Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2025 – 02:10 AM JST

PDB ID	:	8Y30
Title	:	Crystal structure of Staphylococcus aureus RecJ protein in complex with Mg2+
Authors	:	Cheng, K.
Deposited on	:	2024-01-27
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

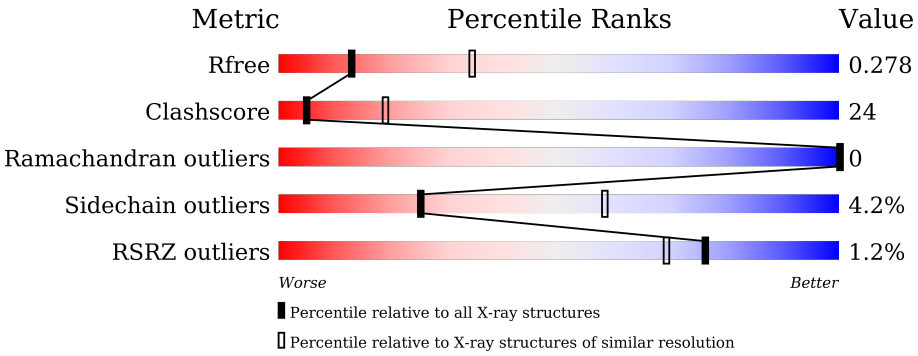
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 <=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	757	62% 35%
1	B	757	61% 35%
1	C	757	64% 34%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18142 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.

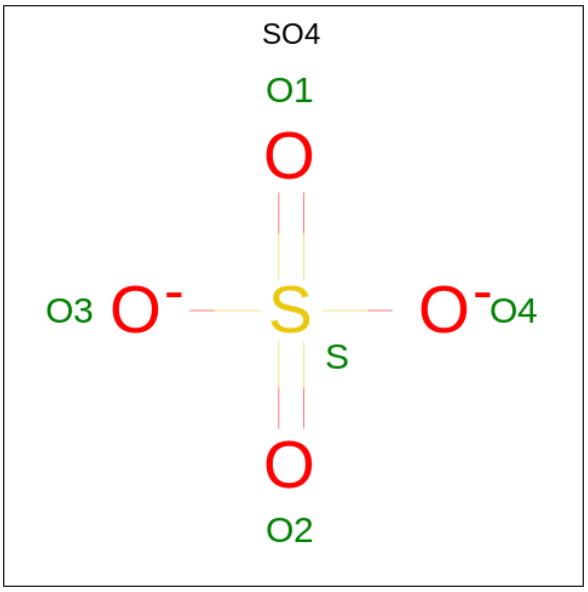
- Molecule 1 is a protein called Single-stranded-DNA-specific exonuclease RecJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total 6012	C 3812	N 1012	O 1163	S 25	0	0	0
1	B	756	Total 6012	C 3812	N 1012	O 1163	S 25	0	0	0
1	C	756	Total 6012	C 3812	N 1012	O 1163	S 25	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

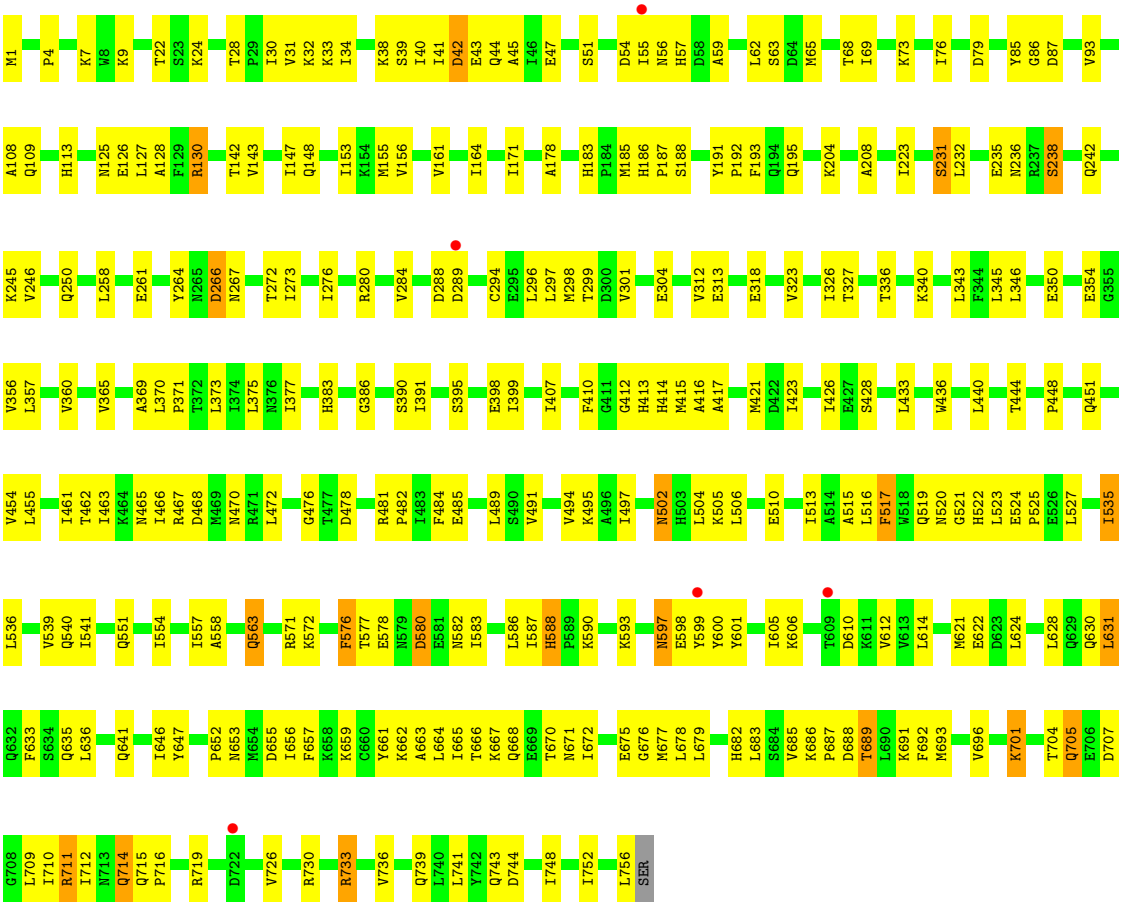
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 15 15	0	0
4	B	18	Total O 18 18	0	0
4	C	22	Total O 22 22	0	0

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.

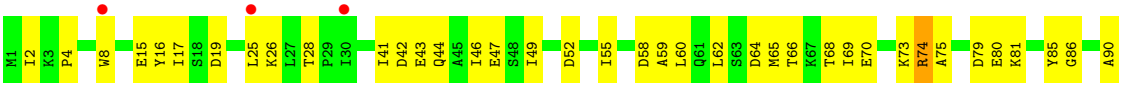
• Molecule 1: Single-stranded-DNA-specific exonuclease RecJ

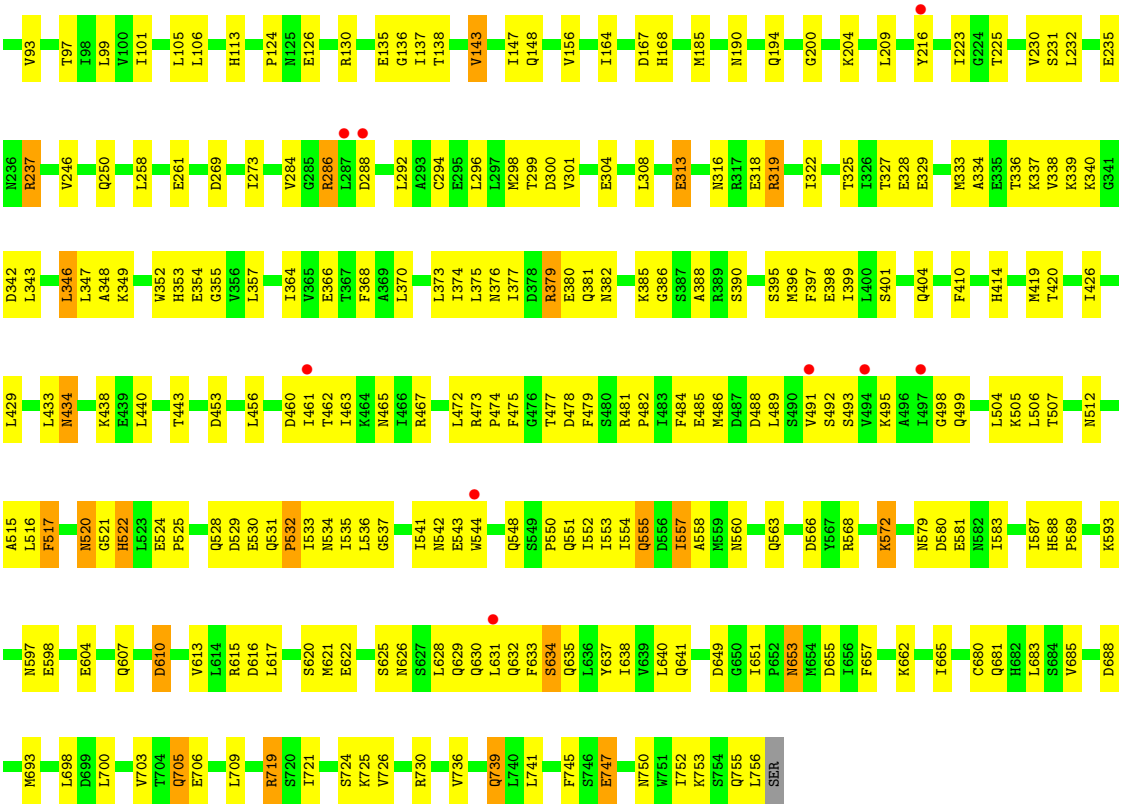
Chain A:



• Molecule 1: Single-stranded-DNA-specific exonuclease RecJ

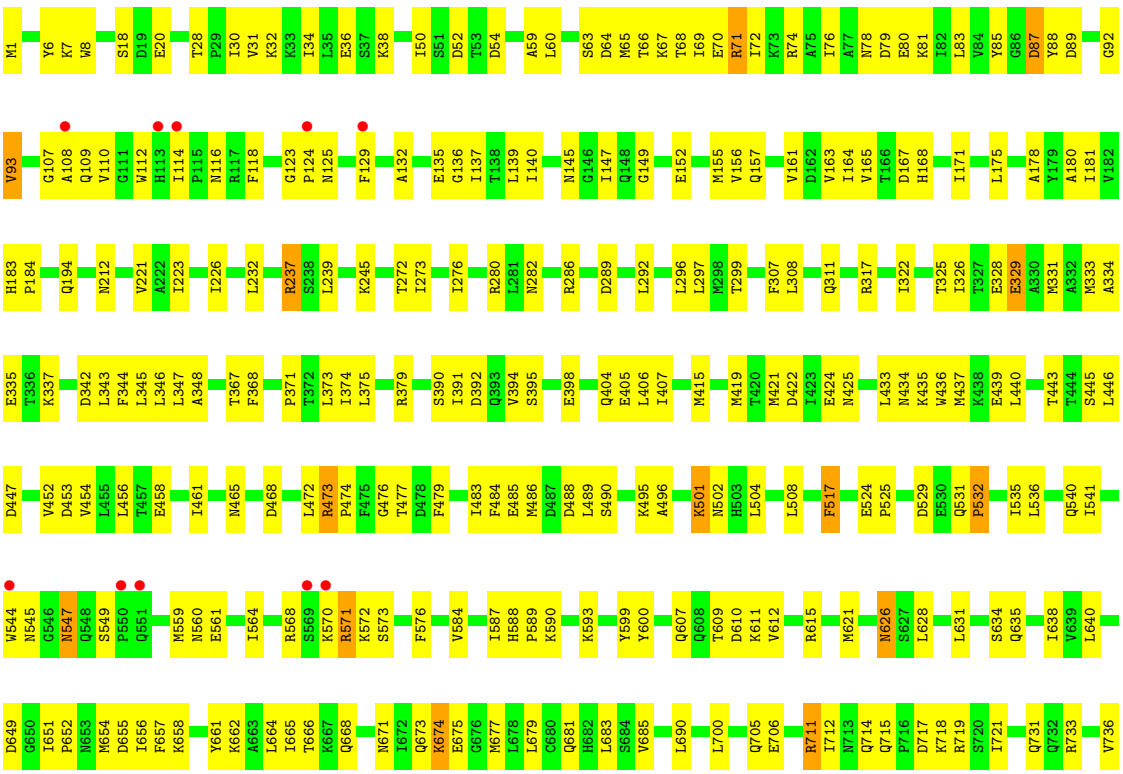
Chain B:





• Molecule 1: Single-stranded-DNA-specific exonuclease RecJ

Chain C:




Q739
L740
F745
K753
L756
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	199.31Å 199.31Å 62.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.00 – 2.80 31.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.00-2.80) 98.8 (31.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.278 0.245 , 0.278	Depositor DCC
R_{free} test set	3538 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	71.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.024 for h,-h-k,-l 0.031 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18142	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	0.53	0/6113	0.65	0/8270
1	B	0.58	1/6113 (0.0%)	0.65	0/8270
1	C	0.55	1/6113 (0.0%)	0.67	2/8270 (0.0%)
All	All	0.56	2/18339 (0.0%)	0.66	2/24810 (0.0%)

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	5
1	B	0	9
1	C	0	13
All	All	0	27

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	PRO	N-CD	-6.04	1.39	1.47
1	C	532	PRO	N-CD	-5.27	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	54	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	329	GLU	N-CA-CB	-5.04	101.52	110.60

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ARG	Sidechain
1	A	571	ARG	Sidechain
1	A	711	ARG	Sidechain
1	A	719	ARG	Sidechain
1	A	733	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	237	ARG	Sidechain
1	B	286	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	379	ARG	Sidechain
1	B	467	ARG	Sidechain
1	B	498	GLY	Peptide
1	B	719	ARG	Sidechain
1	B	74	ARG	Sidechain
1	C	237	ARG	Sidechain
1	C	280	ARG	Sidechain
1	C	317	ARG	Sidechain
1	C	379	ARG	Sidechain
1	C	473	ARG	Peptide,Sidechain
1	C	568	ARG	Sidechain
1	C	571	ARG	Sidechain
1	C	615	ARG	Sidechain
1	C	71	ARG	Sidechain
1	C	711	ARG	Sidechain
1	C	733	ARG	Sidechain
1	C	74	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	6012	0	6057	271	4
1	B	6012	0	6057	355	7
1	C	6012	0	6058	267	7
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	0	0	0
4	A	15	0	0	41	0
4	B	18	0	0	61	0
4	C	22	0	0	76	0
All	All	18142	0	18172	888	12

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 24.

