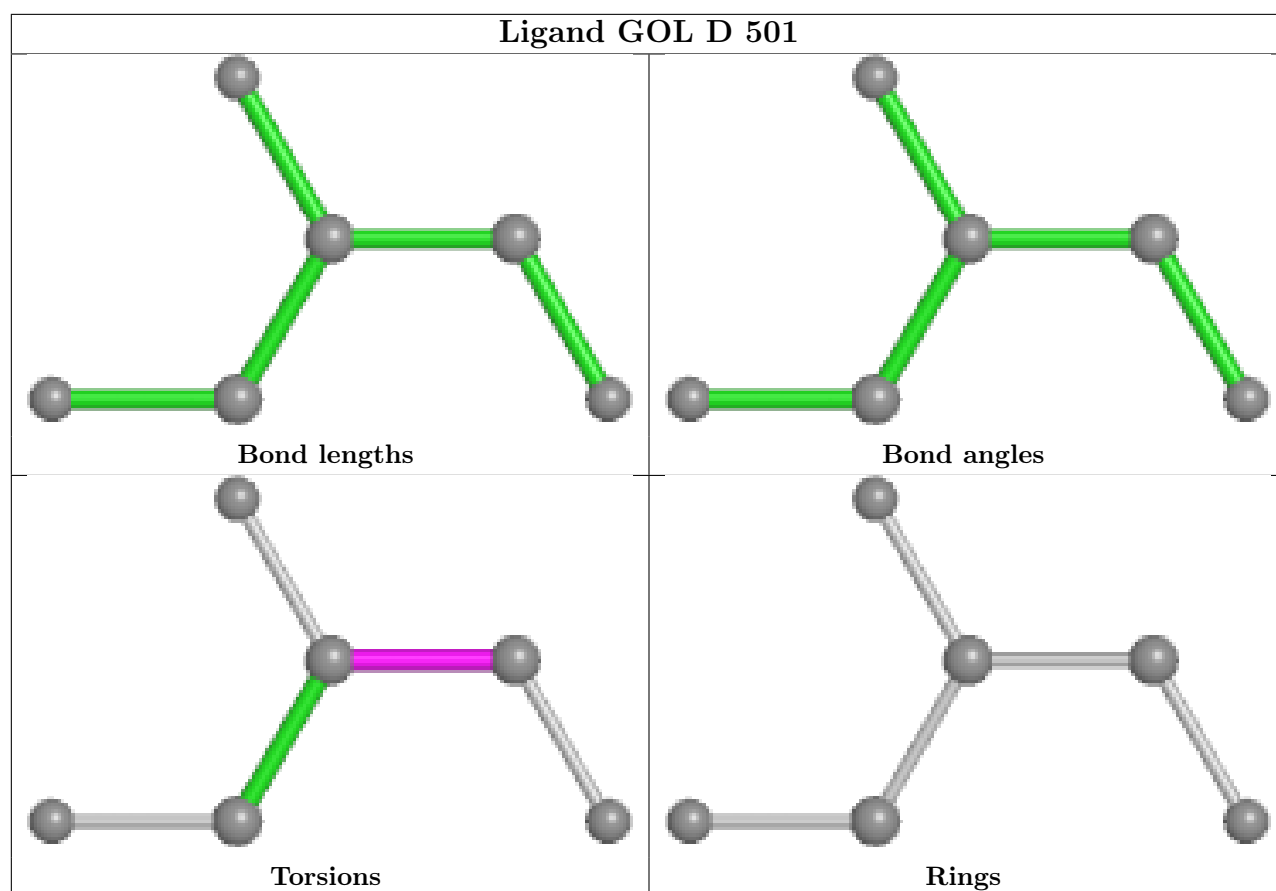
All (22) torsion outliers are listed below:

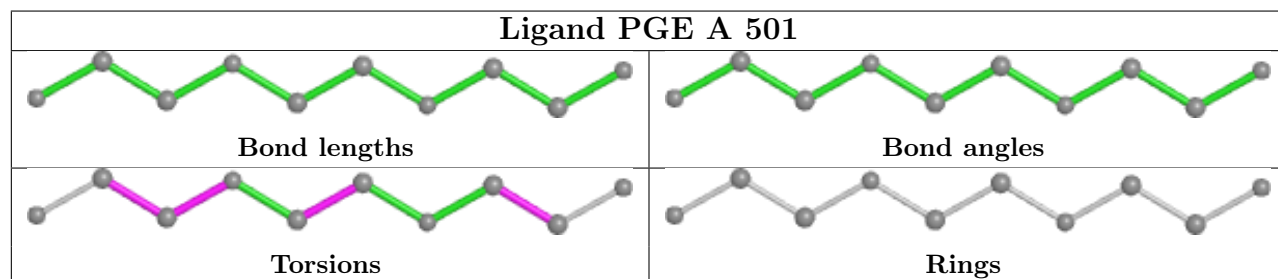
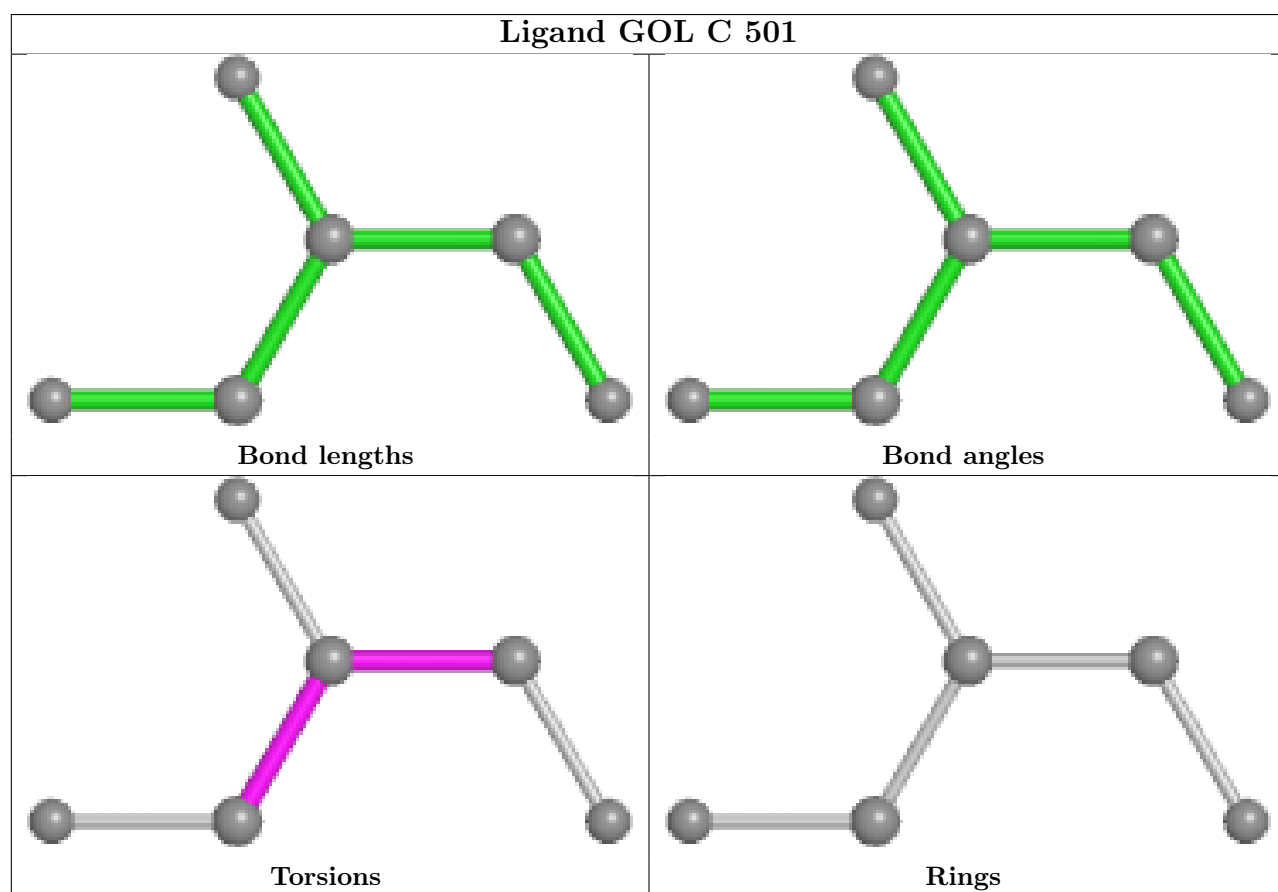
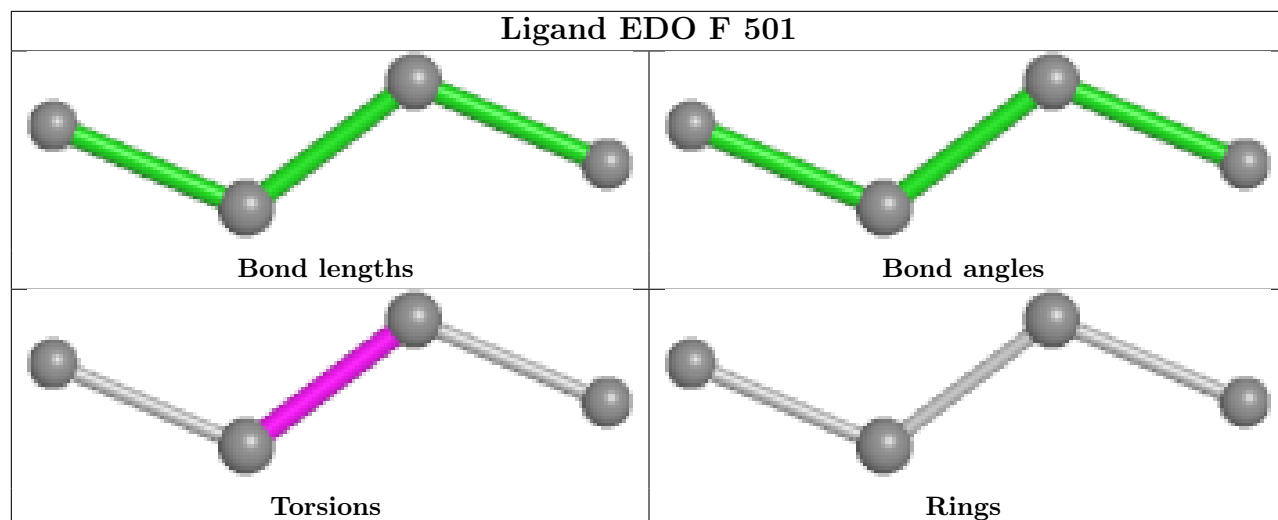
Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	B	501	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	D	501	GOL	O1-C1-C2-O2
3	D	501	GOL	O1-C1-C2-C3
2	A	501	PGE	O2-C3-C4-O3
2	A	501	PGE	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	C	501	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
2	A	501	PGE	O3-C5-C6-O4
3	A	502	GOL	O1-C1-C2-O2
5	F	501	EDO	O1-C1-C2-O2
2	A	501	PGE	C6-C5-O3-C4
3	B	502	GOL	C1-C2-C3-O3
3	C	501	GOL	C1-C2-C3-O3