All (888) 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:461:ILE:HD11	1:B:486:MET:CE	1.51	1.40
1:B:516:LEU:CD1	1:B:551:GLN:HE22	1.38	1.35
1:B:528:GLN:HG3	4:B:904:HOH:O	1.19	1.33
1:B:488:ASP:O	1:B:489:LEU:HD23	1.27	1.26
1:A:655:ASP:OD1	1:A:656:ILE:HD12	1.31	1.26
1:C:611:LYS:HA	4:C:903:HOH:O	1.36	1.22
1:B:709:LEU:HB2	4:B:909:HOH:O	1.39	1.19
1:A:1:MET:CA	4:A:904:HOH:O	1.91	1.17
1:B:461:ILE:CD1	1:B:486:MET:CE	2.26	1.13
1:C:38:LYS:NZ	4:C:901:HOH:O	1.81	1.13
1:B:478:ASP:CA	4:B:902:HOH:O	1.95	1.13
1:B:516:LEU:HD12	1:B:551:GLN:NE2	1.65	1.11
1:B:489:LEU:HB2	4:B:901:HOH:O	1.50	1.11
1:B:485:GLU:HA	4:B:908:HOH:O	1.48	1.11
1:C:544:TRP:HE1	1:C:549:SER:HB2	0.97	1.11
1:B:709:LEU:HD12	4:B:909:HOH:O	1.50	1.11
1:B:478:ASP:CG	4:B:902:HOH:O	1.88	1.10
1:B:462:THR:HG23	4:B:913:HOH:O	1.51	1.10
1:B:588:HIS:CD2	1:B:589:PRO:HD2	1.87	1.10
1:C:540:GLN:HB3	4:C:906:HOH:O	1.50	1.09
1:B:440:LEU:HA	1:B:443:THR:HG22	1.33	1.09
1:B:631:LEU:HD11	1:B:633:PHE:HB3	1.28	1.09
1:B:461:ILE:CD1	1:B:486:MET:HE1	1.82	1.09
1:C:447:ASP:N	4:C:904:HOH:O	1.85	1.09
1:B:461:ILE:HD11	1:B:486:MET:HE2	1.22	1.08
1:C:483:ILE:N	4:C:902:HOH:O	1.83	1.08
1:B:366:GLU:O	1:B:366:GLU:OE1	1.71	1.08
1:C:486:MET:HA	4:C:910:HOH:O	1.53	1.07
1:B:588:HIS:HD2	1:B:589:PRO:HD2	0.96	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:CD2	1:A:506:LEU:HD11	1.84	1.07
1:B:485:GLU:CA	4:B:908:HOH:O	2.00	1.07
1:B:478:ASP:N	4:B:902:HOH:O	1.85	1.06
1:C:665:ILE:HA	1:C:712:ILE:CD1	1.85	1.06
1:B:488:ASP:C	1:B:489:LEU:HD23	1.75	1.06
1:B:347:LEU:HD12	1:B:374:ILE:HD11	1.08	1.05
1:B:491:VAL:HG23	1:B:529:ASP:HA	1.37	1.05
1:B:69:ILE:HG22	1:B:73:LYS:HD2	1.38	1.04
1:B:440:LEU:HA	1:B:443:THR:CG2	1.86	1.04
1:B:17:ILE:N	4:B:905:HOH:O	1.89	1.04
1:A:289:ASP:CA	4:A:909:HOH:O	2.06	1.04
1:B:327:THR:HG22	4:B:914:HOH:O	1.58	1.04
1:B:486:MET:HB2	1:B:535:ILE:HD11	1.40	1.04
1:B:625:SER:O	1:B:629:GLN:HG3	1.57	1.03
1:A:1:MET:N	4:A:904:HOH:O	1.86	1.03
1:B:516:LEU:CD1	1:B:551:GLN:NE2	2.20	1.03
1:B:486:MET:N	4:B:908:HOH:O	1.92	1.03
1:A:350:GLU:N	4:A:905:HOH:O	1.90	1.03
1:A:655:ASP:OD1	1:A:656:ILE:CD1	2.06	1.03
1:C:544:TRP:HE1	1:C:549:SER:CB	1.70	1.02
1:B:516:LEU:HD12	1:B:551:GLN:HE22	0.85	1.01
1:B:535:ILE:HD12	1:B:535:ILE:O	1.59	1.01
1:A:289:ASP:HB3	4:A:909:HOH:O	1.58	1.01
1:B:531:GLN:CB	4:B:904:HOH:O	2.08	1.01
1:A:258:LEU:HD11	1:A:280:ARG:HD3	1.40	0.99
1:B:533:ILE:O	4:B:901:HOH:O	1.81	0.99
1:A:127:LEU:N	4:A:908:HOH:O	1.96	0.99
1:B:531:GLN:HB2	4:B:904:HOH:O	1.61	0.99
1:B:347:LEU:HD12	1:B:374:ILE:CD1	1.93	0.99
1:B:301:VAL:HG23	1:B:304:GLU:OE2	1.61	0.99
1:B:301:VAL:O	1:B:304:GLU:HG2	1.62	0.98
1:C:483:ILE:HG13	4:C:902:HOH:O	1.61	0.98
1:A:504:LEU:HD21	1:A:506:LEU:HD11	1.41	0.98
1:B:621:MET:N	4:B:906:HOH:O	1.89	0.97
1:A:261:GLU:HB3	1:A:313:GLU:HG3	1.46	0.97
1:A:69:ILE:HD11	1:A:208:ALA:HB1	1.47	0.96
1:A:662:LYS:O	1:A:665:ILE:CD1	2.14	0.95
1:C:489:LEU:HA	4:C:914:HOH:O	1.66	0.95
1:B:489:LEU:CB	4:B:901:HOH:O	2.11	0.95
1:B:620:SER:CA	4:B:906:HOH:O	2.13	0.95
1:A:1:MET:HA	4:A:904:HOH:O	1.60	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:OE1	4:A:902:HOH:O	1.82	0.95
1:B:49:ILE:HD12	1:B:479:PHE:CE2	2.02	0.94
1:A:523:LEU:N	4:A:901:HOH:O	1.95	0.94
1:C:483:ILE:CG1	4:C:902:HOH:O	2.15	0.94
1:C:610:ASP:O	4:C:903:HOH:O	1.84	0.94
1:C:452:VAL:HG11	1:C:485:GLU:HB2	1.47	0.94
1:C:544:TRP:NE1	1:C:549:SER:HB2	1.81	0.93
1:B:588:HIS:HD2	1:B:589:PRO:CD	1.81	0.93
1:C:311:GLN:N	4:C:911:HOH:O	1.98	0.92
1:A:497:ILE:HG13	1:A:505:LYS:HE3	1.50	0.92
1:C:700:LEU:HA	1:C:719:ARG:HH21	1.32	0.92
1:B:709:LEU:CB	4:B:909:HOH:O	2.05	0.92
1:B:288:ASP:OD1	4:B:903:HOH:O	1.86	0.92
1:C:85:TYR:CE2	4:C:918:HOH:O	2.21	0.92
1:B:488:ASP:O	1:B:489:LEU:CD2	2.16	0.92
1:B:491:VAL:CG2	1:B:529:ASP:HA	1.99	0.92
1:C:540:GLN:OE1	4:C:906:HOH:O	1.88	0.92
1:B:528:GLN:O	4:B:904:HOH:O	1.87	0.91
1:B:489:LEU:N	4:B:901:HOH:O	2.04	0.91
1:B:617:LEU:HD23	1:B:640:LEU:HD22	1.48	0.91
1:A:24:LYS:NZ	1:A:43:GLU:OE2	2.04	0.91
1:C:718:LYS:HA	4:C:908:HOH:O	1.70	0.90
1:B:42:ASP:O	1:B:46:ILE:HG13	1.71	0.90
1:C:116:ASN:O	4:C:907:HOH:O	1.90	0.90
1:C:483:ILE:CB	4:C:902:HOH:O	2.20	0.89
1:B:373:LEU:HD12	1:B:388:ALA:HB2	1.53	0.89
1:B:461:ILE:CD1	1:B:486:MET:HE2	1.97	0.89
1:C:299:THR:HG21	1:C:308:LEU:HD12	1.55	0.89
1:B:493:SER:OG	1:B:507:THR:HB	1.73	0.88
1:A:289:ASP:C	4:A:909:HOH:O	2.12	0.88
1:C:156:VAL:HG22	1:C:161:VAL:HB	1.55	0.88
1:C:447:ASP:CA	4:C:904:HOH:O	2.20	0.88
1:B:349:LYS:CA	1:B:377:ILE:HD12	2.04	0.88
1:B:653:ASN:HB2	1:B:655:ASP:OD1	1.72	0.88
1:A:641:GLN:HG2	4:A:906:HOH:O	1.73	0.87
1:C:434:ASN:HB3	4:C:913:HOH:O	1.74	0.87
1:C:665:ILE:HA	1:C:712:ILE:HD11	1.55	0.87
1:A:284:VAL:O	1:A:288:ASP:O	1.92	0.87
1:B:478:ASP:CB	4:B:902:HOH:O	2.11	0.87
1:C:371:PRO:HG3	1:C:394:VAL:HG21	1.56	0.87
1:C:717:ASP:O	4:C:908:HOH:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:LYS:HD3	4:C:917:HOH:O	1.72	0.87
1:C:64:ASP:O	1:C:68:THR:OG1	1.91	0.87
1:B:124:PRO:O	4:B:907:HOH:O	1.90	0.86
1:B:352:TRP:O	1:B:376:ASN:ND2	2.08	0.86
1:C:435:LYS:NZ	4:C:905:HOH:O	1.87	0.86
1:C:446:LEU:O	1:C:447:ASP:OD1	1.94	0.86
1:C:610:ASP:N	4:C:912:HOH:O	2.06	0.86
1:B:706:GLU:O	4:B:909:HOH:O	1.93	0.86
1:B:347:LEU:CD1	1:B:374:ILE:HD11	2.00	0.85
1:A:605:ILE:O	4:A:907:HOH:O	1.93	0.85
1:C:654:MET:O	1:C:658:LYS:HG2	1.75	0.85
1:C:668:GLN:OE1	1:C:668:GLN:HA	1.74	0.85
1:A:398:GLU:CB	4:A:902:HOH:O	2.23	0.85
1:B:683:LEU:O	1:B:685:VAL:HG13	1.77	0.84
1:B:625:SER:OG	1:B:755:GLN:OE1	1.95	0.84
1:A:289:ASP:CB	4:A:909:HOH:O	2.14	0.82
1:B:620:SER:HA	4:B:906:HOH:O	1.76	0.82
1:C:116:ASN:OD1	4:C:907:HOH:O	1.96	0.82
1:B:429:LEU:HG	1:B:433:LEU:CD1	2.08	0.82
1:B:621:MET:HE2	1:B:736:VAL:HA	1.60	0.82
1:A:670:THR:HB	1:A:675:GLU:OE1	1.78	0.82
1:B:709:LEU:CD1	4:B:909:HOH:O	2.11	0.82
1:B:530:GLU:OE1	1:B:530:GLU:HA	1.77	0.82
1:B:581:GLU:O	1:B:607:GLN:NE2	2.11	0.82
1:B:461:ILE:HD11	1:B:486:MET:HE1	1.40	0.81
1:B:515:ALA:HB1	1:B:554:ILE:HD11	1.61	0.81
1:B:485:GLU:C	4:B:908:HOH:O	2.10	0.81
1:B:621:MET:CE	1:B:736:VAL:HA	2.11	0.81
1:A:662:LYS:O	1:A:665:ILE:HD12	1.78	0.81
1:B:657:PHE:CE1	1:B:693:MET:HG2	2.16	0.81
1:A:665:ILE:HD12	1:A:666:THR:N	1.96	0.80
1:C:485:GLU:O	4:C:910:HOH:O	1.97	0.80
1:A:504:LEU:HD23	1:A:506:LEU:HD11	1.63	0.80
1:B:429:LEU:HG	1:B:433:LEU:HD11	1.60	0.80
1:C:490:SER:N	4:C:914:HOH:O	2.12	0.80
1:A:688:ASP:HA	1:A:691:LYS:HD3	1.62	0.79
1:C:609:THR:C	4:C:912:HOH:O	2.21	0.79
1:B:631:LEU:CD1	1:B:633:PHE:HD2	1.97	0.78
1:B:301:VAL:HG23	1:B:304:GLU:CD	2.02	0.78
1:B:440:LEU:CA	1:B:443:THR:HG22	2.14	0.78
1:B:491:VAL:HG23	1:B:491:VAL:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:SER:HA	1:B:414:HIS:CD2	2.18	0.78
1:C:544:TRP:NE1	1:C:549:SER:CB	2.44	0.77
1:C:700:LEU:HD23	1:C:719:ARG:NH2	1.97	0.77
1:C:545:ASN:OD1	1:C:545:ASN:O	2.03	0.77
1:B:347:LEU:HB2	1:B:374:ILE:CD1	2.14	0.76
1:B:725:LYS:H	1:B:725:LYS:HD2	1.51	0.76
1:A:662:LYS:O	1:A:665:ILE:HD11	1.83	0.76
1:C:407:ILE:HG23	1:C:419:MET:HE3	1.67	0.76
1:C:665:ILE:HG22	1:C:712:ILE:HD13	1.68	0.76
1:C:486:MET:HG3	4:C:910:HOH:O	1.87	0.75
1:B:504:LEU:HB2	1:B:521:GLY:HA2	1.68	0.75
1:A:54:ASP:OD2	1:A:242:GLN:NE2	2.20	0.75
1:B:81:LYS:HZ1	1:B:136:GLY:HA3	1.50	0.75
1:C:621:MET:HE2	1:C:739:GLN:HB2	1.67	0.75
1:C:486:MET:CA	4:C:910:HOH:O	2.21	0.75
1:C:621:MET:HE2	1:C:739:GLN:CB	2.17	0.74
1:B:64:ASP:O	1:B:68:THR:OG1	2.04	0.74
1:B:631:LEU:HD12	1:B:633:PHE:HD2	1.51	0.74
1:C:700:LEU:HD23	1:C:719:ARG:HH21	1.50	0.74
1:A:494:VAL:HG23	1:A:506:LEU:HD21	1.68	0.74
1:B:81:LYS:NZ	1:B:135:GLU:O	2.18	0.74
1:C:334:ALA:HB1	1:C:345:LEU:HD13	1.70	0.74
1:B:343:LEU:O	1:B:370:LEU:HD22	1.88	0.74
1:A:289:ASP:N	4:A:909:HOH:O	2.18	0.74
1:A:294:CYS:SG	1:A:298:MET:CE	2.76	0.74
1:A:294:CYS:SG	1:A:298:MET:HE1	2.28	0.73
1:B:553:ILE:O	4:B:912:HOH:O	2.06	0.73
1:C:32:LYS:HE3	1:C:36:GLU:OE2	1.87	0.73
1:A:398:GLU:HB2	4:A:902:HOH:O	1.87	0.73
1:C:308:LEU:O	4:C:911:HOH:O	2.06	0.73
1:A:504:LEU:CD2	1:A:506:LEU:CD1	2.65	0.73
1:B:349:LYS:C	1:B:377:ILE:HD12	2.08	0.73
1:C:60:LEU:HD23	1:C:65:MET:CE	2.19	0.73
1:A:504:LEU:HD23	1:A:506:LEU:CD1	2.19	0.73
1:B:572:LYS:O	1:B:572:LYS:HD3	1.89	0.73
1:C:1:MET:HE2	1:C:634:SER:HB3	1.70	0.72
1:C:453:ASP:OD2	4:C:902:HOH:O	2.07	0.72
1:C:661:TYR:O	1:C:665:ILE:HG23	1.89	0.72
1:C:665:ILE:CA	1:C:712:ILE:CD1	2.67	0.72
1:A:451:GLN:NE2	4:A:913:HOH:O	2.22	0.72
1:A:705:GLN:HB2	1:A:710:ILE:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:MET:HE1	1:B:739:GLN:HB2	1.71	0.72
1:B:328:GLU:N	4:B:914:HOH:O	2.22	0.72
1:A:679:LEU:HD12	1:A:682:HIS:CE1	2.24	0.72
1:C:504:LEU:N	4:C:915:HOH:O	2.22	0.72
1:B:531:GLN:HB3	4:B:904:HOH:O	1.78	0.71
1:C:116:ASN:CB	4:C:907:HOH:O	2.38	0.71
1:A:68:THR:HG23	1:A:164:ILE:HD13	1.72	0.71
1:C:52:ASP:OD1	1:C:52:ASP:O	2.07	0.71
1:C:665:ILE:CA	1:C:712:ILE:HD11	2.21	0.71
1:B:463:ILE:HD11	1:B:550:PRO:HD3	1.72	0.71
1:A:30:ILE:HG21	1:A:465:ASN:O	1.91	0.71
1:B:456:LEU:HB3	1:B:486:MET:CE	2.21	0.71
1:A:655:ASP:OD1	1:A:656:ILE:N	2.24	0.71
1:C:486:MET:HB3	1:C:489:LEU:HD11	1.73	0.71
1:A:659:LYS:O	1:A:683:LEU:HD21	1.90	0.71
1:B:44:GLN:N	4:B:911:HOH:O	2.23	0.71
1:C:434:ASN:CB	4:C:913:HOH:O	2.33	0.71
1:C:540:GLN:CB	4:C:906:HOH:O	2.23	0.71
1:C:610:ASP:CA	4:C:912:HOH:O	2.39	0.71
1:A:659:LYS:C	1:A:662:LYS:HG2	2.11	0.70
1:B:461:ILE:CG1	1:B:486:MET:HE1	2.21	0.70
1:A:125:ASN:C	4:A:908:HOH:O	2.29	0.70
1:B:617:LEU:CD2	1:B:640:LEU:HD22	2.20	0.70
1:C:434:ASN:CA	4:C:913:HOH:O	2.39	0.70
1:B:327:THR:CG2	4:B:914:HOH:O	2.26	0.70
1:B:552:ILE:O	4:B:910:HOH:O	2.09	0.70
1:B:700:LEU:HD11	1:B:721:ILE:HA	1.71	0.70
1:B:65:MET:O	1:B:69:ILE:HG13	1.91	0.70
1:C:1:MET:SD	1:C:560:ASN:HA	2.32	0.70
1:A:494:VAL:HG23	1:A:506:LEU:CD2	2.21	0.70
1:B:493:SER:OG	1:B:507:THR:CB	2.39	0.70
1:C:573:SER:N	4:C:919:HOH:O	2.25	0.69
1:A:398:GLU:HB3	4:A:902:HOH:O	1.86	0.69
1:A:128:ALA:N	4:A:908:HOH:O	2.07	0.69
1:B:16:TYR:C	4:B:905:HOH:O	2.24	0.69
1:A:125:ASN:O	4:A:908:HOH:O	2.10	0.69
1:A:289:ASP:O	4:A:909:HOH:O	2.05	0.69
1:A:653:ASN:OD1	4:A:910:HOH:O	2.09	0.69
1:A:661:TYR:O	1:A:665:ILE:HG13	1.93	0.69
1:B:620:SER:OG	1:B:622:GLU:HG2	1.92	0.69
1:B:617:LEU:HD23	1:B:640:LEU:CD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:GLN:O	4:C:903:HOH:O	2.10	0.69
1:B:461:ILE:O	1:B:461:ILE:HG22	1.93	0.69
1:C:584:VAL:HG13	1:C:612:VAL:HG13	1.74	0.69
1:A:463:ILE:HD12	1:A:463:ILE:H	1.58	0.69
1:A:350:GLU:CB	4:A:905:HOH:O	2.41	0.68
1:B:631:LEU:CD1	1:B:633:PHE:HB3	2.15	0.68
1:B:301:VAL:N	1:B:304:GLU:OE2	2.17	0.68
1:A:246:VAL:HG13	1:A:250:GLN:HG3	1.75	0.68
1:B:478:ASP:OD1	4:B:902:HOH:O	2.04	0.68
1:B:516:LEU:HD11	1:B:551:GLN:HE22	1.49	0.68
1:B:382:ASN:OD1	1:B:382:ASN:O	2.11	0.68
1:A:535:ILE:HG12	1:A:554:ILE:HG12	1.76	0.68
1:B:485:GLU:HB2	1:B:536:LEU:HD11	1.76	0.68
1:B:579:ASN:OD1	1:B:579:ASN:O	2.11	0.68
1:B:610:ASP:HB3	1:B:634:SER:HB2	1.75	0.68
1:B:382:ASN:O	1:B:382:ASN:CG	2.31	0.67
1:C:753:LYS:HA	1:C:756:LEU:HD12	1.75	0.67
1:B:535:ILE:O	4:B:908:HOH:O	2.11	0.67
1:B:620:SER:HB2	4:B:906:HOH:O	1.94	0.67
1:A:188:SER:HA	1:B:379:ARG:NE	2.09	0.67
1:B:485:GLU:HB2	1:B:536:LEU:CD1	2.25	0.67
1:B:346:LEU:HD21	1:B:426:ILE:HG23	1.77	0.67
1:B:347:LEU:HB2	1:B:374:ILE:HD13	1.77	0.67
1:A:69:ILE:HD11	1:A:208:ALA:CB	2.25	0.67
1:A:659:LYS:O	1:A:662:LYS:HG2	1.93	0.67
1:C:331:MET:HE1	1:C:367:THR:HG21	1.75	0.67
1:C:671:ASN:HB3	1:C:674:LYS:HG2	1.74	0.66
1:C:706:GLU:HB2	1:C:711:ARG:HH12	1.60	0.66
1:C:434:ASN:O	4:C:913:HOH:O	2.12	0.66
1:C:78:ASN:HB2	1:C:80:GLU:HG3	1.75	0.66
1:A:350:GLU:HG3	4:A:905:HOH:O	1.95	0.66
1:C:436:TRP:O	1:C:439:GLU:HG3	1.95	0.66
1:A:709:LEU:N	1:A:709:LEU:HD22	2.11	0.66
1:B:485:GLU:HA	1:B:536:LEU:HD12	1.76	0.66
1:C:116:ASN:CG	4:C:907:HOH:O	2.34	0.66
1:C:665:ILE:HA	1:C:712:ILE:HD12	1.76	0.66
1:B:354:GLU:HA	1:B:357:LEU:HG	1.78	0.65
1:B:327:THR:C	4:B:914:HOH:O	2.33	0.65
1:B:725:LYS:H	1:B:725:LYS:CD	2.09	0.65
1:A:667:LYS:O	1:A:668:GLN:HB2	1.95	0.65
1:B:492:SER:HB2	1:B:507:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASN:HB3	4:C:907:HOH:O	1.95	0.65
1:C:489:LEU:CA	4:C:914:HOH:O	2.34	0.65
1:B:318:GLU:O	1:B:322:ILE:HG13	1.97	0.65
1:C:147:ILE:HG21	1:C:171:ILE:HA	1.78	0.65
1:A:641:GLN:NE2	4:A:906:HOH:O	1.92	0.65
1:B:81:LYS:NZ	1:B:136:GLY:HA3	2.12	0.64
1:B:698:LEU:HD23	1:B:703:VAL:HG23	1.77	0.64
1:C:486:MET:CB	4:C:910:HOH:O	2.44	0.64
1:B:460:ASP:HA	4:B:913:HOH:O	1.96	0.64
1:A:656:ILE:HD12	1:A:656:ILE:H	1.62	0.64
1:B:301:VAL:CG2	1:B:304:GLU:CD	2.65	0.64
1:A:705:GLN:CB	1:A:710:ILE:HD13	2.28	0.64
1:B:349:LYS:HA	1:B:377:ILE:HD12	1.80	0.64
1:B:587:ILE:HD11	1:B:593:LYS:HG2	1.79	0.64
1:C:517:PHE:O	4:C:915:HOH:O	2.15	0.64
1:B:81:LYS:HZ2	1:B:135:GLU:C	2.00	0.64
1:A:93:VAL:HG12	1:A:297:LEU:HD12	1.78	0.63
1:A:502:ASN:OD1	4:A:912:HOH:O	2.15	0.63
1:C:66:THR:O	1:C:69:ILE:HG12	1.97	0.63
1:C:325:THR:O	1:C:328:GLU:HB3	1.98	0.63
1:B:68:THR:HG23	1:B:164:ILE:HG21	1.80	0.63
1:B:327:THR:CB	4:B:914:HOH:O	2.46	0.63
1:B:340:LYS:HG2	1:B:340:LYS:O	1.98	0.63
1:B:537:GLY:HA2	1:B:555:GLN:HG2	1.79	0.63
1:C:328:GLU:O	4:C:909:HOH:O	2.15	0.63
1:B:395:SER:HA	1:B:414:HIS:HD2	1.61	0.63
1:A:1:MET:HG3	4:A:904:HOH:O	1.97	0.63
1:C:715:GLN:HA	1:C:715:GLN:OE1	1.97	0.63
1:A:665:ILE:HD12	1:A:666:THR:H	1.63	0.63
1:B:516:LEU:N	4:B:910:HOH:O	1.93	0.63
1:B:535:ILE:HD12	1:B:535:ILE:C	2.19	0.63
1:A:280:ARG:NH2	1:A:313:GLU:OE2	2.32	0.63
1:C:700:LEU:HA	1:C:719:ARG:NH2	2.09	0.63
1:A:232:LEU:HD12	1:A:476:GLY:HA3	1.81	0.63
1:A:659:LYS:O	1:A:662:LYS:HE3	1.98	0.63
1:B:49:ILE:HD12	1:B:479:PHE:CD2	2.34	0.62
1:C:446:LEU:N	4:C:921:HOH:O	2.31	0.62
1:A:646:ILE:HD12	1:A:733:ARG:HG2	1.81	0.62
1:B:465:ASN:OD1	4:B:913:HOH:O	2.15	0.62
1:B:506:LEU:HB2	1:B:515:ALA:HB3	1.81	0.62
1:C:232:LEU:HD22	1:C:476:GLY:HA3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:CD1	1:B:633:PHE:CD2	2.81	0.62
1:C:165:VAL:HG23	1:C:181:ILE:HA	1.82	0.62
1:A:484:PHE:CE2	1:A:539:VAL:HG22	2.34	0.62
1:B:491:VAL:CG2	1:B:491:VAL:O	2.46	0.62
1:A:187:PRO:O	1:B:379:ARG:HD2	2.00	0.62
1:C:593:LYS:NZ	4:C:917:HOH:O	2.19	0.62
1:A:515:ALA:O	1:A:516:LEU:HD12	1.99	0.61
1:C:28:THR:HG23	1:C:30:ILE:HG22	1.81	0.61
1:B:8:TRP:CD2	1:B:536:LEU:HD22	2.35	0.61
1:B:607:GLN:O	1:B:607:GLN:HG2	2.01	0.61
1:A:40:ILE:HG23	1:A:45:ALA:HB1	1.81	0.61
1:B:147:ILE:HG23	1:B:148:GLN:HG3	1.82	0.61
1:C:307:PHE:CZ	1:C:311:GLN:NE2	2.68	0.61
1:B:543:GLU:HA	1:B:548:GLN:HG2	1.82	0.61
1:C:60:LEU:HD23	1:C:65:MET:HE1	1.81	0.61
1:C:664:LEU:O	1:C:712:ILE:HD11	2.00	0.61
1:C:540:GLN:CG	4:C:906:HOH:O	2.48	0.61
1:B:375:LEU:HD23	1:B:386:GLY:HA3	1.82	0.61
1:A:1:MET:CG	4:A:904:HOH:O	2.49	0.60
1:B:299:THR:CG2	1:B:304:GLU:HG3	2.31	0.60
1:B:429:LEU:HG	1:B:433:LEU:HD12	1.83	0.60
1:B:626:ASN:O	1:B:630:GLN:HG2	2.02	0.60
1:B:463:ILE:HD11	1:B:550:PRO:CD	2.31	0.60
1:C:60:LEU:HD23	1:C:65:MET:HE2	1.83	0.60
1:B:456:LEU:HB3	1:B:486:MET:HE2	1.83	0.60
1:A:621:MET:HE1	1:A:736:VAL:HA	1.83	0.60
1:C:1:MET:HE1	1:C:634:SER:HA	1.83	0.60
1:C:93:VAL:HG22	1:C:297:LEU:HD12	1.84	0.60
1:C:486:MET:CG	4:C:910:HOH:O	2.48	0.60
1:B:294:CYS:SG	1:B:298:MET:HE2	2.42	0.60
1:A:294:CYS:SG	1:A:298:MET:HE3	2.41	0.59
1:B:489:LEU:CA	4:B:901:HOH:O	2.38	0.59
1:B:520:ASN:HA	1:B:522:HIS:CE1	2.37	0.59
1:B:597:ASN:OD1	1:B:598:GLU:HG3	2.02	0.59
1:C:570:LYS:HA	1:C:570:LYS:HE2	1.85	0.59
1:A:599:TYR:HD2	1:A:605:ILE:HG23	1.68	0.59
1:A:743:GLN:HG2	1:A:744:ASP:H	1.66	0.59
1:B:349:LYS:HA	1:B:377:ILE:CD1	2.31	0.59
1:C:588:HIS:CE1	1:C:589:PRO:HG2	2.37	0.59
1:B:4:PRO:HG3	1:B:558:ALA:HB2	1.85	0.59
1:B:284:VAL:HG11	1:B:292:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:TRP:CD1	1:C:549:SER:HB3	2.38	0.59
1:A:284:VAL:HG12	1:A:289:ASP:O	2.03	0.58
1:A:375:LEU:HD23	1:A:386:GLY:HA3	1.85	0.58
1:C:329:GLU:C	4:C:909:HOH:O	2.40	0.58
1:A:365:VAL:HG22	1:A:370:LEU:O	2.02	0.58
1:C:700:LEU:HD11	1:C:721:ILE:HA	1.85	0.58
1:C:337:LYS:HG2	1:C:342:ASP:OD2	2.03	0.58
1:A:40:ILE:HG23	1:A:45:ALA:CB	2.34	0.58
1:B:461:ILE:HG12	1:B:486:MET:HE1	1.85	0.58
1:C:68:THR:CG2	1:C:164:ILE:HG21	2.34	0.58
1:C:245:LYS:HE2	1:C:245:LYS:HA	1.85	0.58
1:C:572:LYS:N	4:C:919:HOH:O	2.36	0.58
1:A:42:ASP:HB2	1:A:44:GLN:OE1	2.04	0.58
1:B:49:ILE:CD1	1:B:479:PHE:CD2	2.87	0.58
1:C:524:GLU:N	1:C:525:PRO:HD2	2.18	0.58
1:B:485:GLU:CB	1:B:536:LEU:CD1	2.82	0.58
1:C:373:LEU:HG	1:C:375:LEU:HD21	1.85	0.58
1:A:440:LEU:HG	1:A:444:THR:HB	1.87	0.57
1:A:54:ASP:OD1	1:A:55:ILE:N	2.37	0.57
1:B:615:ARG:HD2	1:B:616:ASP:OD1	2.03	0.57
1:A:44:GLN:CD	1:A:44:GLN:H	2.06	0.57
1:A:369:ALA:CB	1:A:448:PRO:HG3	2.34	0.57
1:B:106:LEU:HD11	1:B:209:LEU:HB3	1.86	0.57
1:B:566:ASP:HA	1:B:745:PHE:CE1	2.39	0.57
1:C:85:TYR:HE2	4:C:918:HOH:O	1.74	0.57
1:A:610:ASP:HA	1:A:633:PHE:HA	1.87	0.57
1:B:294:CYS:SG	1:B:298:MET:CE	2.92	0.57
1:A:39:SER:O	1:A:41:ILE:HG12	2.05	0.57
1:B:456:LEU:HB3	1:B:486:MET:HE3	1.86	0.57
1:A:522:HIS:C	4:A:901:HOH:O	2.34	0.57
1:C:668:GLN:OE1	1:C:668:GLN:CA	2.47	0.57
1:B:563:GLN:HE21	1:B:635:GLN:HB3	1.69	0.57
1:C:405:GLU:HG2	1:C:406:LEU:HG	1.86	0.57
1:B:288:ASP:CG	4:B:903:HOH:O	2.36	0.57
1:B:336:THR:O	1:B:336:THR:HG22	2.05	0.57
1:C:395:SER:HB3	1:C:398:GLU:HG2	1.87	0.57
1:A:156:VAL:HG22	1:A:161:VAL:HB	1.87	0.56
1:A:223:ILE:HA	1:A:273:ILE:CG2	2.35	0.56
1:C:593:LYS:CD	4:C:917:HOH:O	2.40	0.56
1:C:662:LYS:O	1:C:666:THR:HG23	2.05	0.56
1:A:4:PRO:HG3	1:A:558:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LYS:CA	1:B:377:ILE:CD1	2.80	0.56
1:B:486:MET:HB2	1:B:535:ILE:CD1	2.25	0.56
1:C:541:ILE:O	4:C:916:HOH:O	2.17	0.56
1:B:299:THR:HG21	1:B:304:GLU:HG3	1.88	0.56
1:A:463:ILE:O	1:A:467:ARG:HG3	2.05	0.56
1:C:473:ARG:HG2	1:C:473:ARG:HH11	1.71	0.56
1:A:494:VAL:O	1:A:495:LYS:HD2	2.06	0.56
1:C:331:MET:N	4:C:909:HOH:O	2.38	0.56
1:C:655:ASP:OD1	1:C:656:ILE:N	2.38	0.56
1:A:628:LEU:O	1:A:631:LEU:HB2	2.05	0.56
1:A:665:ILE:CD1	1:A:666:THR:HG23	2.35	0.56
1:C:714:GLN:O	1:C:715:GLN:OE1	2.23	0.56
1:B:301:VAL:CG2	1:B:304:GLU:OE2	2.47	0.56
1:B:610:ASP:N	1:B:610:ASP:OD1	2.38	0.56
1:C:30:ILE:CG2	1:C:465:ASN:HB3	2.36	0.56
1:C:664:LEU:C	1:C:712:ILE:HD11	2.26	0.56
1:B:2:ILE:HG21	1:B:557:ILE:HD13	1.88	0.56
1:B:554:ILE:HD12	4:B:910:HOH:O	2.06	0.56
1:A:54:ASP:CG	1:A:242:GLN:HE22	2.10	0.55
1:A:126:GLU:HG2	1:A:130:ARG:HD2	1.88	0.55
1:B:390:SER:HB2	1:B:396:MET:HG2	1.88	0.55
1:B:232:LEU:HD21	1:B:474:PRO:HB2	1.88	0.55
1:A:563:GLN:HB3	1:A:635:GLN:HG3	1.89	0.55
1:B:343:LEU:O	1:B:370:LEU:CD2	2.53	0.55
1:A:350:GLU:CG	4:A:905:HOH:O	2.54	0.55
1:B:375:LEU:HD23	1:B:386:GLY:CA	2.36	0.55
1:A:147:ILE:HG23	1:A:148:GLN:HG2	1.88	0.55
1:A:692:PHE:O	1:A:696:VAL:HG13	2.07	0.55
1:B:364:ILE:HG23	1:B:368:PHE:HD2	1.71	0.54
1:B:485:GLU:CA	1:B:536:LEU:HD12	2.37	0.54
1:A:54:ASP:HA	1:A:238:SER:OG	2.08	0.54
1:B:399:ILE:CD1	1:B:433:LEU:HD23	2.37	0.54
1:C:232:LEU:HD21	1:C:474:PRO:HB2	1.88	0.54
1:C:572:LYS:CA	4:C:919:HOH:O	2.54	0.54
1:A:412:GLY:HA3	1:A:417:ALA:HA	1.90	0.54
1:B:628:LEU:HD13	1:B:752:ILE:HG23	1.89	0.54
1:C:1:MET:HE2	1:C:634:SER:CB	2.37	0.54
1:C:392:ASP:HA	1:C:415:MET:HE2	1.90	0.54
1:A:191:TYR:CD1	1:A:192:PRO:HD2	2.42	0.54
1:A:354:GLU:HA	1:A:357:LEU:HG	1.90	0.54
1:B:698:LEU:CD2	1:B:703:VAL:HG23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:OG	1:A:186:HIS:HB3	2.07	0.53
1:C:30:ILE:HG23	1:C:31:VAL:N	2.23	0.53
1:B:580:ASP:OD2	1:B:583:ILE:N	2.36	0.53
1:C:299:THR:CG2	1:C:308:LEU:HD12	2.34	0.53
1:C:621:MET:HE2	1:C:739:GLN:HB3	1.90	0.53
1:A:336:THR:O	1:A:340:LYS:HG3	2.09	0.53
1:C:717:ASP:C	4:C:908:HOH:O	2.41	0.53
1:A:54:ASP:HB2	1:A:242:GLN:HE22	1.72	0.53
1:A:467:ARG:O	1:A:470:ASN:HB2	2.08	0.53
1:B:399:ILE:HG12	1:B:433:LEU:HD23	1.91	0.53
1:B:587:ILE:CG2	1:B:615:ARG:HH21	2.22	0.53
1:C:677:MET:O	1:C:681:GLN:HG3	2.09	0.53
1:B:42:ASP:O	1:B:46:ILE:CG1	2.53	0.53
1:B:504:LEU:HB3	1:B:517:PHE:HB3	1.90	0.53
1:C:440:LEU:HA	1:C:443:THR:HG22	1.90	0.53
1:C:485:GLU:HA	1:C:536:LEU:HD12	1.91	0.53
1:A:540:GLN:HE21	1:A:551:GLN:HE21	1.57	0.53
1:B:346:LEU:CD2	1:B:426:ILE:HG23	2.39	0.53
1:B:462:THR:CG2	4:B:913:HOH:O	2.30	0.53
1:B:481:ARG:HG3	1:B:482:PRO:HD2	1.89	0.53
1:A:55:ILE:HD12	1:A:238:SER:HB2	1.90	0.53
1:B:489:LEU:CD1	1:B:535:ILE:HG13	2.38	0.53
1:C:609:THR:OG1	4:C:912:HOH:O	2.19	0.53
1:B:535:ILE:C	1:B:535:ILE:CD1	2.78	0.52
1:A:463:ILE:HG23	1:A:541:ILE:HD13	1.90	0.52
1:C:28:THR:HG21	1:C:465:ASN:HA	1.91	0.52
1:B:237:ARG:NH2	1:B:472:LEU:O	2.42	0.52
1:B:489:LEU:HD11	1:B:535:ILE:HG13	1.89	0.52
1:B:631:LEU:HD22	1:B:632:GLN:N	2.24	0.52
1:C:116:ASN:C	4:C:907:HOH:O	2.43	0.52
1:C:373:LEU:HG	1:C:375:LEU:CD2	2.40	0.52
1:A:524:GLU:HB3	1:A:525:PRO:HD3	1.91	0.52
1:B:185:MET:HG2	1:B:194:GLN:HB3	1.90	0.52
1:B:709:LEU:CG	4:B:909:HOH:O	2.35	0.52
1:A:7:LYS:NZ	1:A:606:LYS:O	2.42	0.52
1:A:350:GLU:HB2	4:A:905:HOH:O	2.07	0.52
1:A:662:LYS:HG3	1:A:663:ALA:N	2.25	0.52
1:B:621:MET:HE3	1:B:736:VAL:HA	1.90	0.52
1:A:614:LEU:HD13	1:A:636:LEU:HD11	1.92	0.52
1:A:741:LEU:C	1:A:741:LEU:HD13	2.30	0.52
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:LYS:HD2	1:B:725:LYS:N	2.23	0.52
1:C:434:ASN:C	4:C:913:HOH:O	2.48	0.52
1:C:89:ASP:OD1	1:C:92:GLY:N	2.42	0.52
1:C:226:ILE:HD12	1:C:273:ILE:HD12	1.92	0.52
1:B:68:THR:HG23	1:B:164:ILE:HD13	1.91	0.52
1:B:385:LYS:HD2	1:B:420:THR:OG1	2.10	0.52
1:B:535:ILE:O	1:B:535:ILE:CD1	2.46	0.52
1:A:593:LYS:HE3	1:A:600:TYR:CD2	2.45	0.51
1:C:718:LYS:HD3	4:C:908:HOH:O	2.10	0.51
1:B:81:LYS:HE3	1:B:136:GLY:C	2.31	0.51
1:B:85:TYR:HE1	1:B:113:HIS:HD1	1.57	0.51
1:C:157:GLN:HE21	1:C:163:VAL:H	1.57	0.51
1:C:477:THR:C	1:C:479:PHE:H	2.13	0.51
1:B:15:GLU:HB3	1:B:41:ILE:HD13	1.92	0.51
1:B:465:ASN:N	1:B:465:ASN:HD22	2.08	0.51
1:C:125:ASN:N	4:C:918:HOH:O	2.43	0.51
1:C:572:LYS:C	4:C:919:HOH:O	2.49	0.51
1:C:572:LYS:HB2	4:C:919:HOH:O	2.09	0.51
1:C:626:ASN:C	1:C:626:ASN:HD22	2.14	0.51
1:C:652:PRO:O	1:C:657:PHE:HE1	1.93	0.51
1:B:300:ASP:N	1:B:300:ASP:OD1	2.43	0.51
1:B:535:ILE:HD12	4:B:908:HOH:O	2.11	0.51
1:A:85:TYR:O	1:A:143:VAL:N	2.43	0.51
1:B:75:ALA:HB1	1:B:80:GLU:HB2	1.93	0.51
1:B:755:GLN:O	1:B:756:LEU:C	2.49	0.51
1:A:605:ILE:H	1:A:630:GLN:HE22	1.57	0.51
1:A:696:VAL:HG12	1:A:726:VAL:HG13	1.91	0.51
1:B:463:ILE:HD11	1:B:550:PRO:N	2.26	0.51
1:C:124:PRO:HA	4:C:918:HOH:O	2.11	0.51
1:C:483:ILE:HB	4:C:902:HOH:O	1.99	0.51
1:A:577:THR:O	1:A:580:ASP:HB2	2.10	0.51
1:B:683:LEU:C	1:B:685:VAL:HG13	2.32	0.51
1:C:1:MET:CE	1:C:634:SER:HA	2.40	0.51
1:A:31:VAL:HG13	1:A:472:LEU:HD11	1.92	0.50
1:B:516:LEU:HD11	1:B:551:GLN:NE2	2.15	0.50
1:A:705:GLN:HB2	1:A:710:ILE:CD1	2.41	0.50
1:A:733:ARG:O	1:A:736:VAL:HG22	2.11	0.50
1:B:66:THR:O	1:B:70:GLU:HG2	2.11	0.50
1:C:308:LEU:C	4:C:911:HOH:O	2.47	0.50
1:A:30:ILE:HG23	1:A:31:VAL:N	2.26	0.50
1:B:231:SER:HA	1:B:477:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:HE1	1:C:346:LEU:HB2	1.76	0.50
1:C:638:ILE:HD12	1:C:745:PHE:CE1	2.46	0.50
1:A:276:ILE:O	1:A:280:ARG:HD2	2.11	0.50
1:B:587:ILE:HG21	1:B:615:ARG:HH21	1.77	0.50
1:B:617:LEU:HD11	1:B:741:LEU:HD11	1.93	0.50
1:C:68:THR:HG23	1:C:164:ILE:CG2	2.42	0.50
1:C:329:GLU:O	1:C:333:MET:HG3	2.12	0.50
1:A:413:HIS:CE1	1:A:416:ALA:HB3	2.47	0.50
1:A:463:ILE:HD12	1:A:463:ILE:N	2.25	0.50
1:A:686:LYS:HB3	1:A:687:PRO:HD2	1.92	0.50
1:B:97:THR:HG23	1:B:298:MET:HG2	1.93	0.50
1:C:123:GLY:O	4:C:918:HOH:O	2.20	0.50
1:A:653:ASN:HB2	1:A:656:ILE:CD1	2.41	0.50
1:A:692:PHE:CE1	1:A:730:ARG:HG3	2.46	0.50
1:B:316:ASN:OD1	1:B:319:ARG:NH1	2.45	0.50
1:C:1:MET:HB3	1:C:559:MET:O	2.12	0.50
1:C:72:ILE:O	1:C:76:ILE:HG13	2.12	0.50
1:A:705:GLN:N	4:A:903:HOH:O	1.83	0.50
1:B:58:ASP:OD1	1:B:59:ALA:N	2.45	0.50
1:B:301:VAL:HB	1:B:304:GLU:CG	2.41	0.50
1:B:460:ASP:C	4:B:913:HOH:O	2.49	0.50
1:C:407:ILE:HG23	1:C:419:MET:CE	2.41	0.50
1:B:81:LYS:NZ	1:B:136:GLY:CA	2.74	0.50
1:C:489:LEU:HD12	1:C:535:ILE:HG13	1.93	0.50
1:C:544:TRP:NE1	1:C:549:SER:HB3	2.24	0.50
1:B:69:ILE:HG22	1:B:73:LYS:CD	2.28	0.50
1:B:489:LEU:O	1:B:532:PRO:HA	2.11	0.50
1:A:491:VAL:HG13	1:A:506:LEU:CD2	2.42	0.49
1:A:599:TYR:CD2	1:A:605:ILE:HG23	2.46	0.49
1:B:456:LEU:O	1:B:486:MET:HG2	2.12	0.49
1:B:553:ILE:HB	4:B:912:HOH:O	2.11	0.49
1:C:30:ILE:HG21	1:C:465:ASN:HB3	1.93	0.49
1:C:736:VAL:O	1:C:740:LEU:HB2	2.11	0.49
1:B:657:PHE:CD1	1:B:693:MET:HG2	2.47	0.49
1:B:662:LYS:O	1:B:665:ILE:HG13	2.12	0.49
1:C:344:PHE:CE1	1:C:346:LEU:HB2	2.46	0.49
1:A:22:THR:HG23	1:A:32:LYS:HD2	1.94	0.49
1:A:709:LEU:HD22	1:A:709:LEU:H	1.76	0.49
1:C:731:GLN:NE2	4:C:922:HOH:O	2.41	0.49
1:A:685:VAL:HG22	1:A:686:LYS:H	1.78	0.49
1:C:34:ILE:O	1:C:38:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:O	1:B:62:LEU:HB2	2.13	0.49
1:B:301:VAL:HB	1:B:304:GLU:CD	2.33	0.49
1:B:353:HIS:HD2	1:B:355:GLY:H	1.60	0.49
1:B:631:LEU:HD11	1:B:633:PHE:CB	2.21	0.49
1:B:225:THR:HG23	1:B:230:VAL:HG23	1.94	0.49
1:B:491:VAL:HG22	1:B:530:GLU:N	2.27	0.49
1:A:399:ILE:HD12	1:A:436:TRP:CE3	2.48	0.49
1:C:30:ILE:HG23	1:C:31:VAL:H	1.78	0.49
1:C:71:ARG:HG3	1:C:139:LEU:HD22	1.95	0.49
1:C:610:ASP:C	4:C:912:HOH:O	2.50	0.48
1:C:456:LEU:HG	1:C:484:PHE:CD1	2.48	0.48
1:A:85:TYR:HE1	1:A:113:HIS:HD2	1.61	0.48
1:A:624:LEU:O	1:A:628:LEU:N	2.45	0.48
1:C:282:ASN:O	1:C:286:ARG:HG3	2.13	0.48
1:A:261:GLU:HB3	1:A:313:GLU:CG	2.32	0.48
1:A:704:THR:CG2	1:A:711:ARG:HB3	2.43	0.48
1:B:15:GLU:HB3	1:B:41:ILE:CD1	2.43	0.48
1:B:55:ILE:O	1:B:235:GLU:HG3	2.13	0.48
1:B:69:ILE:HG23	1:B:209:LEU:HD23	1.96	0.48
1:B:299:THR:HG21	1:B:308:LEU:HD12	1.96	0.48
1:C:31:VAL:HG13	1:C:472:LEU:HD11	1.94	0.48
1:C:587:ILE:HG13	1:C:600:TYR:CD1	2.49	0.48
1:A:576:PHE:CD2	1:A:583:ILE:HG12	2.49	0.48
1:B:60:LEU:HD21	1:B:69:ILE:HD11	1.95	0.48
1:B:680:CYS:HA	1:B:685:VAL:HG22	1.95	0.48
1:C:68:THR:CG2	1:C:164:ILE:HD13	2.44	0.48
1:C:171:ILE:HD13	1:C:175:LEU:HD21	1.95	0.48
1:C:223:ILE:HA	1:C:273:ILE:HG21	1.95	0.48
1:C:564:ILE:HG22	1:C:745:PHE:CZ	2.48	0.48
1:A:712:ILE:HG22	1:A:714:GLN:H	1.77	0.48
1:C:157:GLN:NE2	1:C:163:VAL:H	2.12	0.48
1:A:399:ILE:HG12	1:A:433:LEU:HD22	1.95	0.48
1:A:689:THR:O	1:A:693:MET:HG3	2.14	0.48
1:B:349:LYS:N	1:B:377:ILE:HD12	2.28	0.48
1:B:478:ASP:HA	4:B:902:HOH:O	1.90	0.48
1:C:87:ASP:O	1:C:114:ILE:HD11	2.14	0.48
1:A:54:ASP:CB	1:A:242:GLN:HE22	2.26	0.48
1:B:554:ILE:HD12	1:B:554:ILE:H	1.79	0.48
1:C:237:ARG:NH2	1:C:472:LEU:O	2.46	0.48
1:A:346:LEU:HG	1:A:373:LEU:HB3	1.95	0.48
1:B:327:THR:HB	4:B:914:HOH:O	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ALA:O	1:C:65:MET:SD	2.72	0.48
1:C:63:SER:O	1:C:65:MET:N	2.46	0.48
1:C:335:GLU:HG3	1:C:368:PHE:CE1	2.49	0.48
1:A:326:ILE:HG22	1:A:360:VAL:HG11	1.95	0.47
1:A:57:HIS:ND1	1:A:192:PRO:HB2	2.29	0.47
1:B:68:THR:CG2	1:B:164:ILE:HG21	2.44	0.47
1:C:124:PRO:HG3	1:C:149:GLY:HA3	1.96	0.47
1:C:621:MET:CE	1:C:739:GLN:HB3	2.43	0.47
1:B:333:MET:O	1:B:337:LYS:HG2	2.13	0.47
1:B:401:SER:HA	1:B:404:GLN:OE1	2.14	0.47
1:B:463:ILE:HG23	1:B:541:ILE:HD13	1.96	0.47
1:C:440:LEU:HA	1:C:443:THR:CG2	2.43	0.47
1:C:458:GLU:HA	1:C:461:ILE:HD13	1.96	0.47
1:B:530:GLU:OE1	1:B:530:GLU:CA	2.50	0.47
1:C:163:VAL:O	1:C:178:ALA:HB1	2.14	0.47
1:C:167:ASP:OD1	1:C:168:HIS:N	2.47	0.47
1:C:489:LEU:O	1:C:532:PRO:HA	2.15	0.47
1:A:42:ASP:CB	1:A:44:GLN:OE1	2.63	0.47
1:A:371:PRO:HG3	1:A:391:ILE:HG12	1.97	0.47
1:B:25:LEU:O	1:B:26:LYS:C	2.53	0.47
1:B:101:ILE:HD13	1:B:216:TYR:OH	2.15	0.47
1:B:296:LEU:HA	1:B:308:LEU:HD13	1.95	0.47
1:B:334:ALA:HB3	1:B:368:PHE:CE2	2.50	0.47
1:B:485:GLU:HG3	1:B:536:LEU:HD13	1.95	0.47
1:B:486:MET:H	1:B:535:ILE:HD12	1.78	0.47
1:B:491:VAL:CG2	1:B:529:ASP:CA	2.82	0.47
1:C:64:ASP:HB3	1:C:180:ALA:HB1	1.95	0.47
1:C:447:ASP:C	4:C:904:HOH:O	2.51	0.47
1:B:336:THR:O	1:B:336:THR:CG2	2.62	0.47
1:B:492:SER:OG	1:B:512:ASN:ND2	2.48	0.47
1:B:536:LEU:HD12	1:B:536:LEU:HA	1.79	0.47
1:B:588:HIS:CD2	1:B:589:PRO:CD	2.72	0.47
1:A:125:ASN:ND2	4:A:908:HOH:O	2.48	0.47
1:A:714:GLN:HB3	1:A:715:GLN:H	1.49	0.47
1:B:223:ILE:HA	1:B:273:ILE:HG21	1.96	0.47
1:B:651:ILE:CD1	1:B:730:ARG:HG2	2.44	0.47
1:C:322:ILE:O	1:C:326:ILE:HG13	2.14	0.46
1:C:593:LYS:CE	4:C:917:HOH:O	2.58	0.46
1:A:188:SER:HA	1:B:379:ARG:HE	1.78	0.46
1:A:323:VAL:O	1:A:327:THR:OG1	2.22	0.46
1:A:407:ILE:HG21	1:A:410:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ILE:HD12	1:A:666:THR:HG23	1.97	0.46
1:A:714:GLN:O	1:A:716:PRO:HD3	2.14	0.46
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.79	0.46
1:C:489:LEU:HD12	1:C:535:ILE:CG1	2.46	0.46
1:B:47:GLU:N	4:B:911:HOH:O	1.98	0.46
1:B:200:GLY:O	1:B:204:LYS:HG2	2.15	0.46
1:A:231:SER:OG	1:A:478:ASP:OD2	2.27	0.46
1:B:325:THR:O	1:B:329:GLU:HG3	2.16	0.46
1:C:221:VAL:HG11	1:C:239:LEU:HD13	1.97	0.46
1:A:517:PHE:HE2	1:A:557:ILE:HG22	1.80	0.46
1:C:485:GLU:HG3	1:C:536:LEU:CD1	2.45	0.46
1:A:86:GLY:HA2	1:A:143:VAL:HG23	1.98	0.46
1:A:593:LYS:HE2	1:A:599:TYR:HA	1.98	0.46
1:A:671:ASN:HB2	1:A:709:LEU:CD1	2.45	0.46
1:A:701:LYS:HB2	1:A:701:LYS:NZ	2.30	0.46
1:C:700:LEU:HD23	1:C:719:ARG:CZ	2.45	0.46
1:A:631:LEU:HD12	1:A:633:PHE:HB3	1.97	0.46
1:A:28:THR:HB	1:A:465:ASN:OD1	2.16	0.46
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.82	0.46
1:B:460:ASP:CA	4:B:913:HOH:O	2.58	0.46
1:C:68:THR:HG23	1:C:164:ILE:HD13	1.98	0.46
1:C:116:ASN:O	1:C:118:PHE:N	2.43	0.46
1:C:334:ALA:HB1	1:C:345:LEU:CD1	2.43	0.46
1:B:8:TRP:CE3	1:B:536:LEU:HD22	2.51	0.46
1:B:17:ILE:CB	4:B:905:HOH:O	2.64	0.46
1:B:301:VAL:CB	1:B:304:GLU:CD	2.84	0.46
1:C:28:THR:HG23	1:C:30:ILE:CG2	2.45	0.46
1:A:47:GLU:O	1:A:51:SER:N	2.45	0.46
1:A:153:ILE:HG21	1:A:178:ALA:HB2	1.98	0.46
1:A:423:ILE:HA	1:A:426:ILE:HD11	1.98	0.46
1:A:481:ARG:HG3	1:A:482:PRO:HD2	1.98	0.46
1:A:491:VAL:HG21	1:A:527:LEU:HD22	1.97	0.46
1:A:707:ASP:O	1:A:709:LEU:HD22	2.16	0.46
1:B:81:LYS:HB3	1:B:137:ILE:HD13	1.98	0.46
1:C:347:LEU:HD12	1:C:374:ILE:CD1	2.46	0.46
1:C:422:ASP:HB2	1:C:425:ASN:HD22	1.81	0.46
1:C:454:VAL:HB	1:C:484:PHE:CD1	2.51	0.46
1:B:534:ASN:ND2	1:B:560:ASN:HB2	2.31	0.45
1:B:554:ILE:CD1	4:B:910:HOH:O	2.62	0.45
1:B:631:LEU:C	1:B:631:LEU:HD13	2.36	0.45
1:A:502:ASN:ND2	4:A:912:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:MET:CE	1:A:739:GLN:HB2	2.46	0.45
1:A:301:VAL:HB	1:A:304:GLU:CG	2.47	0.45
1:A:54:ASP:HB2	1:A:242:GLN:NE2	2.31	0.45
1:A:463:ILE:H	1:A:463:ILE:CD1	2.26	0.45
1:A:580:ASP:O	1:A:582:ASN:N	2.45	0.45
1:A:69:ILE:HG23	1:A:73:LYS:HZ2	1.82	0.45
1:B:101:ILE:O	1:B:105:LEU:HG	2.16	0.45
1:B:294:CYS:SG	1:B:298:MET:HE3	2.56	0.45
1:B:535:ILE:CD1	4:B:908:HOH:O	2.65	0.45
1:C:610:ASP:CG	1:C:634:SER:OG	2.54	0.45
1:A:264:TYR:HE1	1:A:266:ASP:O	2.00	0.45
1:B:246:VAL:HG13	1:B:250:GLN:HG3	1.99	0.45
1:B:465:ASN:N	1:B:465:ASN:ND2	2.65	0.45
1:B:747:GLU:HA	1:B:750:ASN:HD22	1.80	0.45
1:C:1:MET:SD	1:C:561:GLU:N	2.79	0.45
1:C:496:ALA:CB	1:C:501:LYS:HG3	2.46	0.45
1:A:147:ILE:HG12	1:A:171:ILE:HG22	1.99	0.45
1:A:346:LEU:HG	1:A:373:LEU:HD23	1.98	0.45
1:B:86:GLY:HA2	1:B:143:VAL:HG23	1.99	0.45
1:A:491:VAL:HG13	1:A:506:LEU:HD22	1.98	0.45
1:A:656:ILE:HD12	1:A:656:ILE:N	2.31	0.45
1:B:461:ILE:HD13	1:B:486:MET:CE	2.36	0.45
1:A:395:SER:OG	4:A:911:HOH:O	2.14	0.44
1:A:672:ILE:O	1:A:676:GLY:N	2.48	0.44
1:C:452:VAL:CG2	1:C:536:LEU:HD11	2.47	0.44
1:C:599:TYR:OH	1:C:607:GLN:HB2	2.16	0.44
1:A:4:PRO:HG3	1:A:558:ALA:CB	2.46	0.44
1:A:520:ASN:HA	1:A:522:HIS:CE1	2.52	0.44
1:B:300:ASP:N	1:B:304:GLU:OE2	2.50	0.44
1:B:397:PHE:CE1	1:B:401:SER:OG	2.71	0.44
1:C:129:PHE:CD2	1:C:152:GLU:HB3	2.53	0.44
1:C:718:LYS:CA	4:C:908:HOH:O	2.47	0.44
1:B:563:GLN:HE21	1:B:635:GLN:CG	2.30	0.44
1:A:68:THR:CG2	1:A:164:ILE:HG21	2.48	0.44
1:A:685:VAL:HG22	1:A:689:THR:CG2	2.48	0.44
1:B:301:VAL:HB	1:B:304:GLU:HG2	2.00	0.44
1:B:657:PHE:HE1	1:B:693:MET:HA	1.83	0.44
1:C:346:LEU:HD12	1:C:433:LEU:HD12	1.99	0.44
1:C:390:SER:OG	1:C:391:ILE:N	2.50	0.44
1:A:59:ALA:O	1:A:65:MET:HG2	2.18	0.44
1:A:659:LYS:O	1:A:662:LYS:CG	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ASP:OD1	1:C:532:PRO:HB3	2.17	0.44
1:C:496:ALA:HB1	1:C:501:LYS:HG3	1.99	0.44
1:A:79:ASP:OD1	1:A:109:GLN:NE2	2.50	0.44
1:B:440:LEU:HD12	1:B:443:THR:HG21	2.00	0.44
1:A:272:THR:O	1:A:276:ILE:HB	2.18	0.44
1:A:652:PRO:HB2	1:A:657:PHE:CE1	2.53	0.44
1:C:655:ASP:O	1:C:658:LYS:HB2	2.18	0.44
1:A:356:VAL:O	1:A:360:VAL:HG23	2.18	0.44
1:A:678:LEU:HD12	1:A:678:LEU:HA	1.79	0.44
1:C:7:LYS:HD2	1:C:8:TRP:H	1.82	0.44
1:C:631:LEU:HD23	1:C:631:LEU:HA	1.88	0.44
1:A:467:ARG:HG2	1:A:541:ILE:CD1	2.48	0.43
1:A:612:VAL:HG13	1:A:636:LEU:HD13	2.00	0.43
1:A:664:LEU:N	1:A:664:LEU:HD22	2.33	0.43
1:B:44:GLN:C	4:B:911:HOH:O	2.56	0.43
1:B:286:ARG:NH1	1:B:355:GLY:O	2.46	0.43
1:C:164:ILE:HG12	1:C:180:ALA:HB3	2.00	0.43
1:C:311:GLN:HB2	4:C:911:HOH:O	2.18	0.43
1:A:79:ASP:O	1:A:79:ASP:OD2	2.35	0.43
1:B:495:LYS:HB2	1:B:505:LYS:HB3	2.00	0.43
1:B:524:GLU:N	1:B:525:PRO:HD2	2.33	0.43
1:B:90:ALA:HA	1:B:93:VAL:HG22	2.00	0.43
1:B:381:GLN:HE21	1:B:381:GLN:HB3	1.59	0.43
1:B:597:ASN:OD1	1:B:597:ASN:C	2.57	0.43
1:C:679:LEU:HD23	1:C:690:LEU:HD11	2.01	0.43
1:A:280:ARG:NE	1:A:313:GLU:OE2	2.51	0.43
1:B:475:PHE:HD1	1:B:479:PHE:O	2.01	0.43
1:C:68:THR:HG23	1:C:164:ILE:HG21	1.99	0.43
1:C:547:ASN:HD22	1:C:547:ASN:N	2.16	0.43
1:A:183:HIS:HE1	1:A:185:MET:HE2	1.84	0.43
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.70	0.43
1:C:184:PRO:HB2	1:C:194:GLN:HA	2.01	0.43
1:A:350:GLU:HG2	1:A:377:ILE:HB	2.00	0.43
1:A:582:ASN:HD22	1:A:582:ASN:H	1.66	0.43
1:B:167:ASP:OD1	1:B:168:HIS:N	2.47	0.43
1:C:599:TYR:OH	1:C:607:GLN:NE2	2.44	0.43
1:A:296:LEU:O	1:A:299:THR:HG22	2.18	0.43
1:A:656:ILE:CD1	1:A:656:ILE:H	2.31	0.43
1:B:724:SER:OG	1:B:726:VAL:HG22	2.19	0.43
1:B:615:ARG:O	1:B:641:GLN:N	2.41	0.43
1:C:68:THR:CG2	1:C:164:ILE:CG2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLN:HE21	1:A:668:GLN:HB3	1.64	0.43
1:C:132:ALA:O	1:C:137:ILE:HB	2.19	0.43
1:C:529:ASP:OD2	1:C:531:GLN:NE2	2.52	0.43
1:A:502:ASN:CG	4:A:912:HOH:O	2.57	0.42
1:B:49:ILE:HG23	1:B:479:PHE:HE2	1.84	0.42
1:A:423:ILE:HA	1:A:426:ILE:CD1	2.48	0.42
1:A:461:ILE:CD1	1:A:513:ILE:HD13	2.49	0.42
1:A:85:TYR:O	1:A:142:THR:HA	2.19	0.42
1:A:318:GLU:OE2	1:C:20:GLU:N	2.51	0.42
1:B:434:ASN:O	1:B:438:LYS:HE2	2.19	0.42
1:C:135:GLU:HG3	1:C:136:GLY:N	2.34	0.42
1:C:404:GLN:HA	1:C:407:ILE:HB	2.00	0.42
1:C:504:LEU:HB2	4:C:915:HOH:O	2.19	0.42
1:B:269:ASP:OD2	1:B:473:ARG:NH2	2.52	0.42
1:C:452:VAL:HG22	1:C:536:LEU:HD11	2.01	0.42
1:A:390:SER:HB3	1:A:415:MET:HA	2.02	0.42
1:A:693:MET:O	1:A:696:VAL:HG22	2.19	0.42
1:A:709:LEU:N	1:A:709:LEU:CD2	2.80	0.42
1:B:604:GLU:HA	1:B:630:GLN:HE22	1.85	0.42
1:A:621:MET:CE	1:A:736:VAL:HA	2.50	0.42
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.89	0.42
1:B:348:ALA:C	1:B:377:ILE:HD11	2.40	0.42
1:A:34:ILE:HG23	1:A:38:LYS:HE2	2.02	0.42
1:A:79:ASP:O	1:A:79:ASP:CG	2.58	0.42
1:A:462:THR:O	1:A:466:ILE:HG13	2.20	0.42
1:A:656:ILE:HD13	4:A:910:HOH:O	2.18	0.42
1:B:346:LEU:CD1	1:B:373:LEU:HD23	2.50	0.42
1:B:373:LEU:HD11	1:B:419:MET:SD	2.59	0.42
1:B:563:GLN:HE21	1:B:635:GLN:CB	2.32	0.42
1:B:610:ASP:CB	1:B:634:SER:HB2	2.46	0.42
1:C:665:ILE:N	1:C:712:ILE:HD11	2.35	0.42
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.67	0.42
1:A:454:VAL:HB	1:A:484:PHE:HD1	1.85	0.42
1:B:401:SER:HA	1:B:404:GLN:HG2	2.01	0.42
1:A:187:PRO:O	1:B:379:ARG:HB3	2.20	0.42
1:A:696:VAL:HA	1:A:726:VAL:HG11	2.02	0.42
1:C:79:ASP:O	1:C:109:GLN:NE2	2.53	0.42
1:C:83:LEU:O	1:C:140:ILE:HA	2.19	0.42
1:C:489:LEU:CD1	1:C:535:ILE:CG1	2.98	0.42
1:A:588:HIS:CE1	1:A:590:LYS:HB2	2.54	0.42
1:B:753:LYS:HB2	1:B:753:LYS:HE2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.91	0.41
1:A:76:ILE:HG12	1:A:108:ALA:HB2	2.02	0.41
1:B:43:GLU:HA	1:B:46:ILE:HD12	2.02	0.41
1:C:638:ILE:HG22	1:C:640:LEU:HG	2.02	0.41
1:A:455:LEU:HD22	1:A:485:GLU:O	2.20	0.41
1:A:502:ASN:O	1:A:521:GLY:N	2.46	0.41
1:A:605:ILE:N	1:A:630:GLN:HE22	2.18	0.41
1:C:107:GLY:O	1:C:108:ALA:HB3	2.20	0.41
1:C:736:VAL:HG13	1:C:740:LEU:HD12	2.02	0.41
1:A:126:GLU:C	4:A:908:HOH:O	2.49	0.41
1:B:633:PHE:CE2	1:B:756:LEU:HD11	2.55	0.41
1:B:683:LEU:O	1:B:685:VAL:CG1	2.57	0.41
1:C:334:ALA:CB	1:C:345:LEU:HD13	2.44	0.41
1:B:261:GLU:HB3	1:B:313:GLU:HG3	2.02	0.41
1:B:380:GLU:N	1:B:380:GLU:OE1	2.54	0.41
1:C:334:ALA:O	1:C:337:LYS:N	2.53	0.41
1:A:68:THR:HG23	1:A:164:ILE:HG21	2.03	0.41
1:A:195:GLN:O	1:A:236:ASN:ND2	2.46	0.41
1:A:223:ILE:HA	1:A:273:ILE:HG23	2.01	0.41
1:A:350:GLU:HG2	1:A:377:ILE:O	2.21	0.41
1:A:578:GLU:O	1:A:597:ASN:ND2	2.54	0.41
1:A:691:LYS:HB2	1:A:691:LYS:HE2	1.72	0.41
1:A:704:THR:HG23	1:A:711:ARG:HB3	2.03	0.41
1:B:338:VAL:HG13	1:B:339:LYS:N	2.35	0.41
1:B:404:GLN:HB3	1:B:410:PHE:HE2	1.86	0.41
1:B:414:HIS:CD2	1:B:414:HIS:C	2.94	0.41
1:B:638:ILE:HG22	1:B:640:LEU:HD12	2.02	0.41
1:C:445:SER:C	4:C:921:HOH:O	2.57	0.41
1:C:490:SER:O	1:C:508:LEU:HA	2.20	0.41
1:C:651:ILE:CD1	1:C:731:GLN:HG2	2.50	0.41
1:C:296:LEU:HA	1:C:299:THR:HG22	2.03	0.41
1:A:59:ALA:HB2	1:A:204:LYS:HE3	2.02	0.41
1:A:436:TRP:HZ2	4:A:902:HOH:O	2.03	0.41
1:A:504:LEU:HD23	1:A:506:LEU:HD12	2.02	0.41
1:C:588:HIS:CE1	1:C:590:LYS:HG3	2.56	0.41
1:A:9:LYS:O	1:A:451:GLN:OE1	2.38	0.41
1:A:193:PHE:HE2	1:A:236:ASN:CG	2.24	0.41
1:A:421:MET:HE2	1:A:421:MET:HB2	1.94	0.41
1:A:504:LEU:HB2	1:A:521:GLY:HA2	2.03	0.41
1:B:399:ILE:CG1	1:B:433:LEU:HD23	2.51	0.41
1:B:543:GLU:HG2	1:B:543:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:SER:O	1:B:629:GLN:CG	2.47	0.41
1:A:33:LYS:HD3	1:A:454:VAL:CG1	2.50	0.41
1:A:55:ILE:O	1:A:235:GLU:HG3	2.21	0.41
1:C:50:ILE:HG12	1:C:472:LEU:HD23	2.03	0.41
1:C:272:THR:HA	1:C:276:ILE:HD13	2.01	0.41
1:C:292:LEU:HD12	1:C:308:LEU:HD22	2.02	0.41
1:C:348:ALA:HB2	1:C:375:LEU:HB2	2.02	0.41
1:C:392:ASP:HA	1:C:415:MET:CE	2.51	0.41
1:C:626:ASN:C	1:C:626:ASN:ND2	2.74	0.41
1:A:586:LEU:HB3	1:A:601:TYR:CE1	2.56	0.41
1:A:461:ILE:HD12	1:A:513:ILE:HD13	2.03	0.40
1:B:17:ILE:HB	4:B:905:HOH:O	2.21	0.40
1:B:343:LEU:HD22	1:B:438:LYS:HG3	2.03	0.40
1:B:385:LYS:CG	1:B:420:THR:OG1	2.69	0.40
1:B:484:PHE:HB2	1:B:537:GLY:O	2.21	0.40
1:C:157:GLN:HE21	1:C:163:VAL:N	2.18	0.40
1:C:501:LYS:HB3	1:C:502:ASN:H	1.64	0.40
1:C:683:LEU:O	1:C:685:VAL:HG13	2.21	0.40
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.80	0.40
1:B:429:LEU:CG	1:B:433:LEU:HD11	2.42	0.40
1:B:534:ASN:HD21	1:B:560:ASN:HB2	1.84	0.40
1:B:607:GLN:O	1:B:607:GLN:CG	2.68	0.40
1:B:725:LYS:CD	1:B:725:LYS:N	2.80	0.40
1:C:628:LEU:HD23	1:C:631:LEU:HD12	2.02	0.40
1:A:284:VAL:HG21	1:A:312:VAL:HG22	2.03	0.40
1:B:543:GLU:O	1:B:544:TRP:C	2.59	0.40
1:C:171:ILE:HG13	1:C:183:HIS:CE1	2.56	0.40
1:A:524:GLU:N	4:A:901:HOH:O	1.81	0.40
1:A:587:ILE:HD13	1:A:598:GLU:HB3	2.03	0.40
1:A:741:LEU:HD13	1:A:741:LEU:O	2.20	0.40
1:B:42:ASP:C	1:B:46:ILE:HD11	2.41	0.40
1:B:472:LEU:HD22	1:B:479:PHE:HZ	1.87	0.40
1:B:485:GLU:CA	1:B:536:LEU:CD1	3.00	0.40
1:B:613:VAL:HG22	1:B:637:TYR:HB2	2.03	0.40
1:B:655:ASP:OD1	1:B:655:ASP:N	2.54	0.40
1:C:223:ILE:HA	1:C:273:ILE:CG2	2.51	0.40
1:A:343:LEU:O	1:A:370:LEU:HD22	2.20	0.40
1:A:748:ILE:O	1:A:752:ILE:HG13	2.21	0.40
1:C:343:LEU:HB3	1:C:437:MET:HB3	2.02	0.40