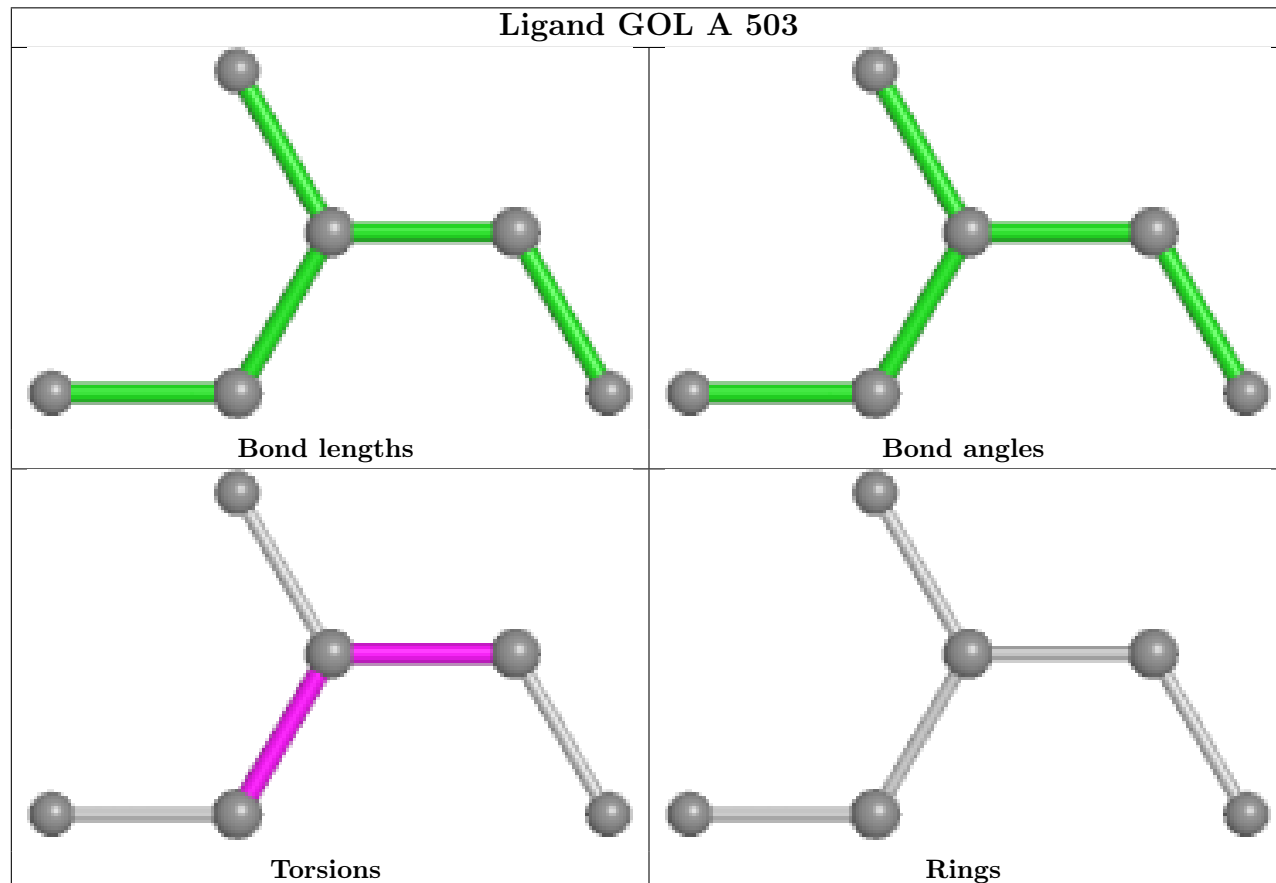
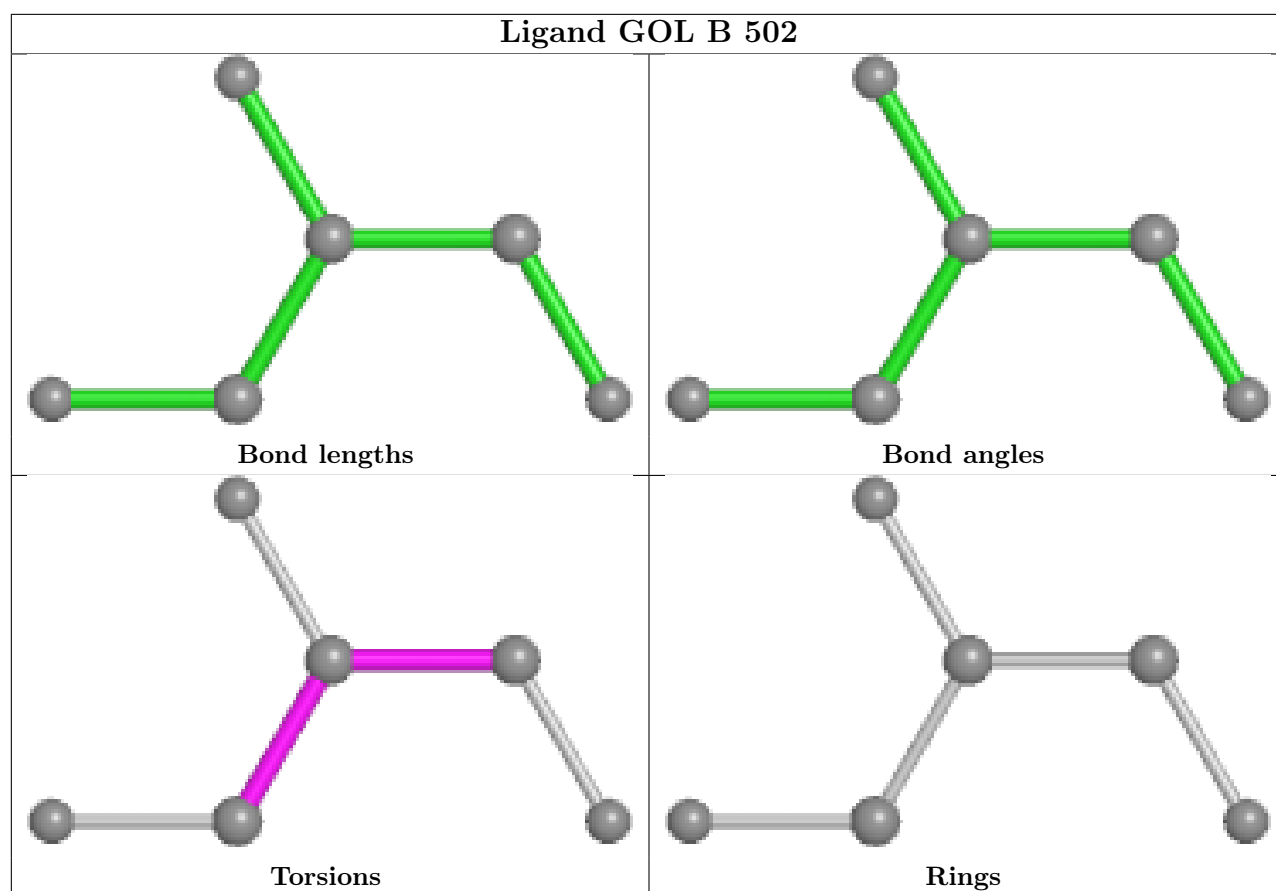
There are no ring outliers.