All (12) 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:B:681:GLN:OE1	1:C:307:PHE:CD1[1_544]	1.68	0.52
1:A:647:TYR:OH	1:A:691:LYS:CD[3_545]	1.74	0.46
1:B:681:GLN:OE1	1:C:307:PHE:CG[1_544]	1.78	0.42
1:A:677:MET:CE	1:A:744:ASP:CB[2_444]	1.79	0.41
1:B:190:ASN:OD1	1:C:67:LYS:N[3_544]	1.88	0.32
1:A:677:MET:CE	1:A:744:ASP:CA[2_444]	1.93	0.27
1:C:649:ASP:OD1	1:C:705:GLN:NE2[2_544]	1.96	0.24
1:B:194:GLN:OE1	1:C:70:GLU:OE1[3_544]	2.03	0.17
1:A:428:SER:OG	1:A:510:GLU:OE1[1_554]	2.08	0.12
1:B:190:ASN:ND2	1:C:66:THR:CB[3_544]	2.12	0.08
1:B:649:ASP:OD1	1:B:705:GLN:NE2[2_434]	2.16	0.04
1:B:42:ASP:OD2	1:C:212:ASN:ND2[3_544]	2.17	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	754/757 (100%)	720 (96%)	34 (4%)	0	100	100
1	B	754/757 (100%)	711 (94%)	43 (6%)	0	100	100
1	C	754/757 (100%)	715 (95%)	39 (5%)	0	100	100
All	All	2262/2271 (100%)	2146 (95%)	116 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	672/673 (100%)	644 (96%)	28 (4%)	25 58
1	B	672/673 (100%)	639 (95%)	33 (5%)	21 52
1	C	672/673 (100%)	648 (96%)	24 (4%)	30 64
All	All	2016/2019 (100%)	1931 (96%)	85 (4%)	25 58