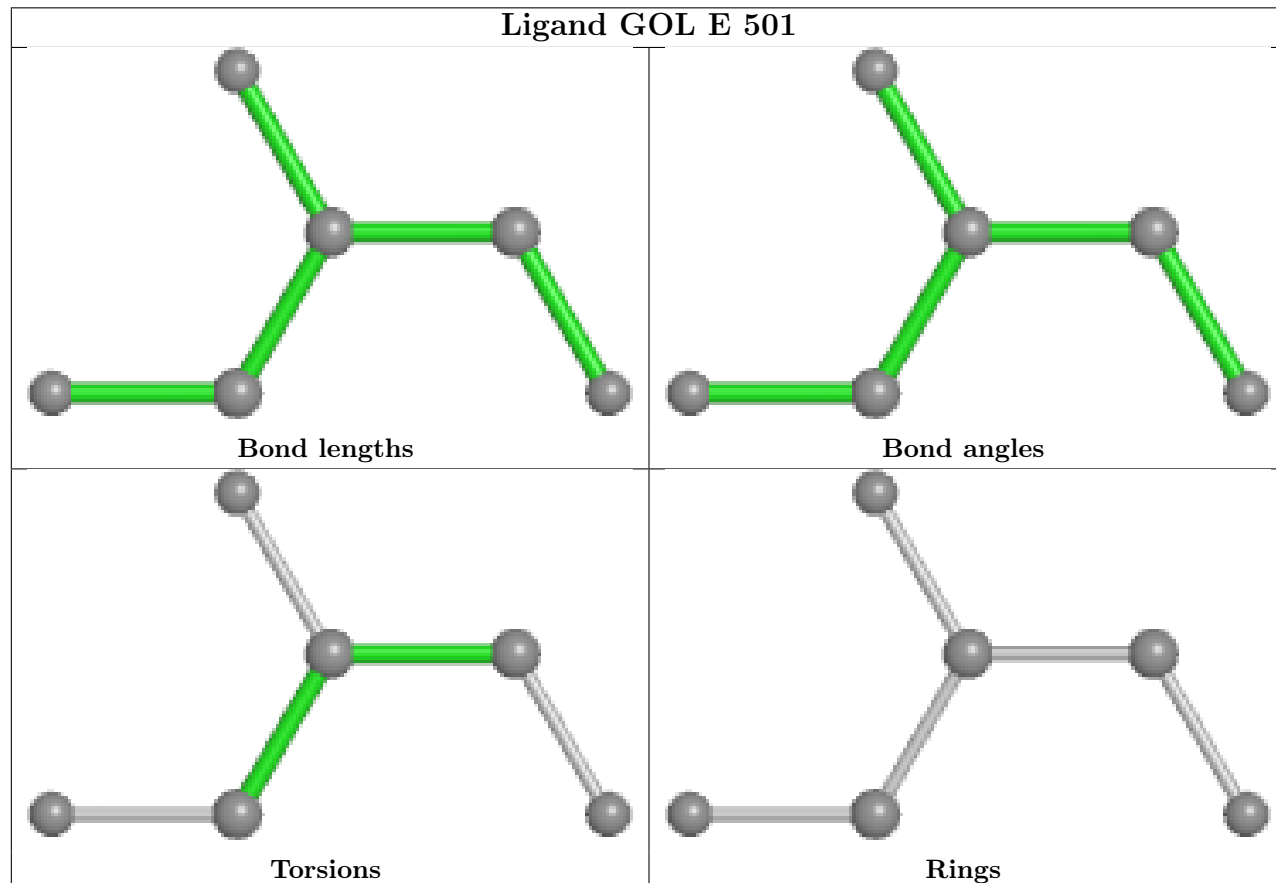
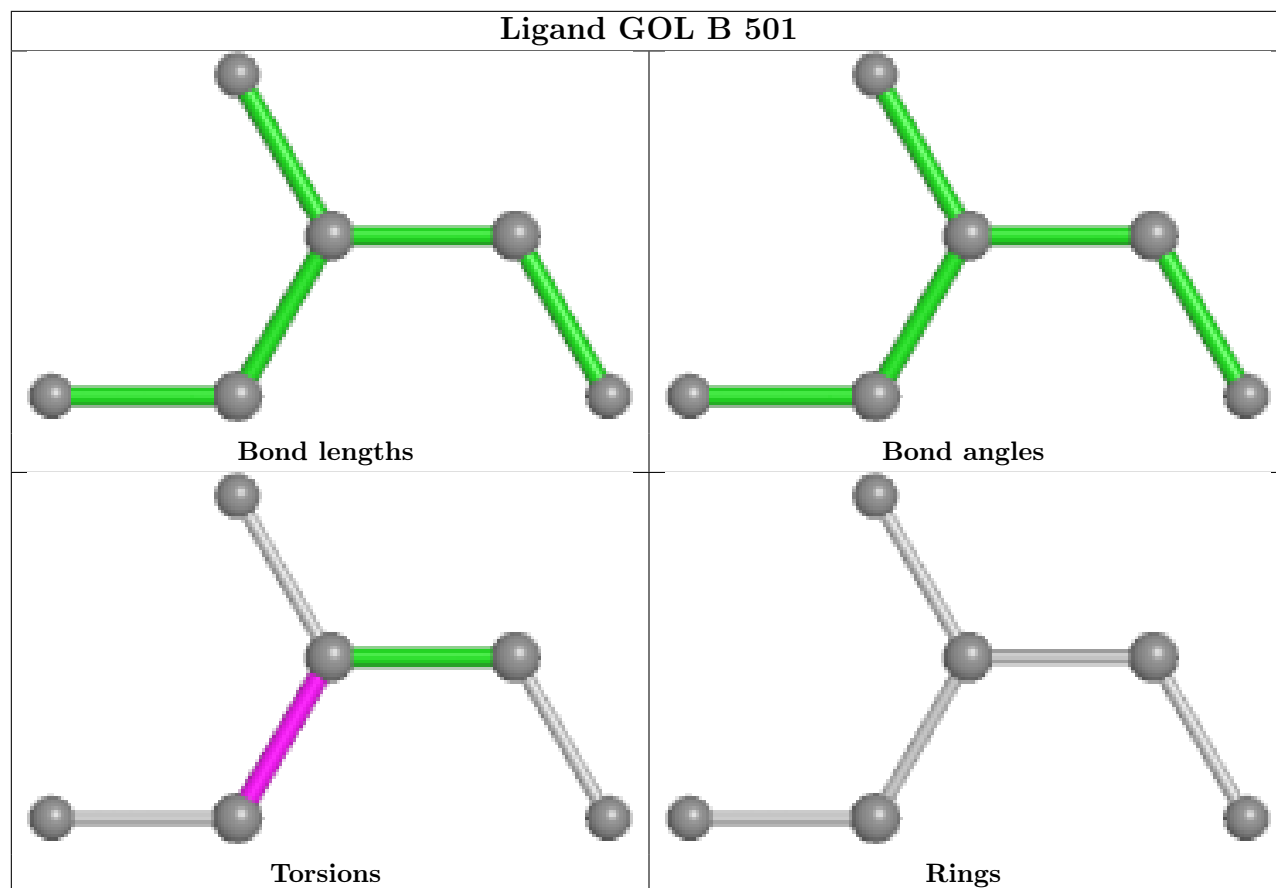
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	468/468 (100%)	0.03	16 (3%)	48	41	31, 70, 148, 235	0
1	B	468/468 (100%)	0.15	17 (3%)	46	39	38, 89, 156, 222	0
1	C	468/468 (100%)	0.30	19 (4%)	42	36	57, 102, 163, 265	0
1	D	468/468 (100%)	0.36	28 (5%)	29	27	41, 103, 183, 239	0
1	E	468/468 (100%)	0.60	25 (5%)	33	29	56, 141, 197, 248	0
1	F	468/468 (100%)	0.62	34 (7%)	22	22	65, 138, 214, 307	0
All	All	2808/2808 (100%)	0.34	139 (4%)	35	31	31, 104, 195, 307	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	VAL	6.4
1	F	100	TYR	6.1
1	F	60	ILE	5.2
1	A	54	ILE	5.1
1	B	100	TYR	5.0
1	E	100	TYR	5.0
1	A	100	TYR	4.9
1	D	100	TYR	4.5
1	C	86	VAL	4.3
1	E	90	ASP	4.3
1	F	62	ALA	4.2
1	F	86	VAL	4.1
1	D	75	PHE	4.1
1	A	86	VAL	4.0
1	C	80	PHE	4.0
1	A	70	ASP	4.0
1	F	79	PHE	4.0
1	C	64	ASP	3.9
1	B	99	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	3.9
1	A	327	PHE	3.8
1	B	398	TYR	3.8
1	B	86	VAL	3.8
1	D	80	PHE	3.6
1	A	398	TYR	3.6
1	F	327	PHE	3.6
1	E	86	VAL	3.5
1	F	295	ALA	3.5
1	B	71	ALA	3.5
1	F	361	PHE	3.5
1	B	327	PHE	3.5
1	C	60	ILE	3.4
1	D	70	ASP	3.4
1	B	80	PHE	3.3
1	F	54	ILE	3.3
1	C	54	ILE	3.2
1	A	93	GLU	3.2
1	E	60	ILE	3.1
1	D	78	PRO	3.1
1	D	54	ILE	3.1
1	F	224	VAL	3.1
1	D	79	PHE	3.1
1	D	74	GLY	3.0
1	A	80	PHE	3.0
1	F	101	GLU	2.9
1	C	79	PHE	2.9
1	D	178	GLY	2.9
1	A	79	PHE	2.9
1	E	396	ASN	2.9
1	F	293	GLU	2.8
1	C	327	PHE	2.8
1	B	183	PRO	2.8
1	C	393	ALA	2.8
1	A	99	GLY	2.8
1	F	372	PHE	2.8
1	F	375	LEU	2.8
1	D	326	HIS	2.8
1	E	54	ILE	2.8
1	E	55	ALA	2.8
1	D	356	ARG	2.7
1	F	328	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	398	TYR	2.6
1	F	47	LYS	2.6
1	F	273	MET	2.6
1	C	326	HIS	2.6
1	E	335	TYR	2.6
1	E	82	GLU	2.6
1	B	54	ILE	2.6
1	F	331	ILE	2.6
1	D	183	PRO	2.6
1	D	71	ALA	2.5
1	E	65	MET	2.5
1	E	51	GLY	2.5
1	D	90	ASP	2.5
1	F	333	LEU	2.5
1	F	115	LEU	2.5
1	F	398	TYR	2.5
1	E	79	PHE	2.4
1	B	332	MET	2.4
1	D	55	ALA	2.4
1	D	69	PRO	2.4
1	D	312	ILE	2.4
1	E	397	LEU	2.4
1	C	59	GLY	2.4
1	D	99	GLY	2.4
1	A	183	PRO	2.4
1	E	327	PHE	2.4
1	C	87	VAL	2.4
1	E	64	ASP	2.4
1	F	90	ASP	2.4
1	A	75	PHE	2.4
1	C	75	PHE	2.4
1	E	393	ALA	2.4
1	B	75	PHE	2.4
1	D	101	GLU	2.4
1	F	71	ALA	2.3
1	F	434	VAL	2.3
1	E	70	ASP	2.3
1	A	328	GLU	2.3
1	B	93	GLU	2.3
1	D	357	ILE	2.3
1	E	102	ARG	2.3
1	E	282	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	73	THR	2.2
1	D	398	TYR	2.2
1	B	400	LEU	2.2
1	F	74	GLY	2.2
1	C	72	GLU	2.2
1	E	92	ILE	2.2
1	F	404	GLU	2.2
1	F	435	PHE	2.2
1	A	101	GLU	2.2
1	A	340	ARG	2.2
1	D	83	PRO	2.2
1	F	64	ASP	2.2
1	E	62	ALA	2.2
1	F	81	ALA	2.2
1	D	53	SER	2.2
1	E	143	ASP	2.2
1	A	71	ALA	2.1
1	C	81	ALA	2.1
1	B	341	SER	2.1
1	D	400	LEU	2.1
1	B	90	ASP	2.1
1	B	161	GLY	2.1
1	C	51	GLY	2.1
1	D	429	LEU	2.1
1	C	210	VAL	2.1
1	C	224	VAL	2.1
1	E	334	ALA	2.1
1	F	28	GLU	2.1
1	D	393	ALA	2.1
1	E	20	ARG	2.1
1	F	410	THR	2.1
1	F	94	PRO	2.0
1	E	72	GLU	2.0
1	F	16	TRP	2.0
1	F	126	PHE	2.0
1	B	87	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

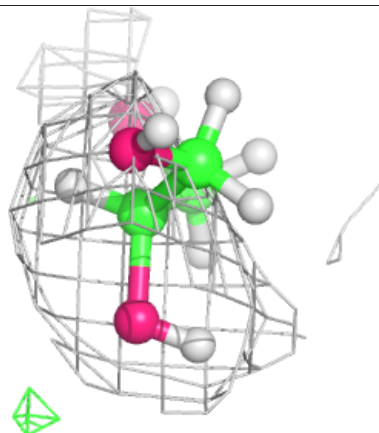
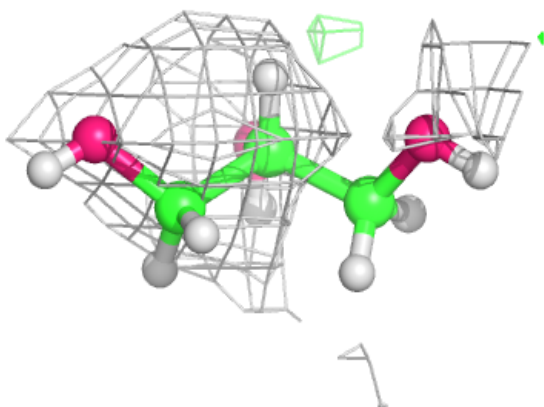
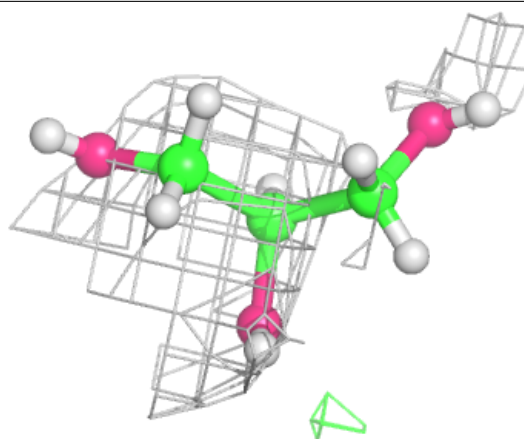
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	502	6/6	0.57	0.17	30,170,175,179	3
3	GOL	C	501	6/6	0.60	0.16	30,130,137,137	3
4	MG	E	503	1/1	0.61	0.22	114,114,114,114	0
3	GOL	B	501	6/6	0.62	0.16	30,118,125,126	3
3	GOL	A	502	6/6	0.73	0.17	30,140,145,146	3
4	MG	E	502	1/1	0.84	0.19	66,66,66,66	0
5	EDO	F	501	4/4	0.85	0.20	30,96,98,99	2
3	GOL	E	501	6/6	0.86	0.13	30,122,131,133	3
3	GOL	D	501	6/6	0.86	0.13	30,103,107,111	3
3	GOL	A	503	6/6	0.89	0.14	30,89,92,92	3
4	MG	B	504	1/1	0.90	0.10	67,67,67,67	0
2	PGE	A	501	10/10	0.90	0.14	30,105,114,114	2
4	MG	D	502	1/1	0.94	0.10	68,68,68,68	0
4	MG	A	505	1/1	0.94	0.12	39,39,39,39	0
4	MG	A	504	1/1	0.95	0.13	49,49,49,49	0
4	MG	F	502	1/1	0.96	0.18	62,62,62,62	0
4	MG	C	502	1/1	0.96	0.16	37,37,37,37	0
4	MG	F	503	1/1	0.97	0.09	68,68,68,68	0
4	MG	D	503	1/1	0.98	0.05	58,58,58,58	0
4	MG	C	503	1/1	0.98	0.05	57,57,57,57	0
4	MG	B	503	1/1	0.98	0.07	41,41,41,41	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.