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	56	ASN
1	A	87	ASP
1	A	155	MET
1	A	231	SER
1	A	238	SER
1	A	245	LYS
1	A	266	ASP
1	A	267	ASN
1	A	383	HIS
1	A	414	HIS
1	A	468	ASP
1	A	502	ASN
1	A	517	PHE
1	A	519	GLN
1	A	535	ILE
1	A	563	GLN
1	A	572	LYS
1	A	576	PHE
1	A	580	ASP
1	A	588	HIS
1	A	597	ASN
1	A	622	GLU
1	A	631	LEU
1	A	689	THR
1	A	701	LYS
1	A	705	GLN
1	A	714	GLN
1	B	19	ASP
1	B	28	THR
1	B	52	ASP
1	B	79	ASP
1	B	99	LEU
1	B	126	GLU

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Mol	Chain	Res	Type
1	B	138	THR
1	B	143	VAL
1	B	156	VAL
1	B	258	LEU
1	B	313	GLU
1	B	342	ASP
1	B	346	LEU
1	B	398	GLU
1	B	434	ASN
1	B	453	ASP
1	B	499	GLN
1	B	517	PHE
1	B	520	ASN
1	B	522	HIS
1	B	542	ASN
1	B	555	GLN
1	B	557	ILE
1	B	568	ARG
1	B	572	LYS
1	B	610	ASP
1	B	634	SER
1	B	653	ASN
1	B	688	ASP
1	B	705	GLN
1	B	719	ARG
1	B	739	GLN
1	B	747	GLU
1	C	6	TYR
1	C	18	SER
1	C	81	LYS
1	C	87	ASP
1	C	88	TYR
1	C	93	VAL
1	C	110	VAL
1	C	112	TRP
1	C	145	ASN
1	C	155	MET
1	C	289	ASP
1	C	421	MET
1	C	424	GLU
1	C	468	ASP
1	C	495	LYS

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Mol	Chain	Res	Type
1	C	501	LYS
1	C	517	PHE
1	C	547	ASN
1	C	571	ARG
1	C	576	PHE
1	C	626	ASN
1	C	673	GLN
1	C	674	LYS
1	C	675	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	242	GLN
1	A	413	HIS
1	A	500	GLN
1	A	519	GLN
1	A	551	GLN
1	A	563	GLN
1	A	582	ASN
1	A	588	HIS
1	A	597	ASN
1	A	630	GLN
1	A	635	GLN
1	A	668	GLN
1	A	750	ASN
1	B	78	ASN
1	B	353	HIS
1	B	381	GLN
1	B	414	HIS
1	B	465	ASN
1	B	512	ASN
1	B	519	GLN
1	B	534	ASN
1	B	540	GLN
1	B	542	ASN
1	B	551	GLN
1	B	555	GLN
1	B	563	GLN
1	B	588	HIS
1	B	630	GLN

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Mol	Chain	Res	Type
1	B	644	HIS
1	B	728	GLN
1	C	78	ASN
1	C	150	HIS
1	C	157	GLN
1	C	169	HIS
1	C	183	HIS
1	C	207	GLN
1	C	242	GLN
1	C	381	GLN
1	C	425	ASN
1	C	503	HIS
1	C	520	ASN
1	C	547	ASN
1	C	607	GLN
1	C	629	GLN
1	C	641	GLN
1	C	743	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 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	SO4	B	805	-	4,4,4	0.47	0	6,6,6	0.05	0
3	SO4	B	804	-	4,4,4	0.41	0	6,6,6	0.04	0
3	SO4	A	805	-	4,4,4	0.49	0	6,6,6	0.08	0
3	SO4	C	805	-	4,4,4	0.48	0	6,6,6	0.05	0
3	SO4	A	804	-	4,4,4	0.51	0	6,6,6	0.05	0
3	SO4	A	803	-	4,4,4	0.47	0	6,6,6	0.05	0
3	SO4	C	804	-	4,4,4	0.44	0	6,6,6	0.05	0
3	SO4	B	803	-	4,4,4	0.45	0	6,6,6	0.04	0
3	SO4	C	803	-	4,4,4	0.42	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

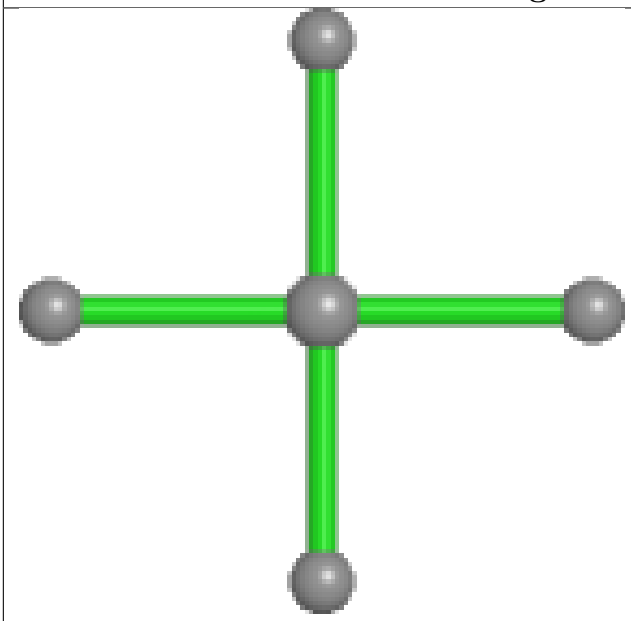
There are no torsion outliers.

There are no ring outliers.

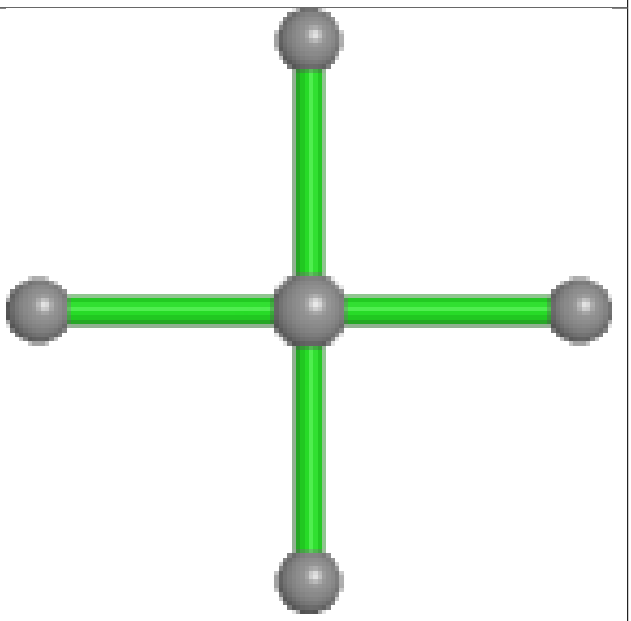
No monomer is involved in short contacts.

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 then 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.

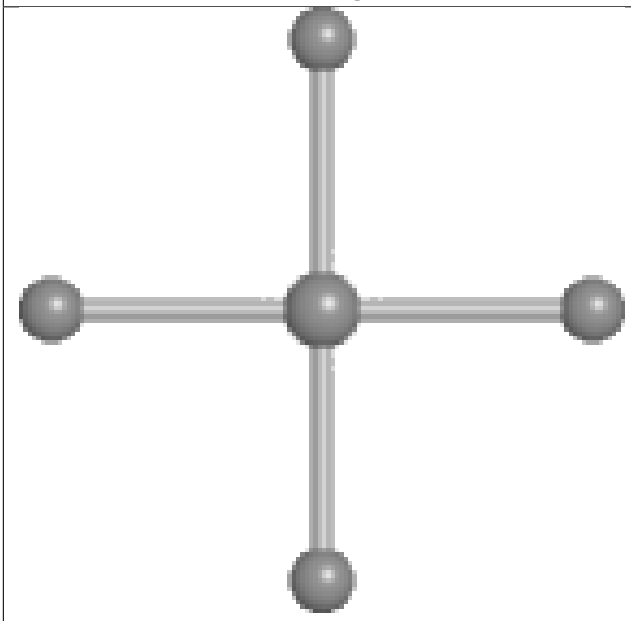
Ligand SO4 B 805



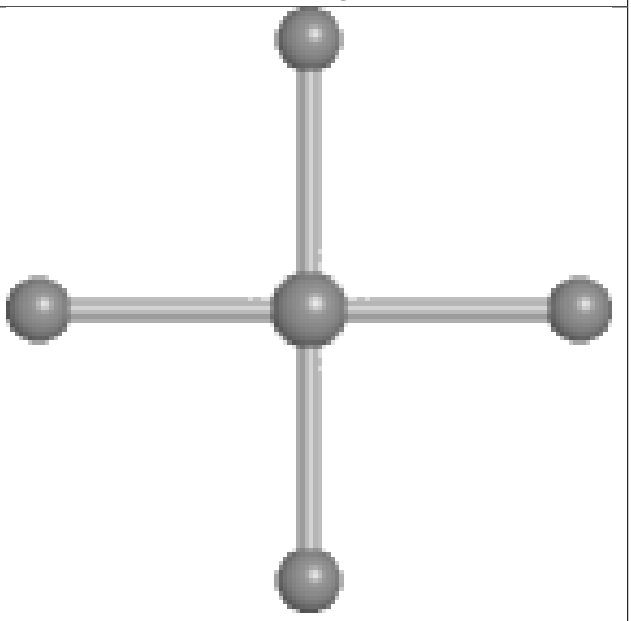
Bond lengths



Bond angles

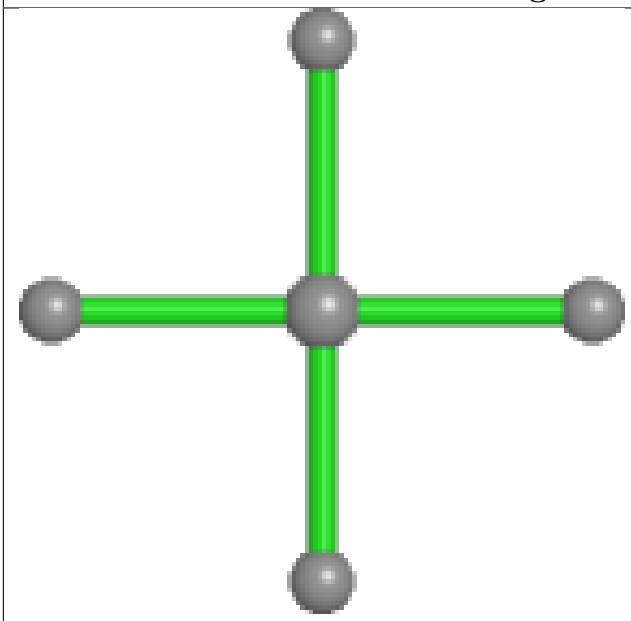


Torsions



Rings

Ligand SO4 B 804



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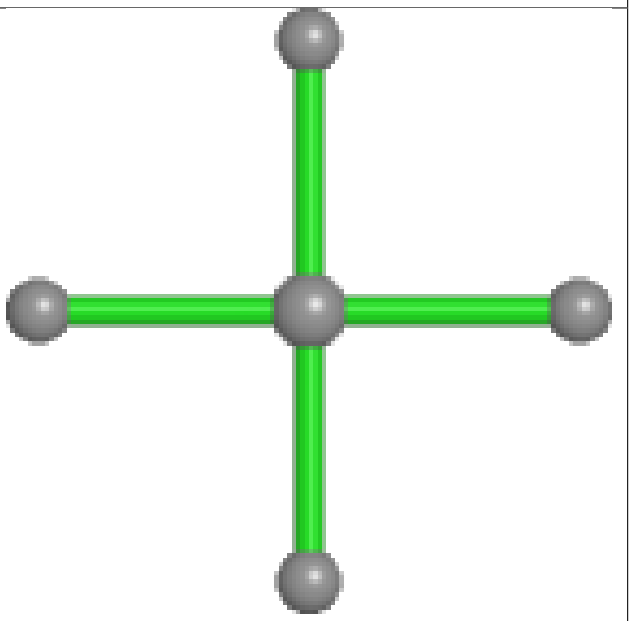

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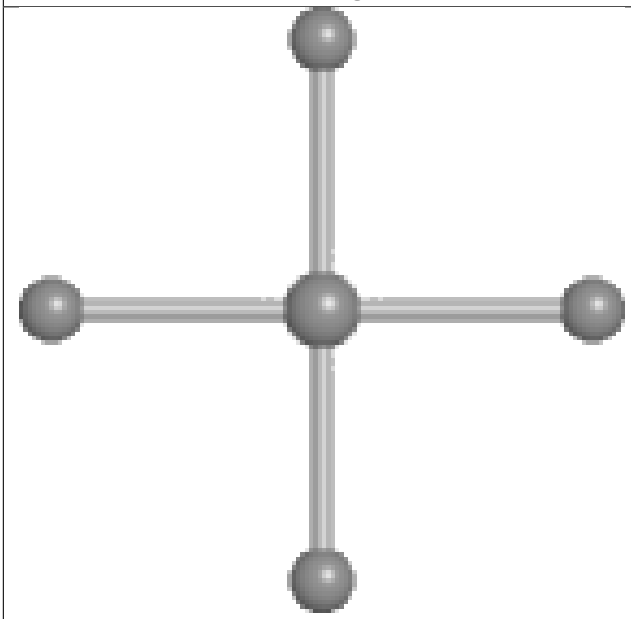

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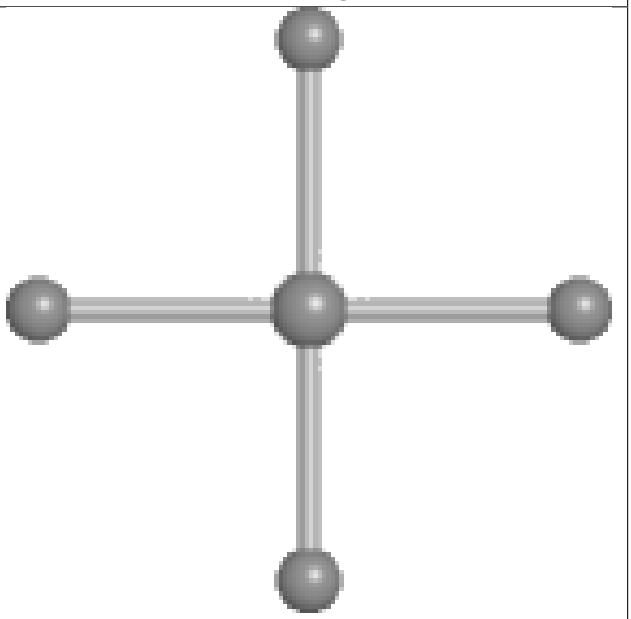
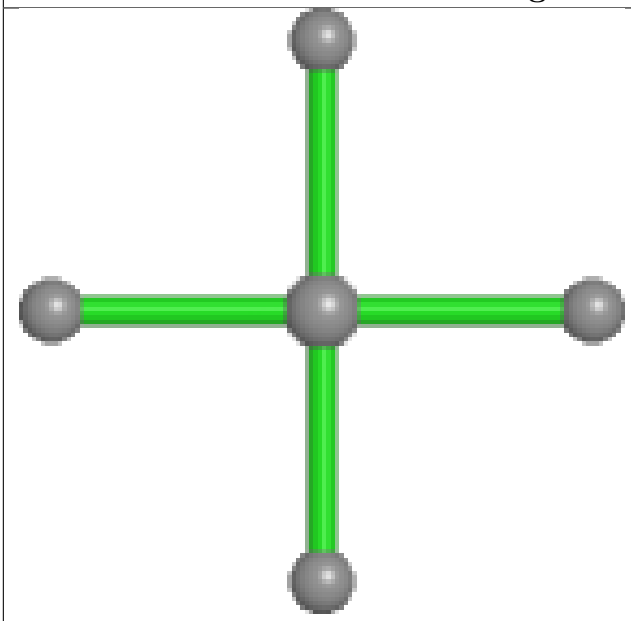
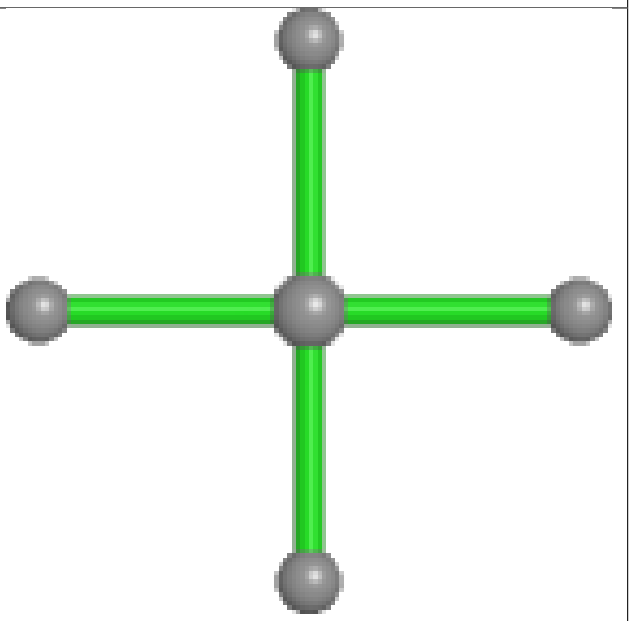