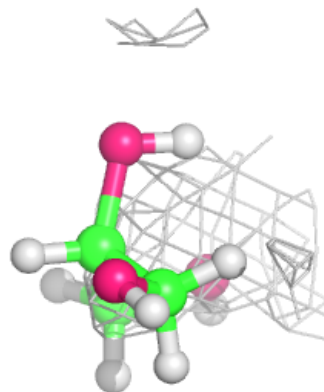
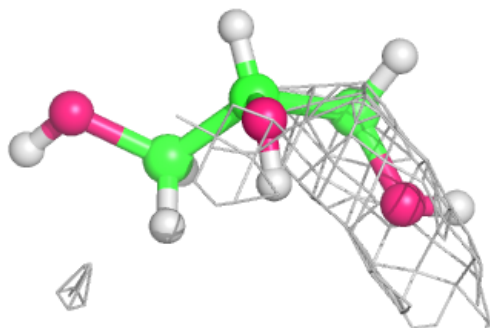
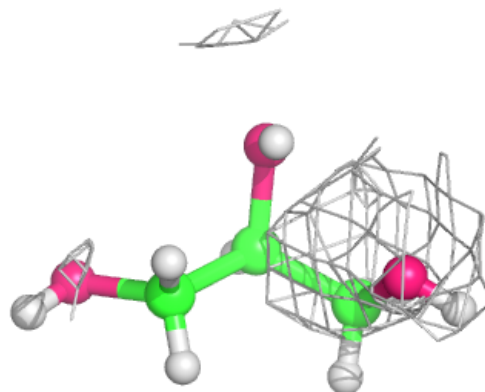
Electron density around GOL B 502:

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



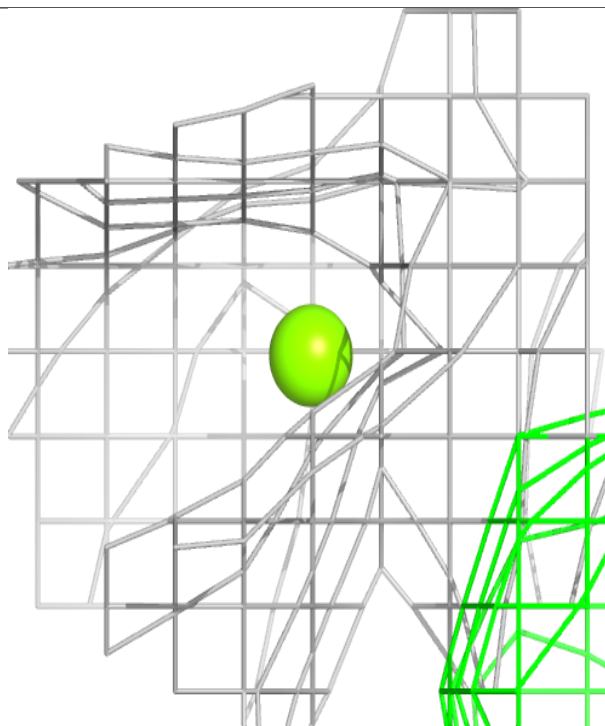
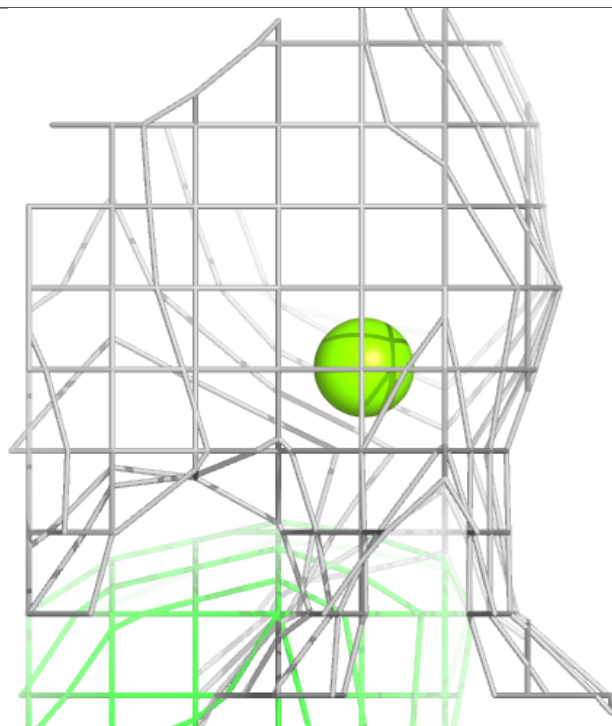
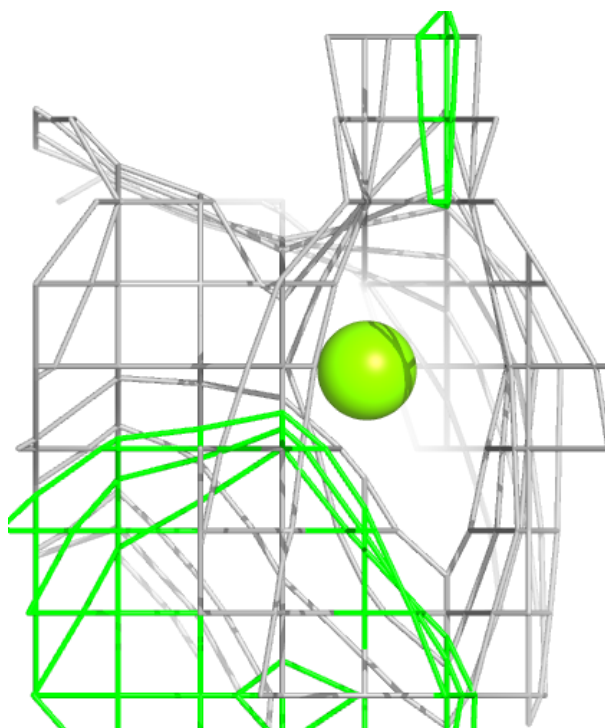
Electron density around GOL C 501:

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



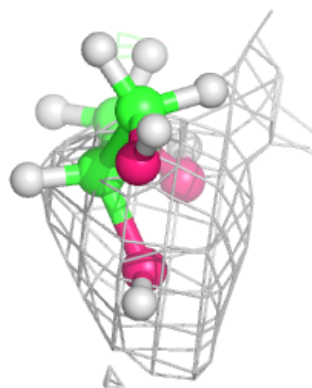
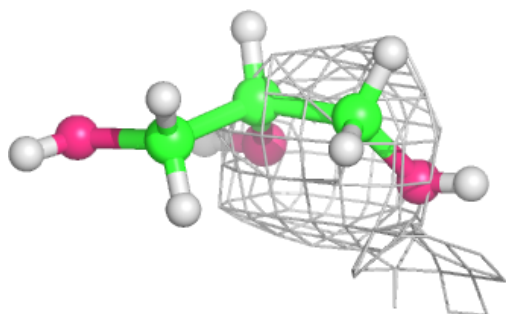
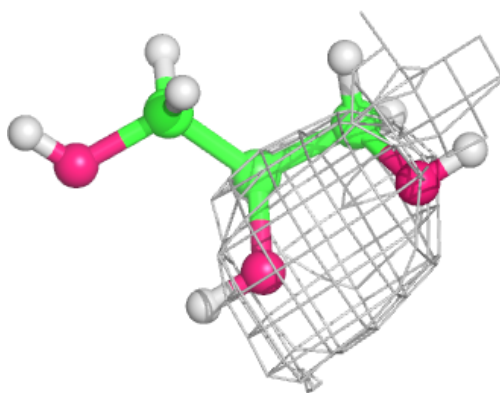
Electron density around MG E 503:

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



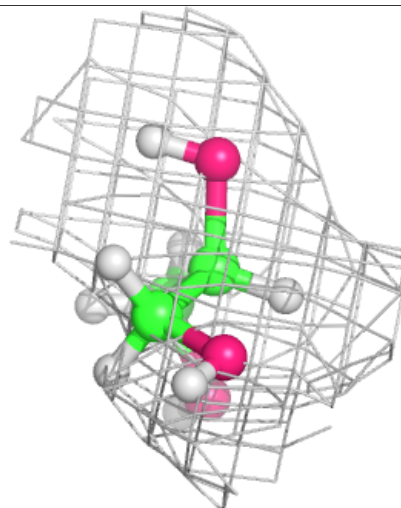
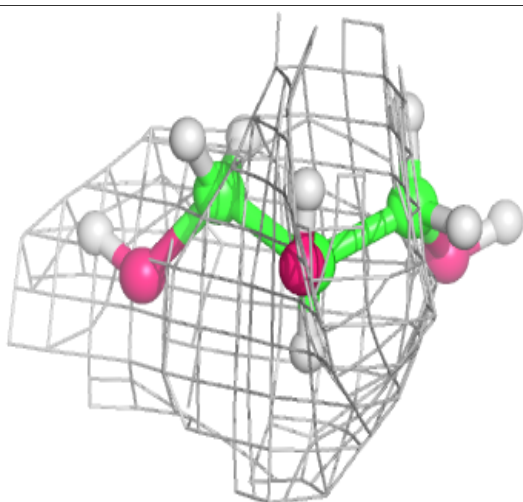
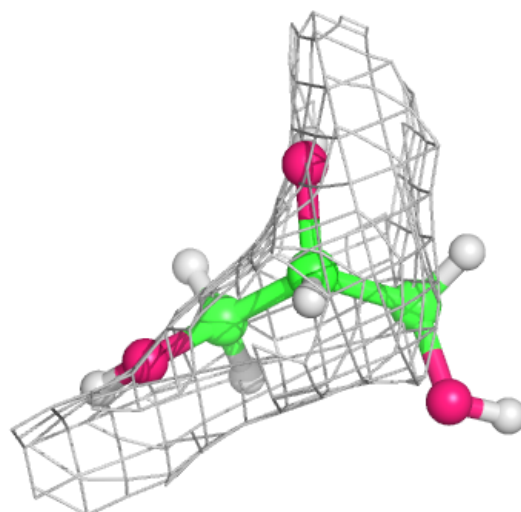
Electron density around GOL B 501:

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



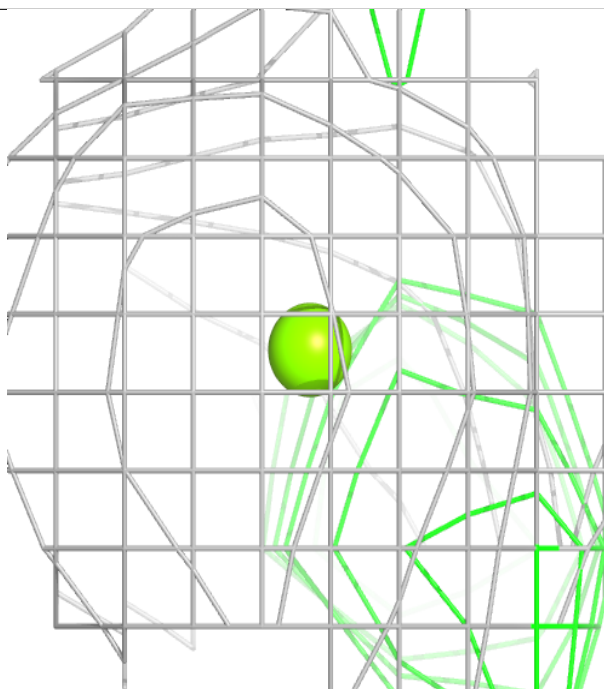
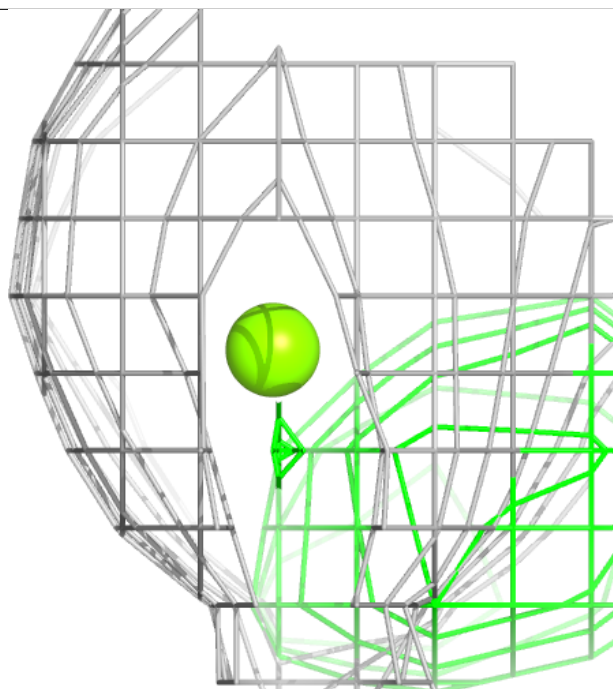
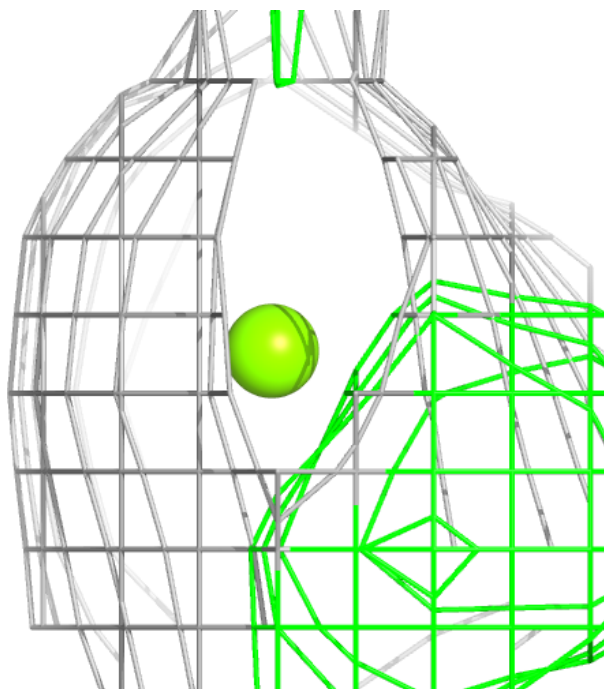
Electron density around GOL A 502:

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



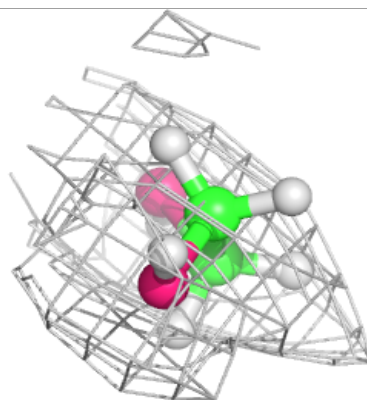
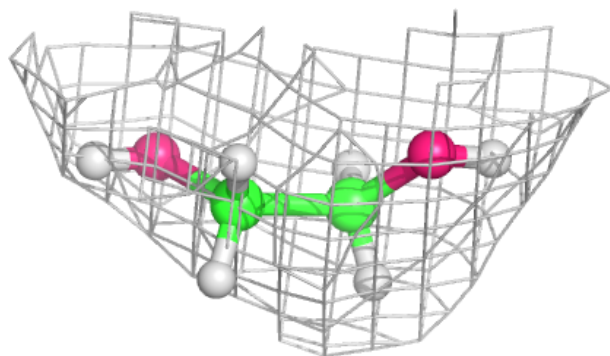
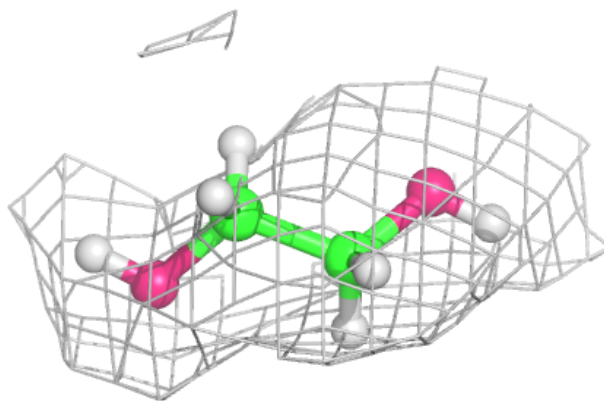
Electron density around MG E 502:

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

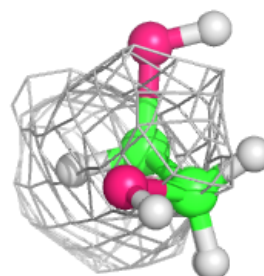
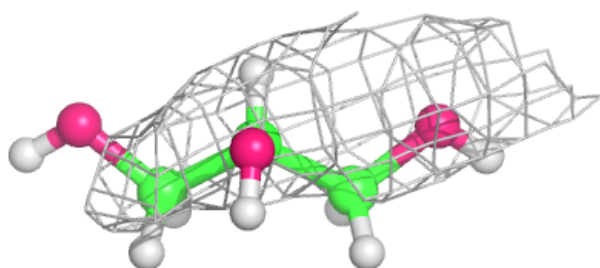
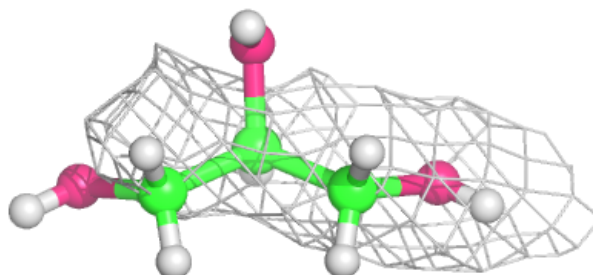


Electron density around EDO F 501:

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

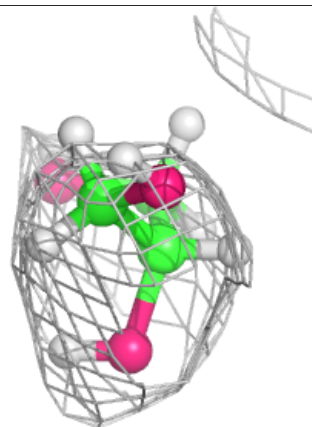
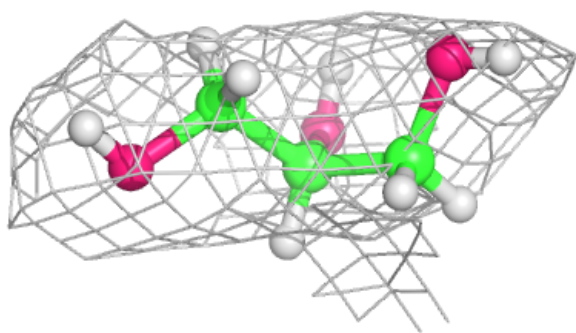
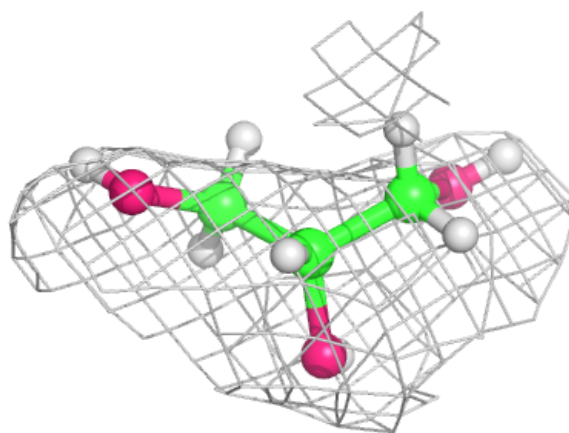
**Electron density around GOL E 501:**

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



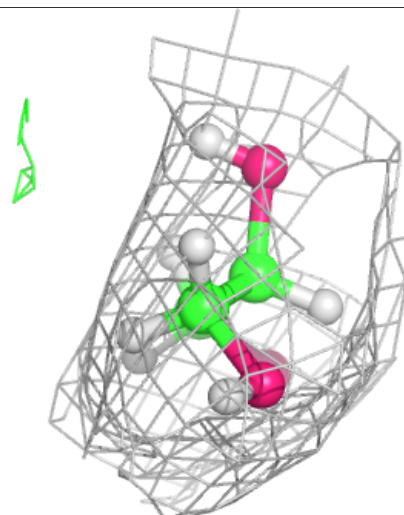
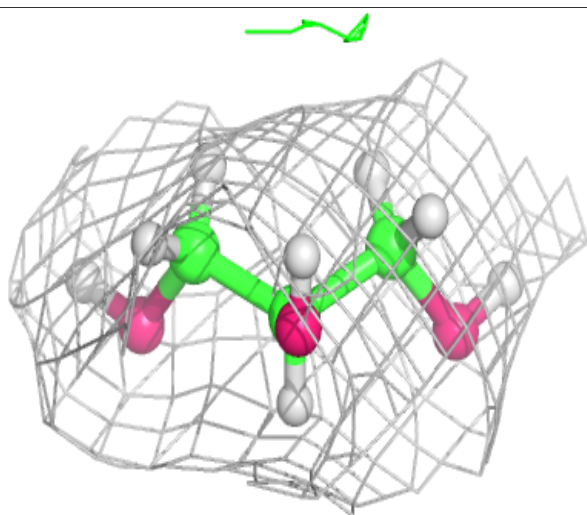
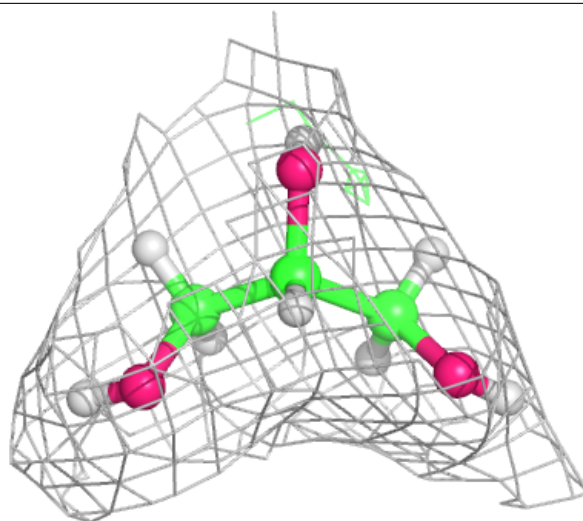
Electron density around GOL D 501:

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



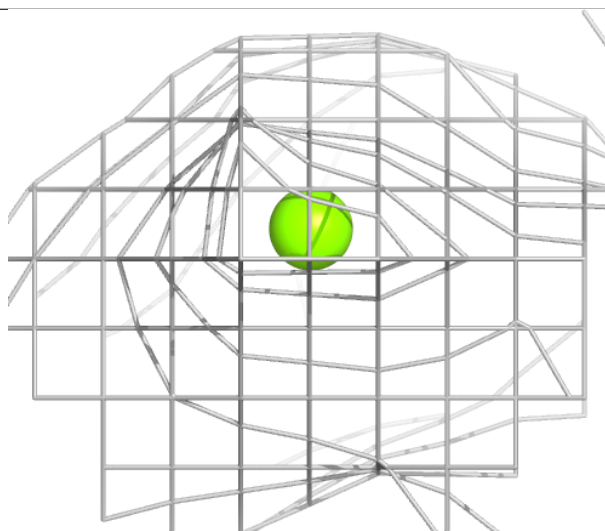
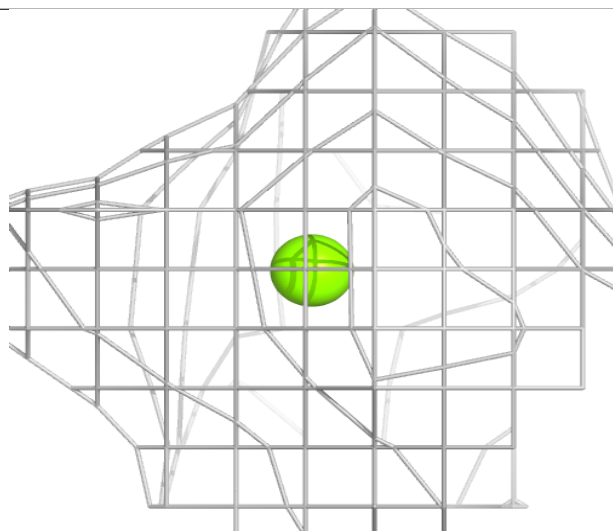
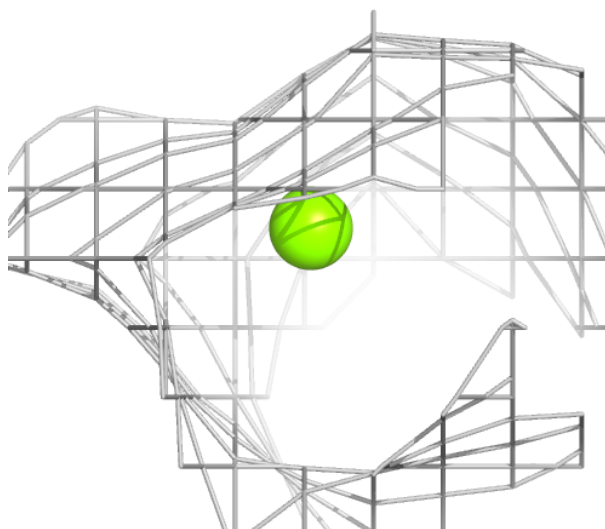
Electron density around GOL A 503:

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



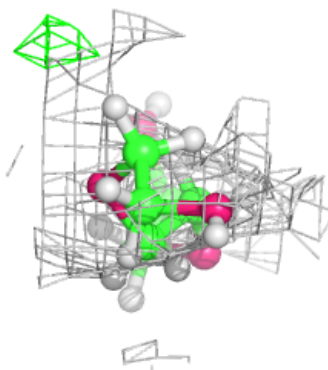
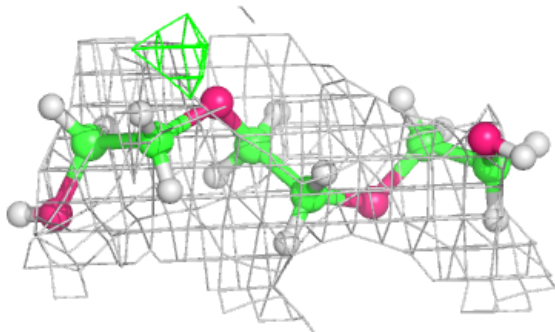
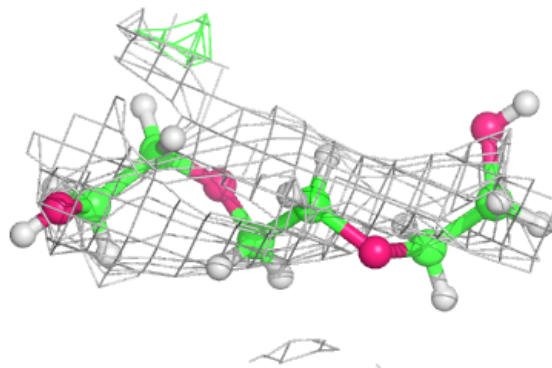
Electron density around MG B 504:

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



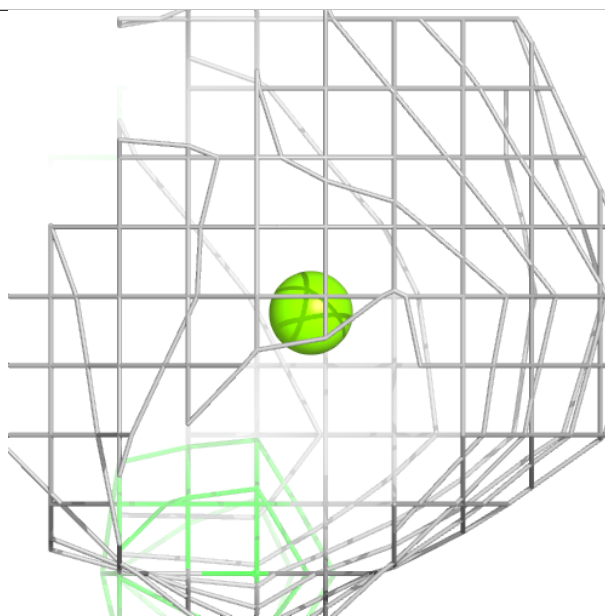
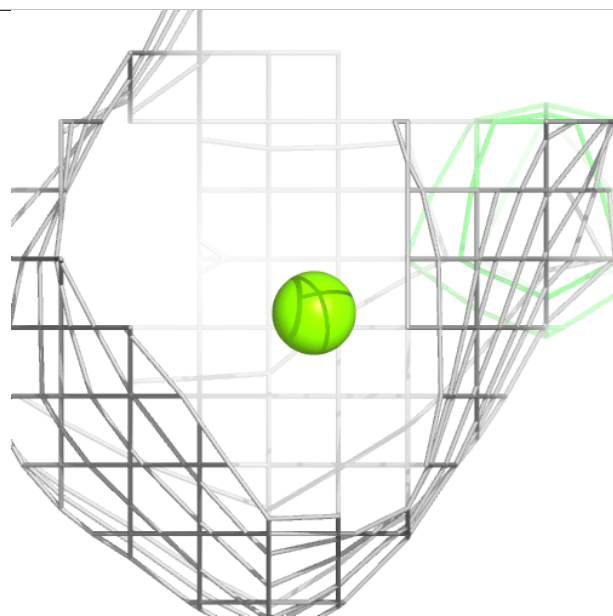
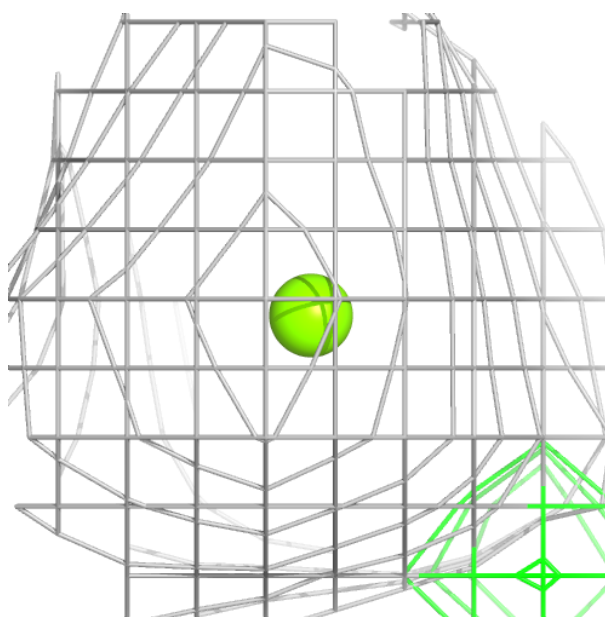
Electron density around PGE A 501:

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



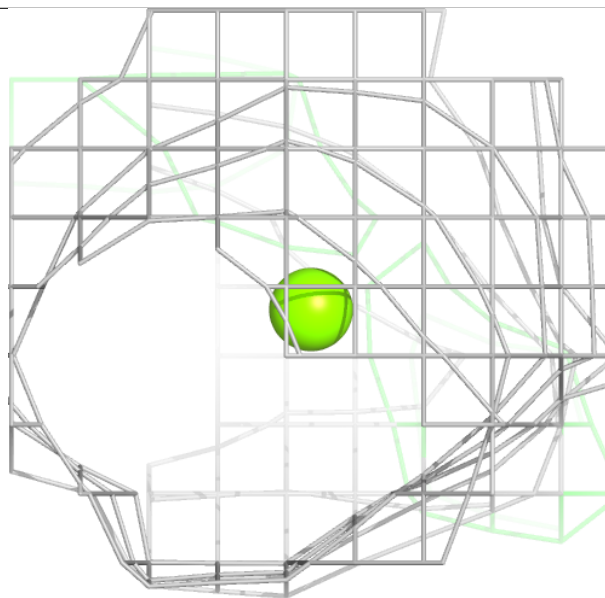
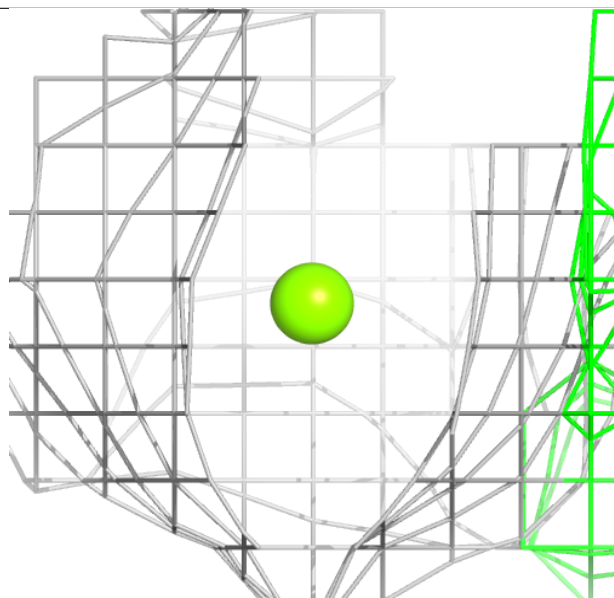
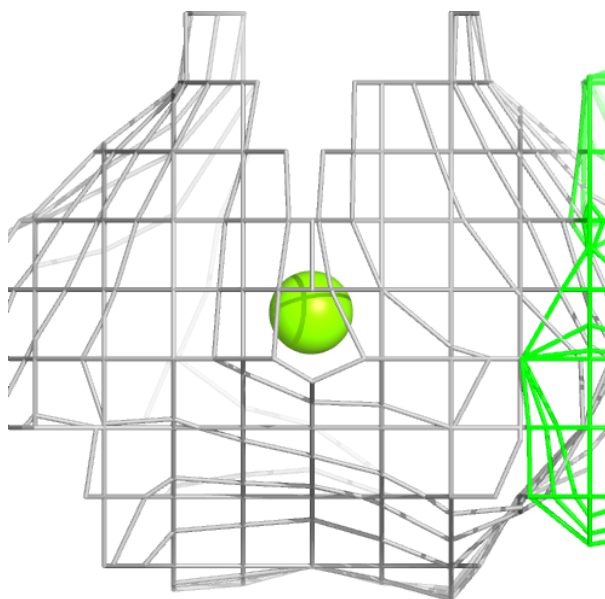
Electron density around MG D 502:

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



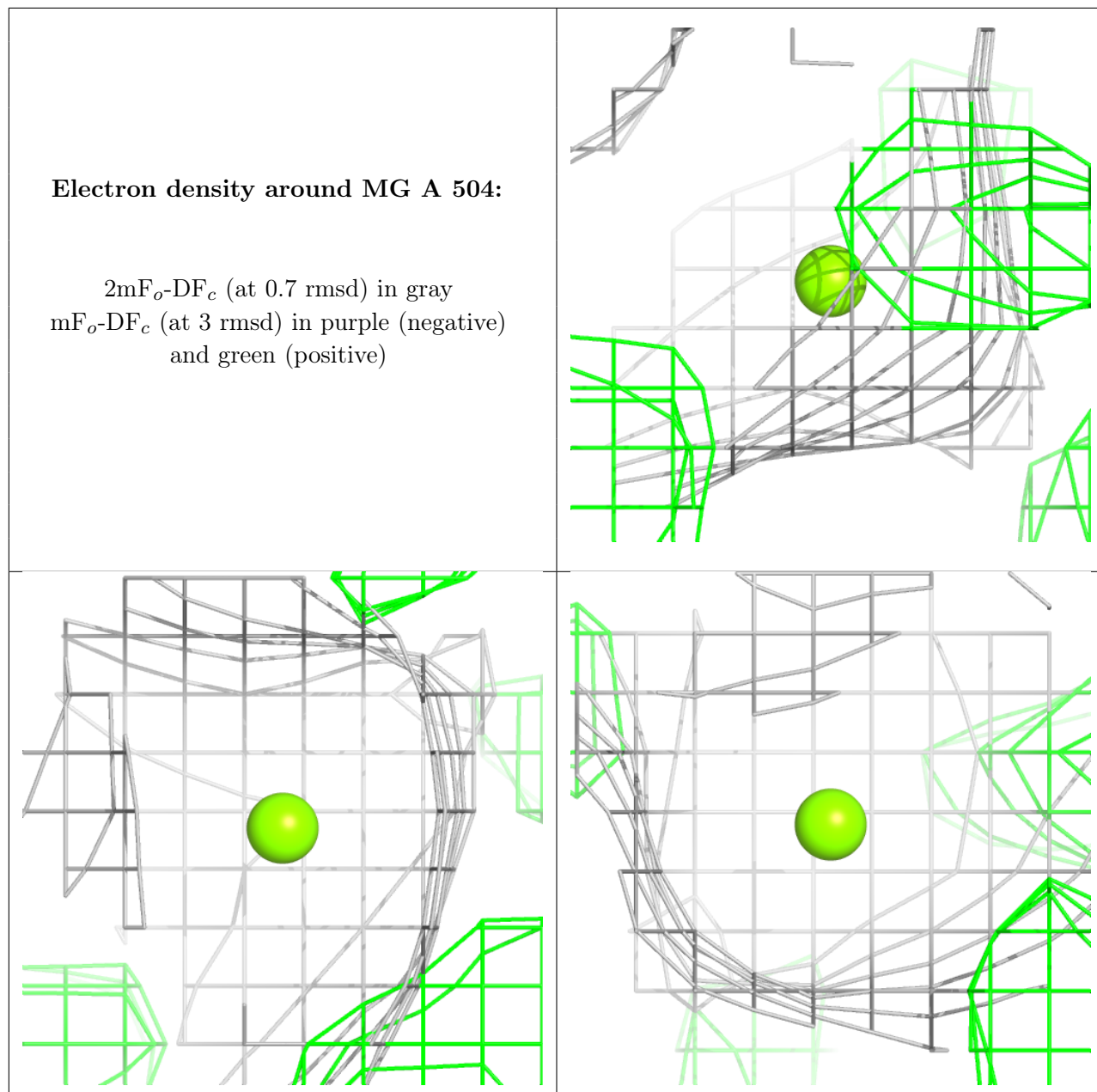
Electron density around MG A 505:

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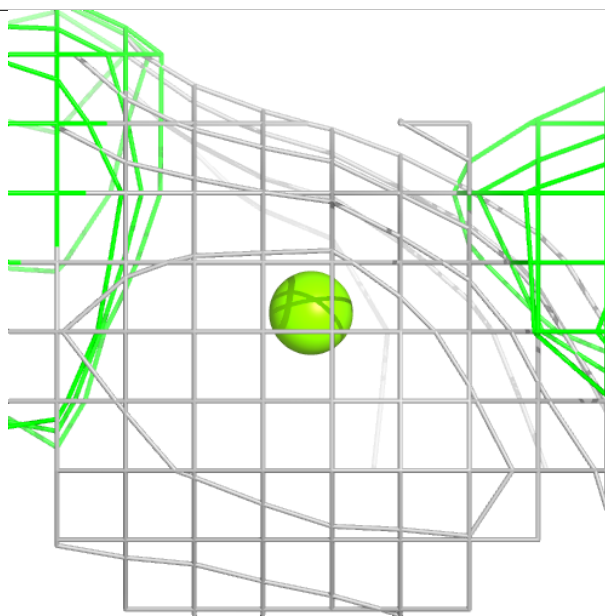
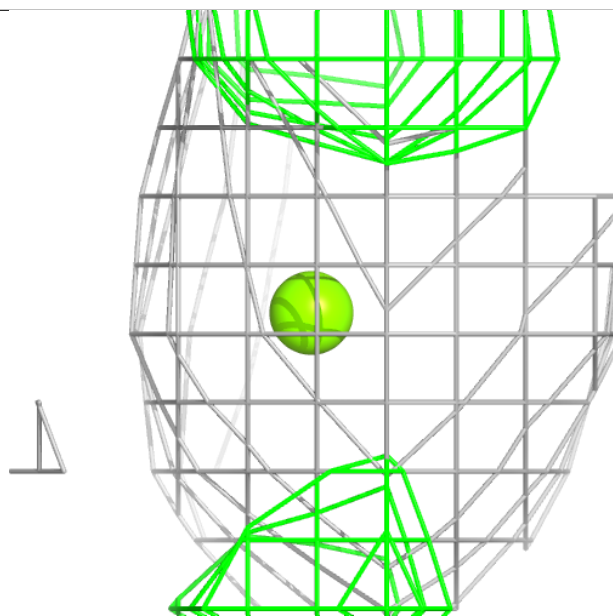
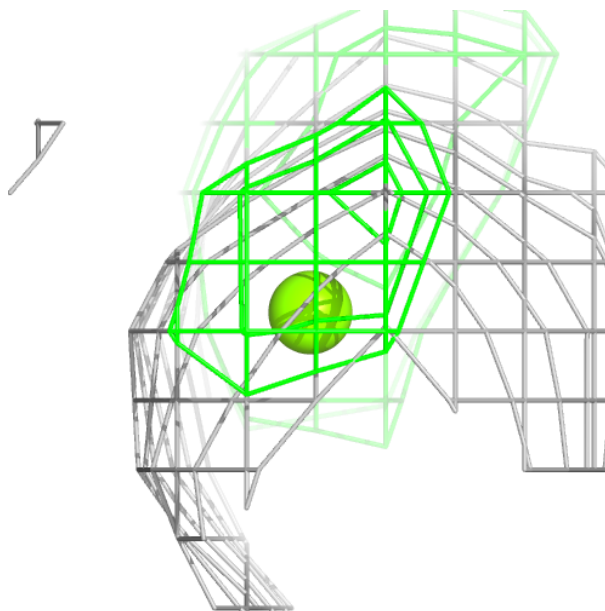
Electron density around MG A 504:

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and green (positive)



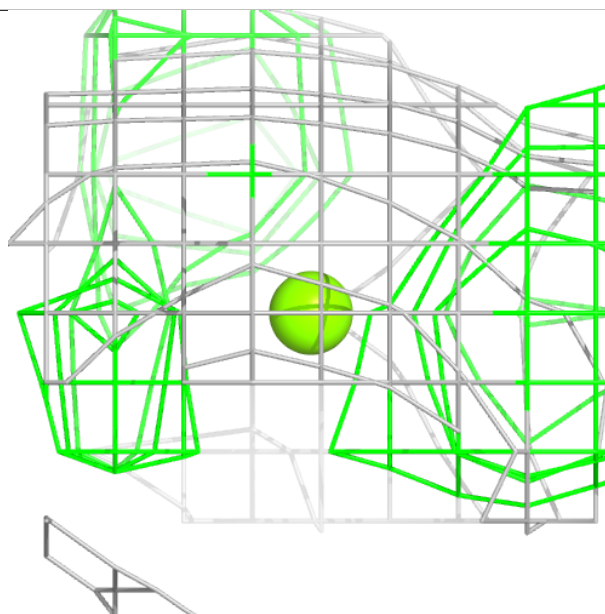
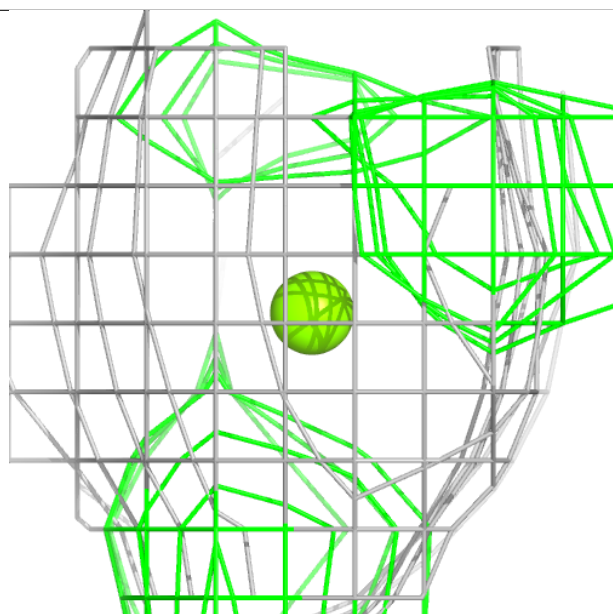
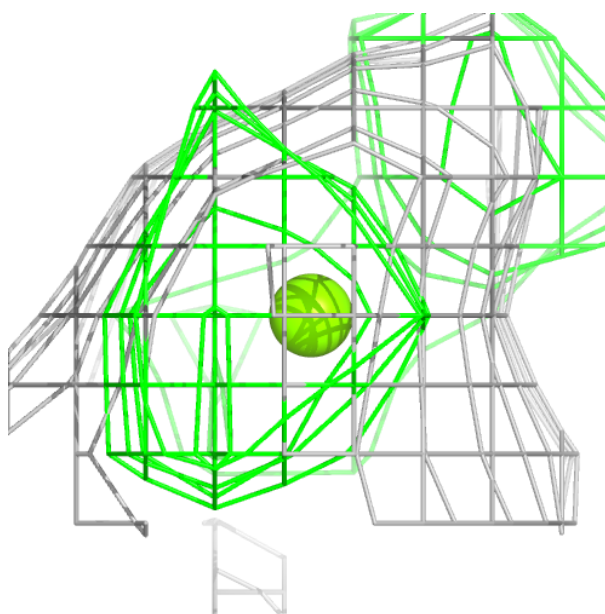
Electron density around MG F 502:

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



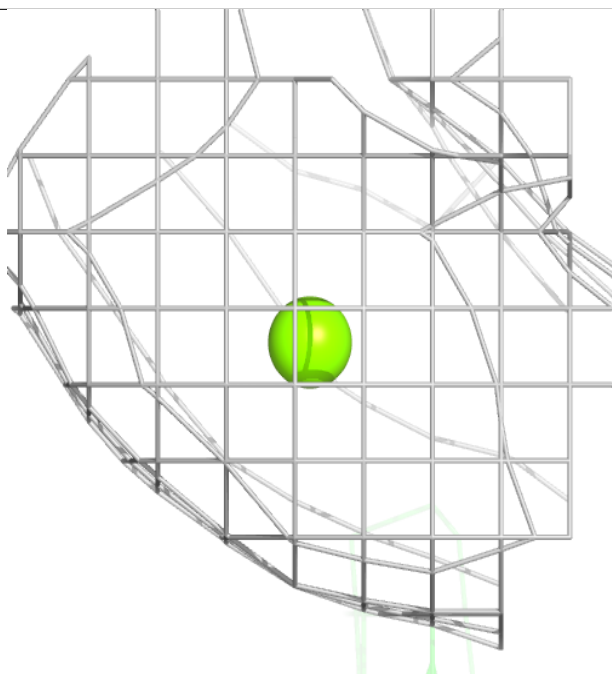
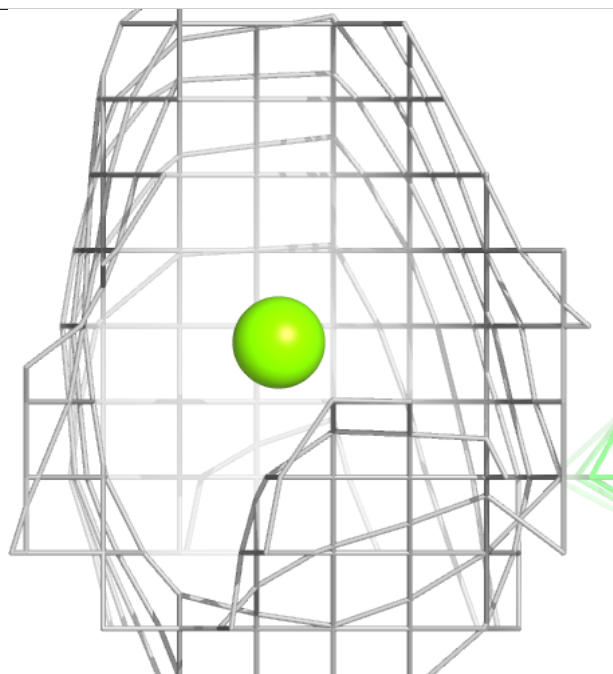
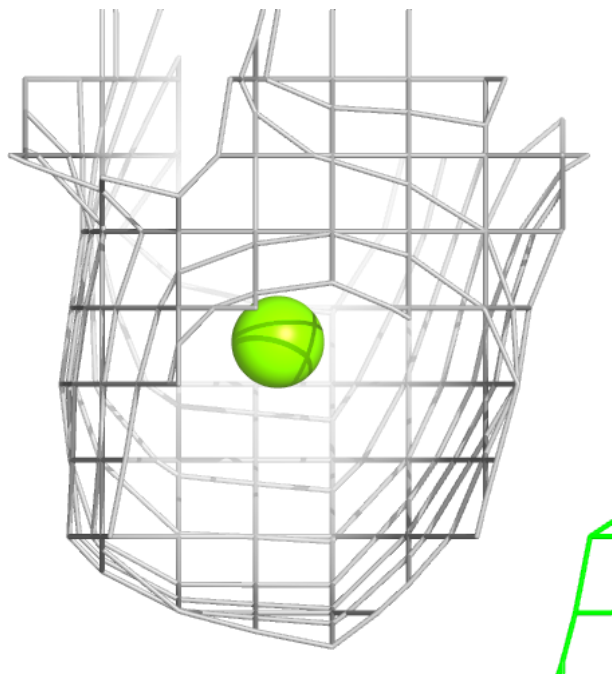
Electron density around MG C 502:

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and green (positive)



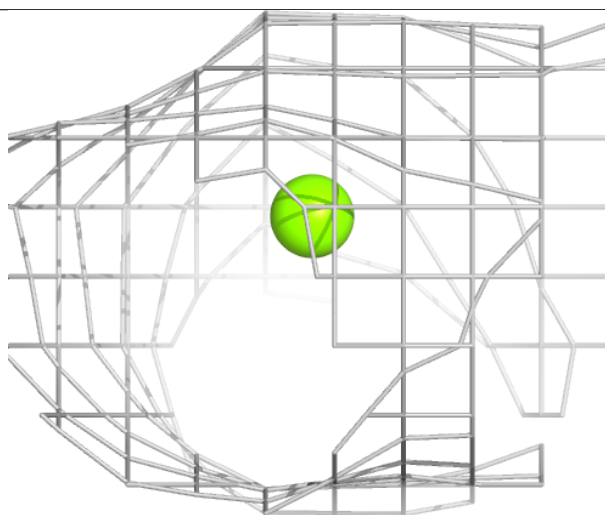
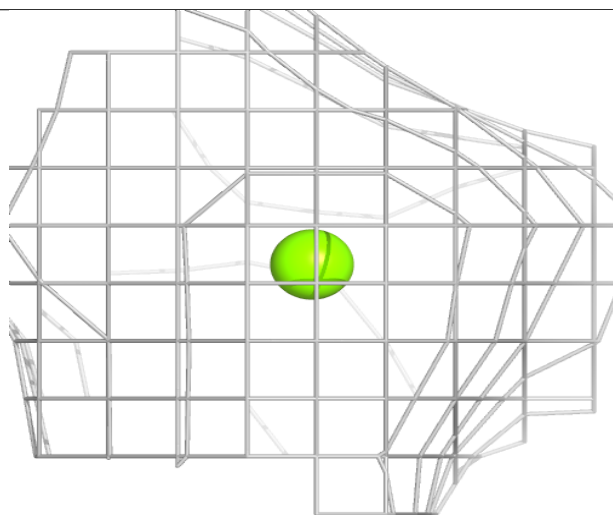
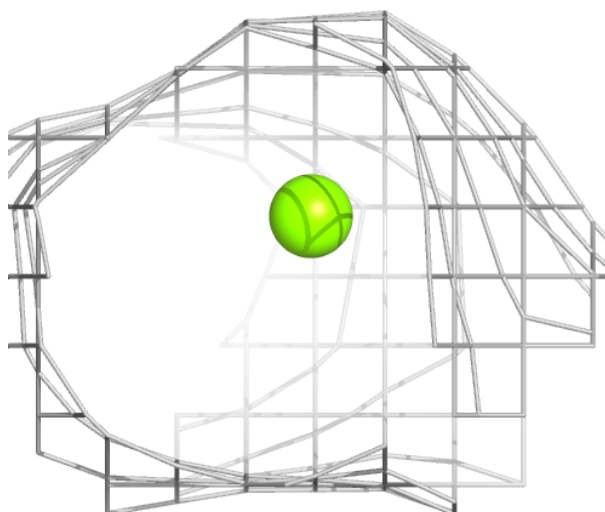
Electron density around MG F 503:

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and green (positive)



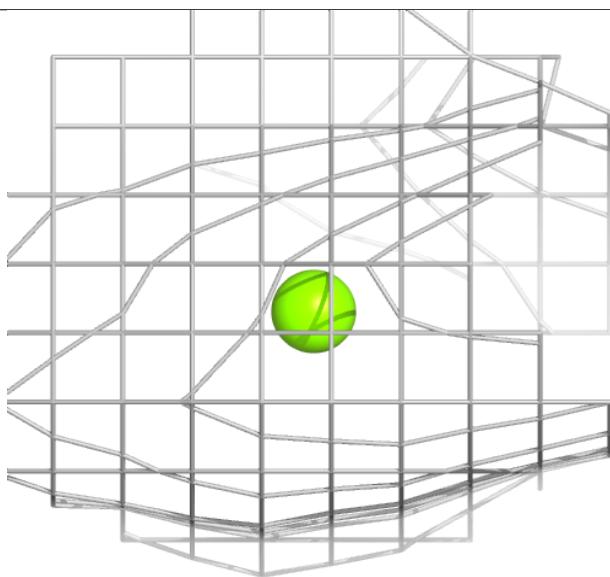
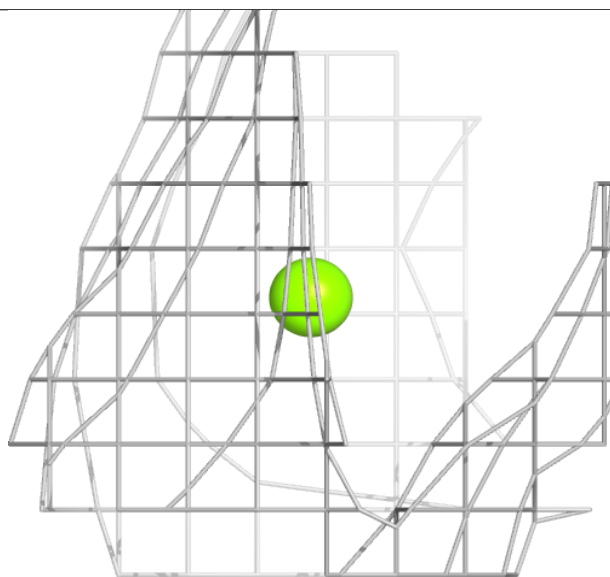
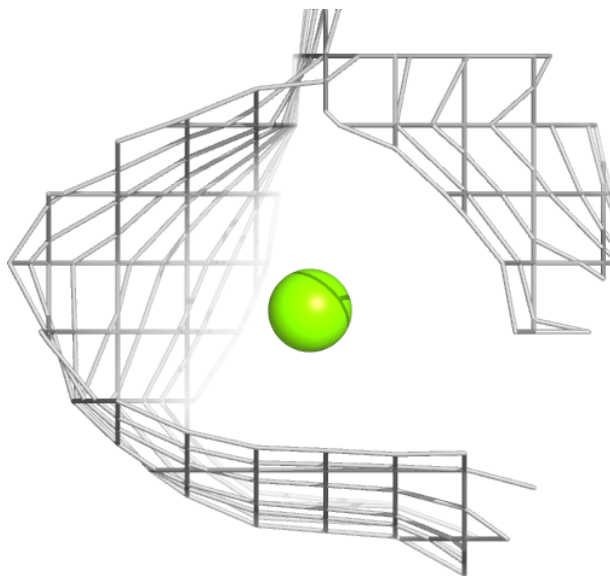
Electron density around MG D 503:

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and green (positive)



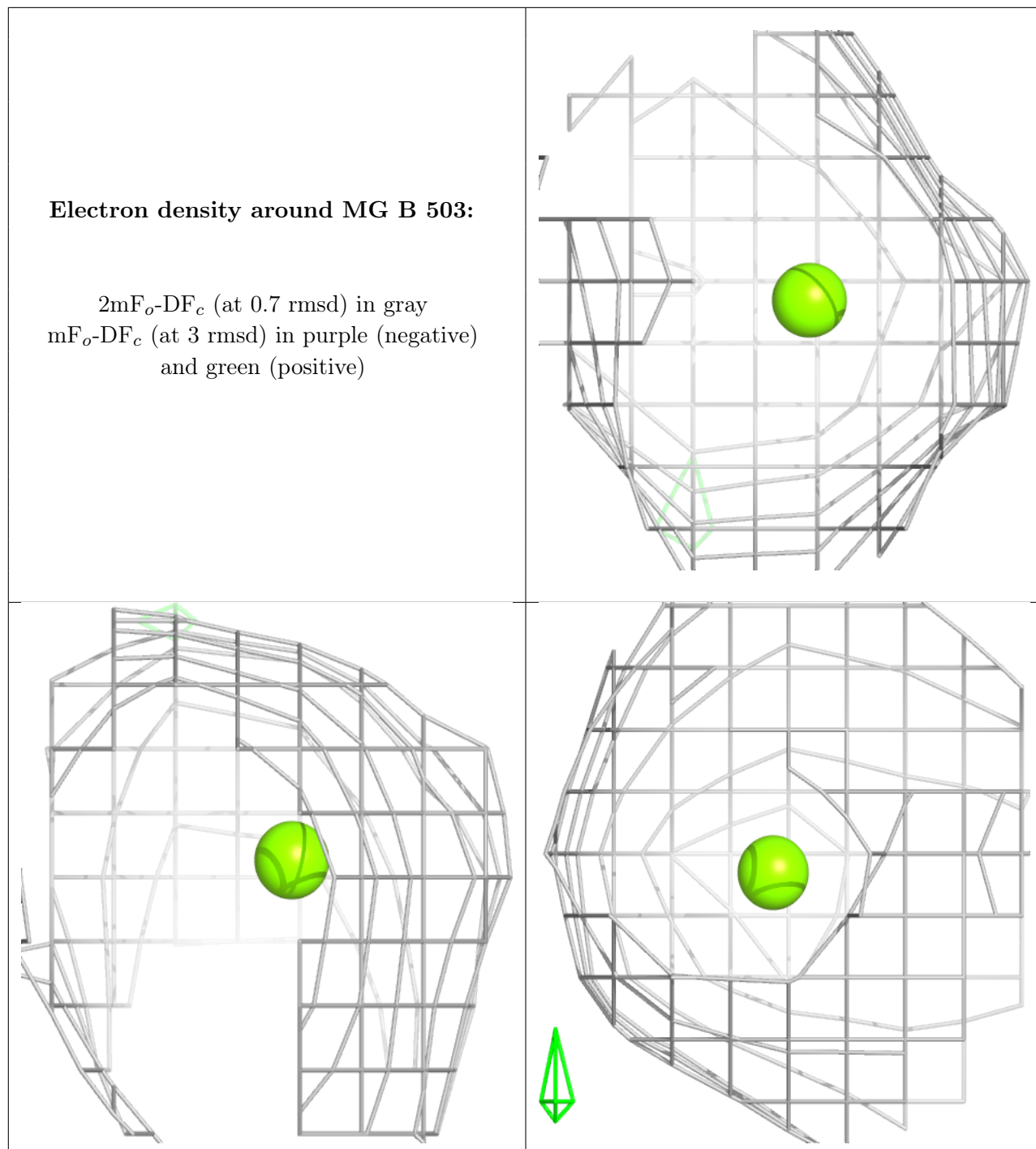
Electron density around MG C 503:

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



Electron density around MG B 503:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.