Rings

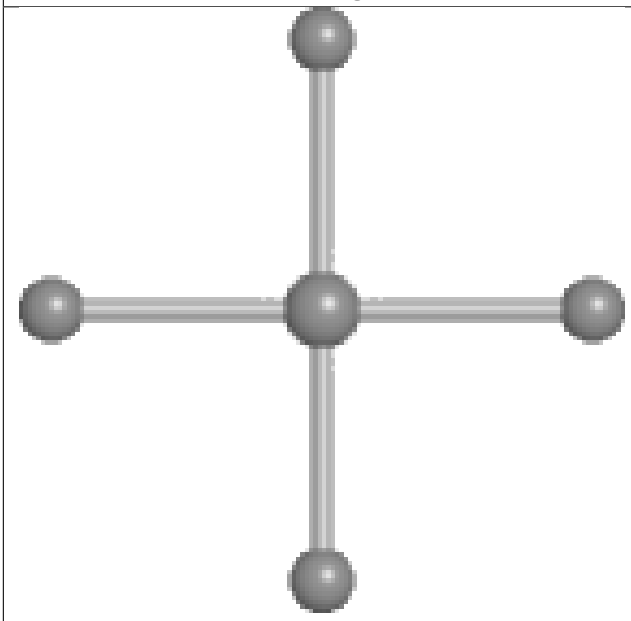
Ligand SO4 A 805



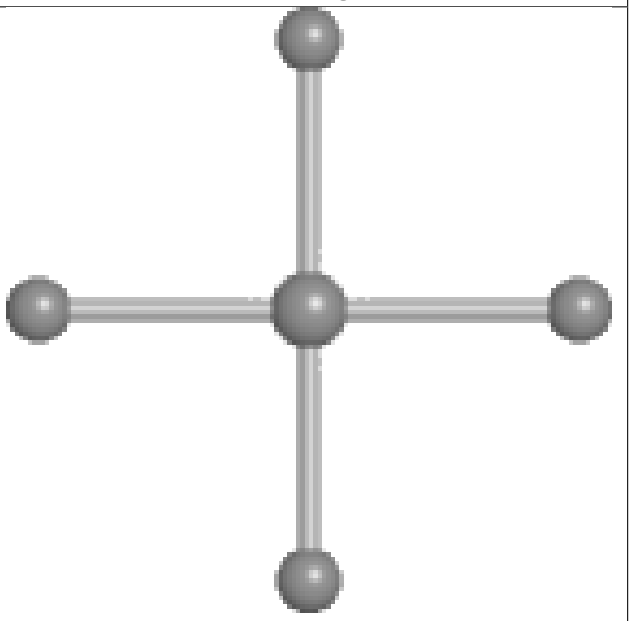
Bond lengths



Bond angles

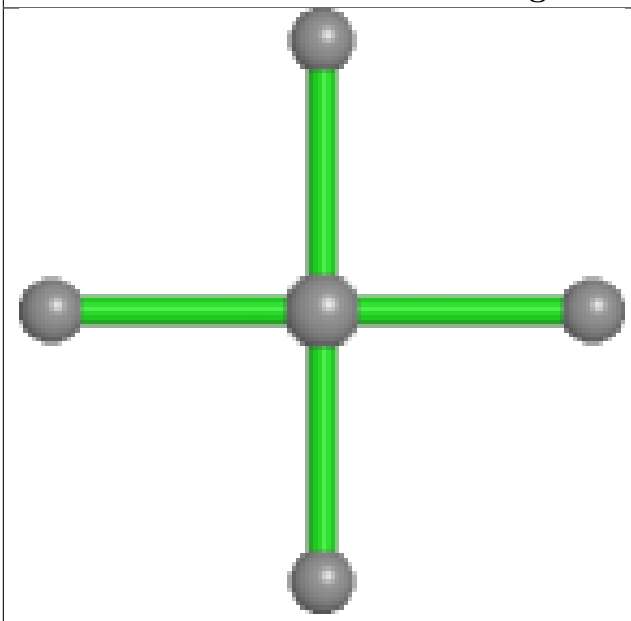


Torsions

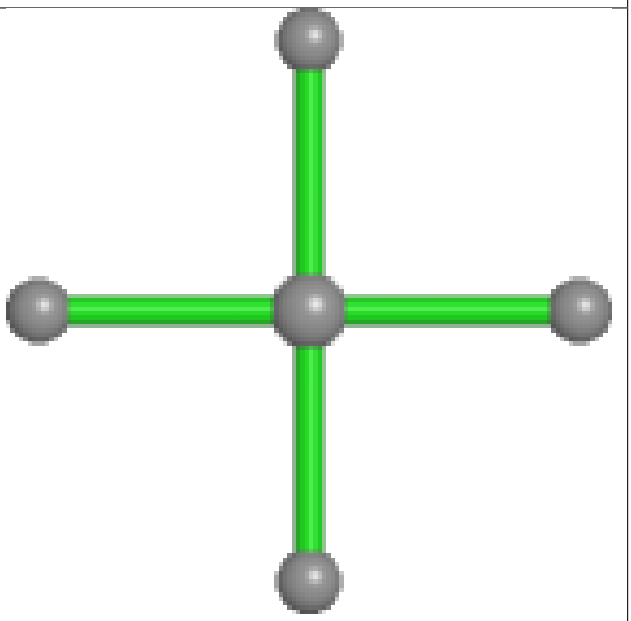


Rings

Ligand SO4 C 805



Bond lengths



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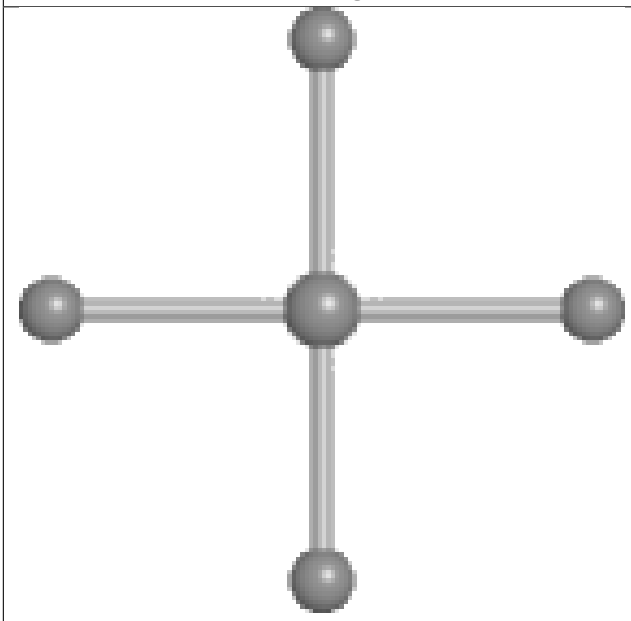

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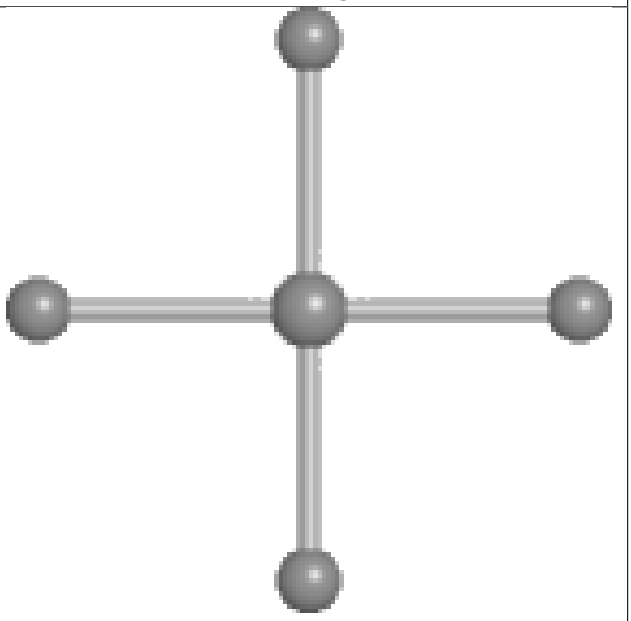
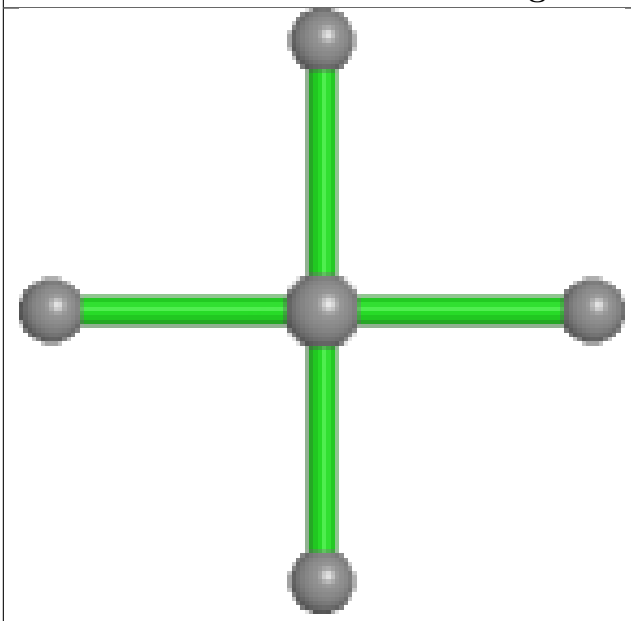


Rings

Ligand SO4 A 804



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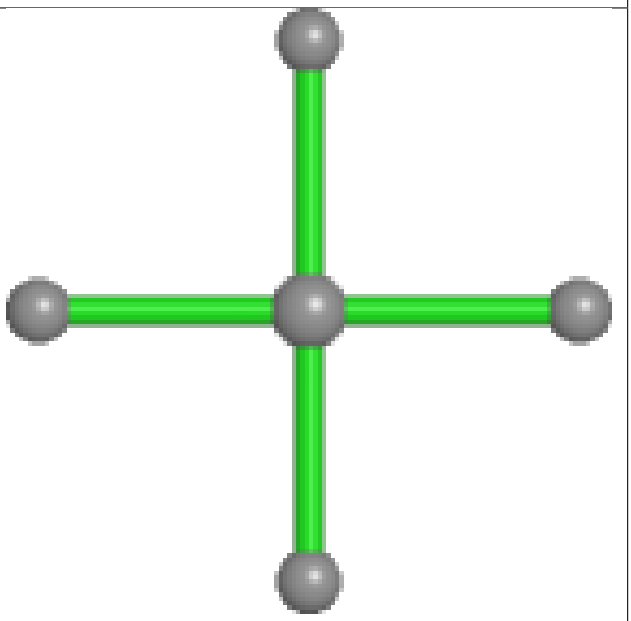

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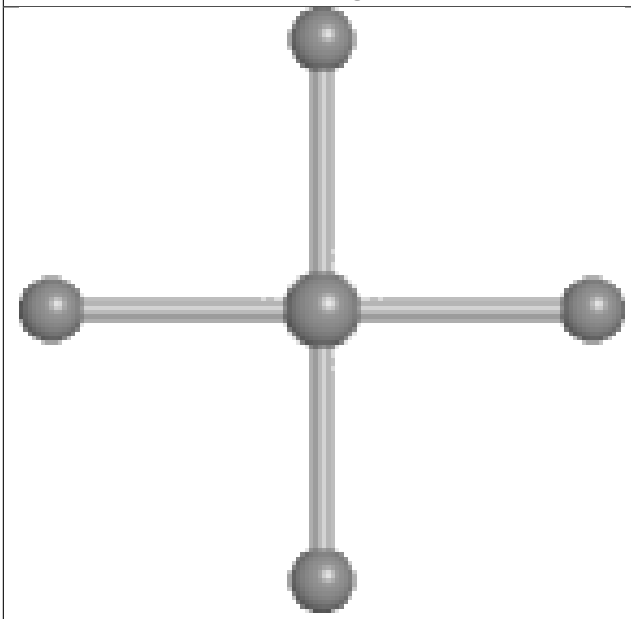

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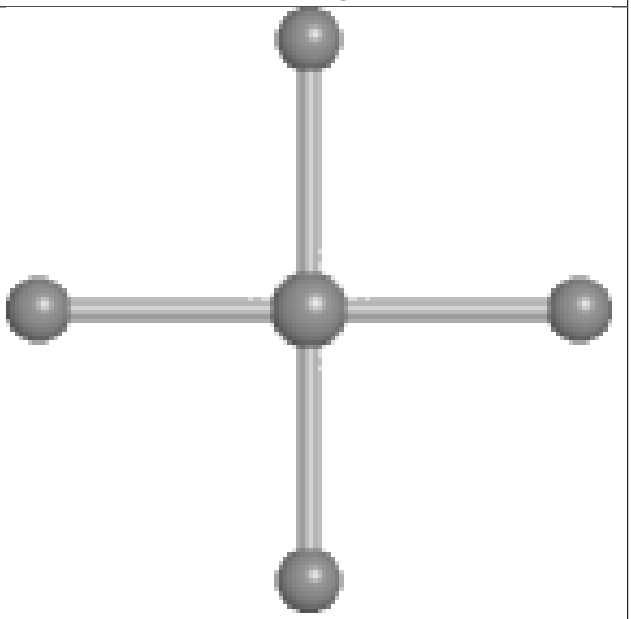
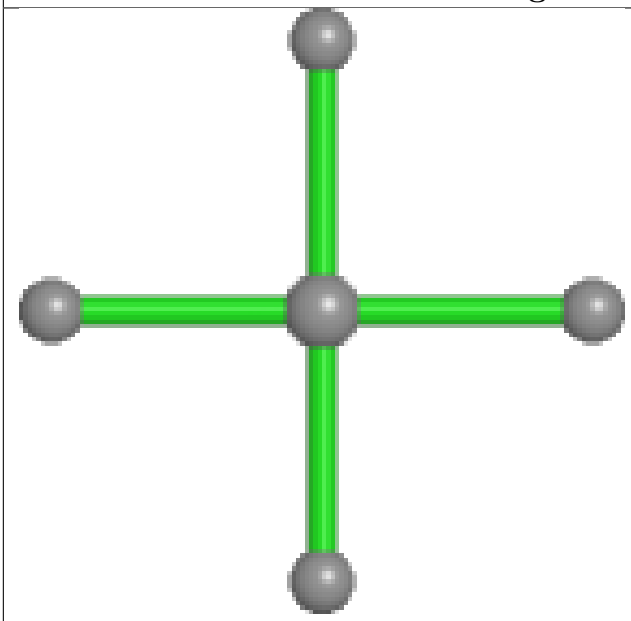


Rings

Ligand SO4 A 803



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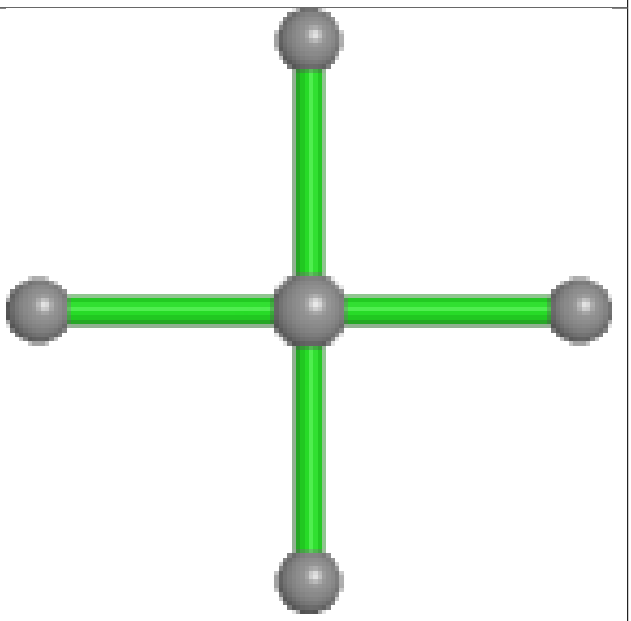

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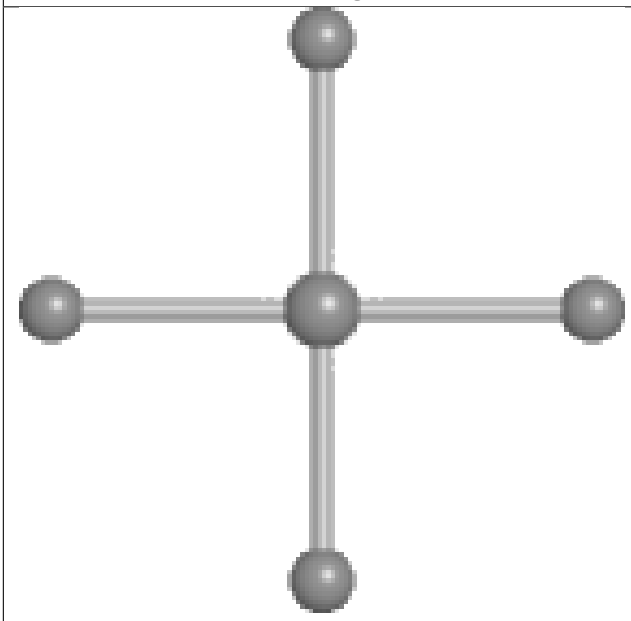

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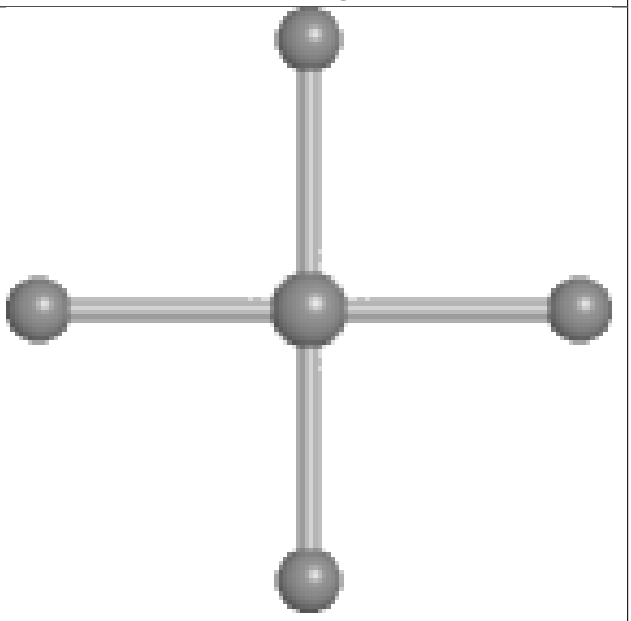
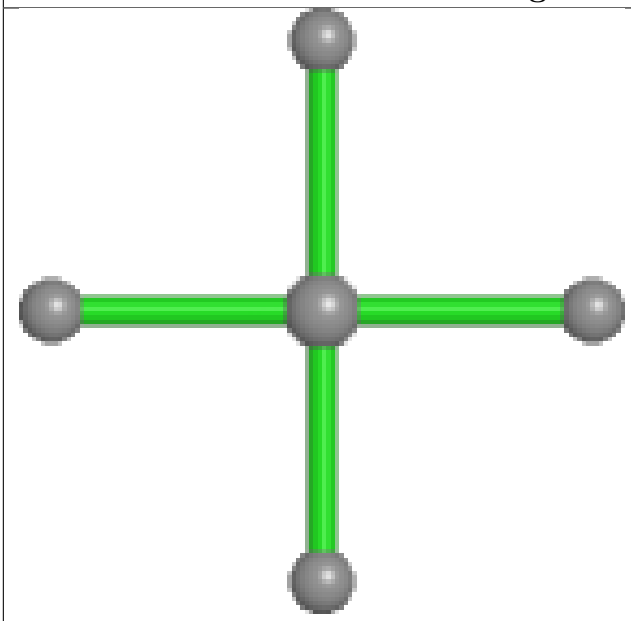
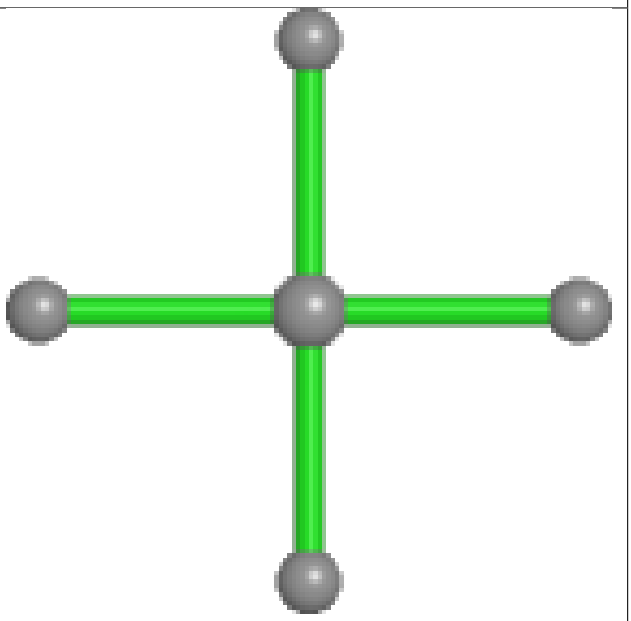


Rings

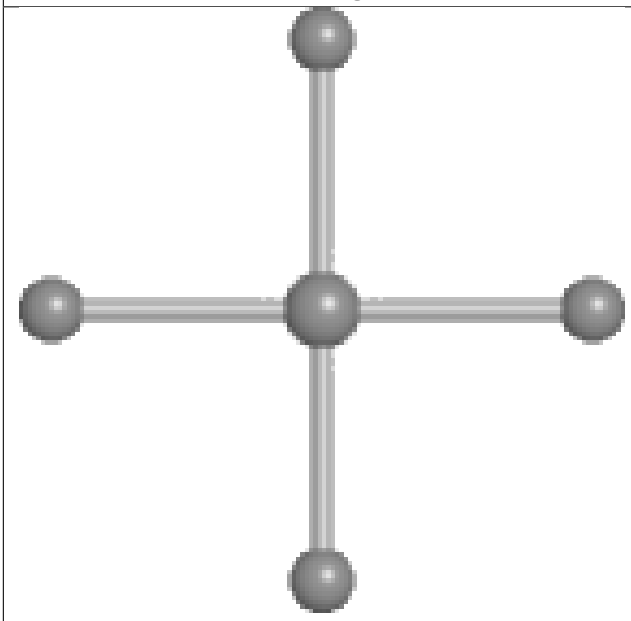
Ligand SO4 C 804



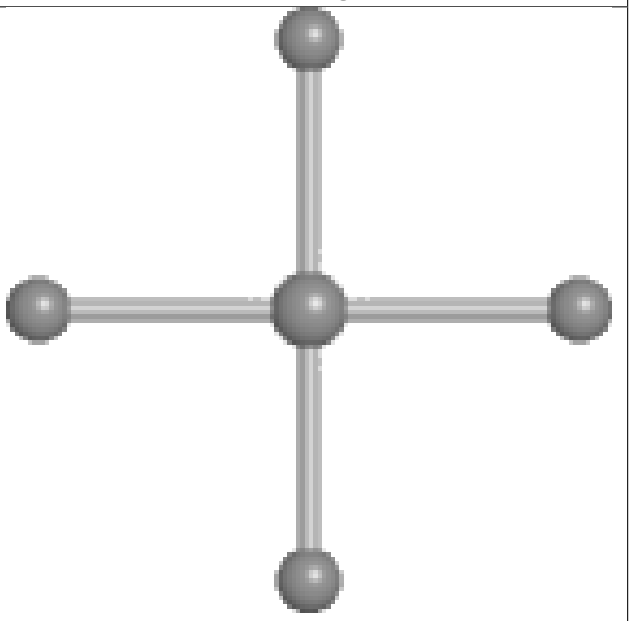
Bond lengths



Bond angles

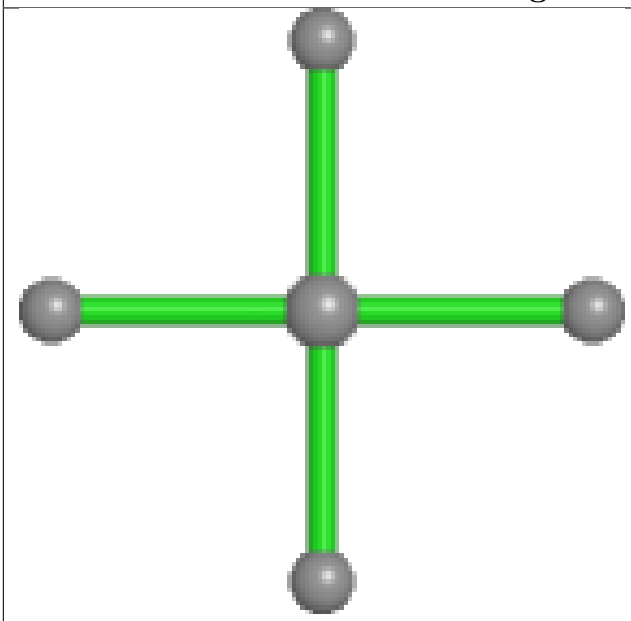


Torsions

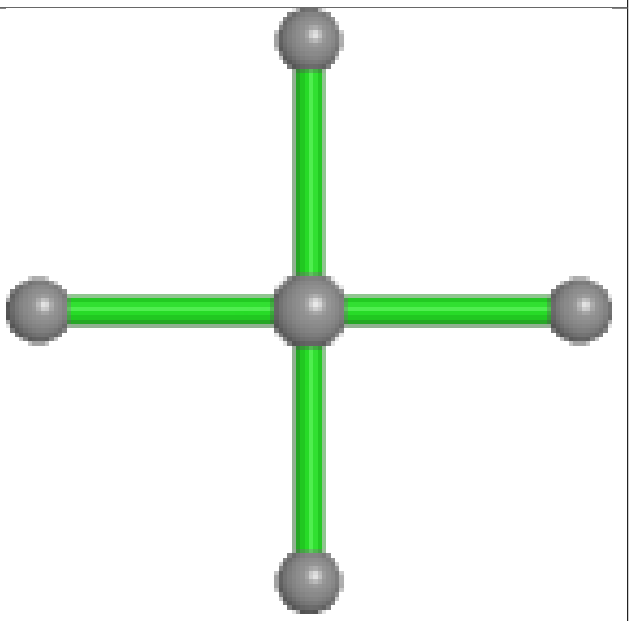


Rings

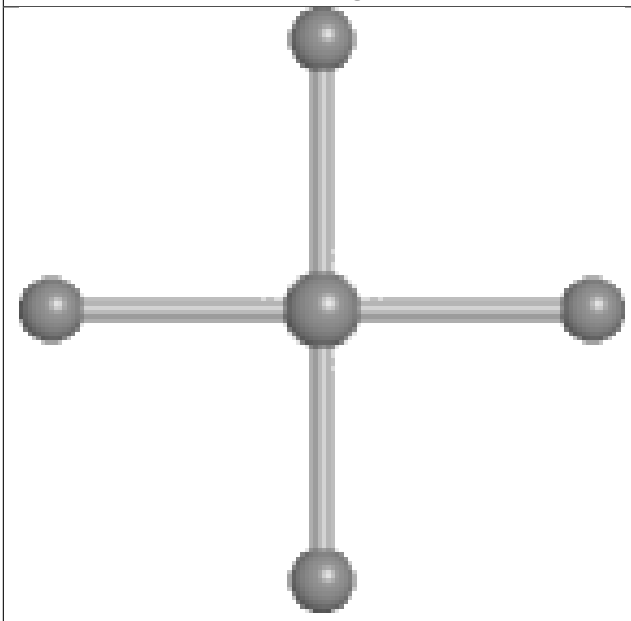
Ligand SO4 B 803



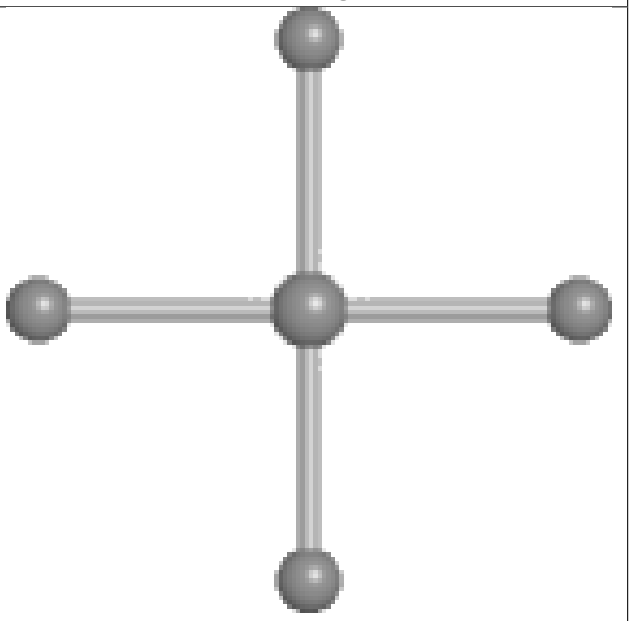
Bond lengths



Bond angles

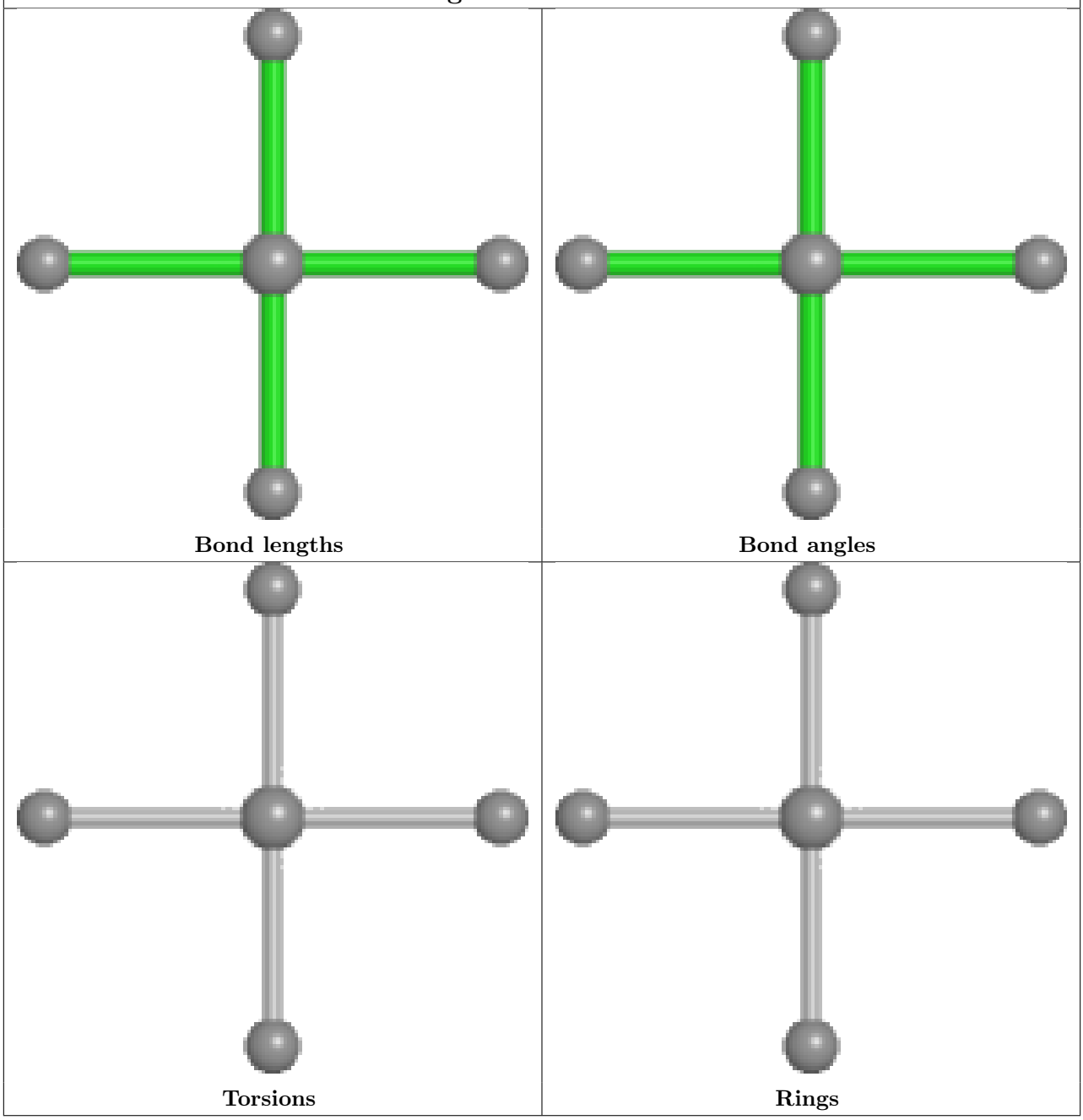


Torsions



Rings

Ligand SO4 C 803



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, 95^{th} 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	756/757 (99%)	0.05	5 (0%)	84	79	41, 63, 89, 110	0
1	B	756/757 (99%)	0.12	12 (1%)	70	63	43, 74, 108, 129	0
1	C	756/757 (99%)	0.14	10 (1%)	74	67	46, 77, 103, 118	0
All	All	2268/2271 (99%)	0.10	27 (1%)	76	69	41, 71, 103, 129	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	569	SER	3.6
1	A	599	TYR	3.3
1	B	216	TYR	2.7
1	A	609	THR	2.7
1	C	124	PRO	2.7
1	C	551	GLN	2.7
1	B	287	LEU	2.7
1	C	129	PHE	2.6
1	B	288	ASP	2.6
1	B	8	TRP	2.5
1	B	461	ILE	2.5
1	B	25	LEU	2.5
1	C	113	HIS	2.4
1	C	108	ALA	2.4
1	B	544	TRP	2.4
1	C	114	ILE	2.4
1	A	55	ILE	2.4
1	B	494	VAL	2.3
1	A	722	ASP	2.2
1	B	631	LEU	2.2
1	B	30	ILE	2.2
1	B	497	ILE	2.2
1	C	544	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	2.1
1	C	550	PRO	2.0
1	B	491	VAL	2.0
1	C	570	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

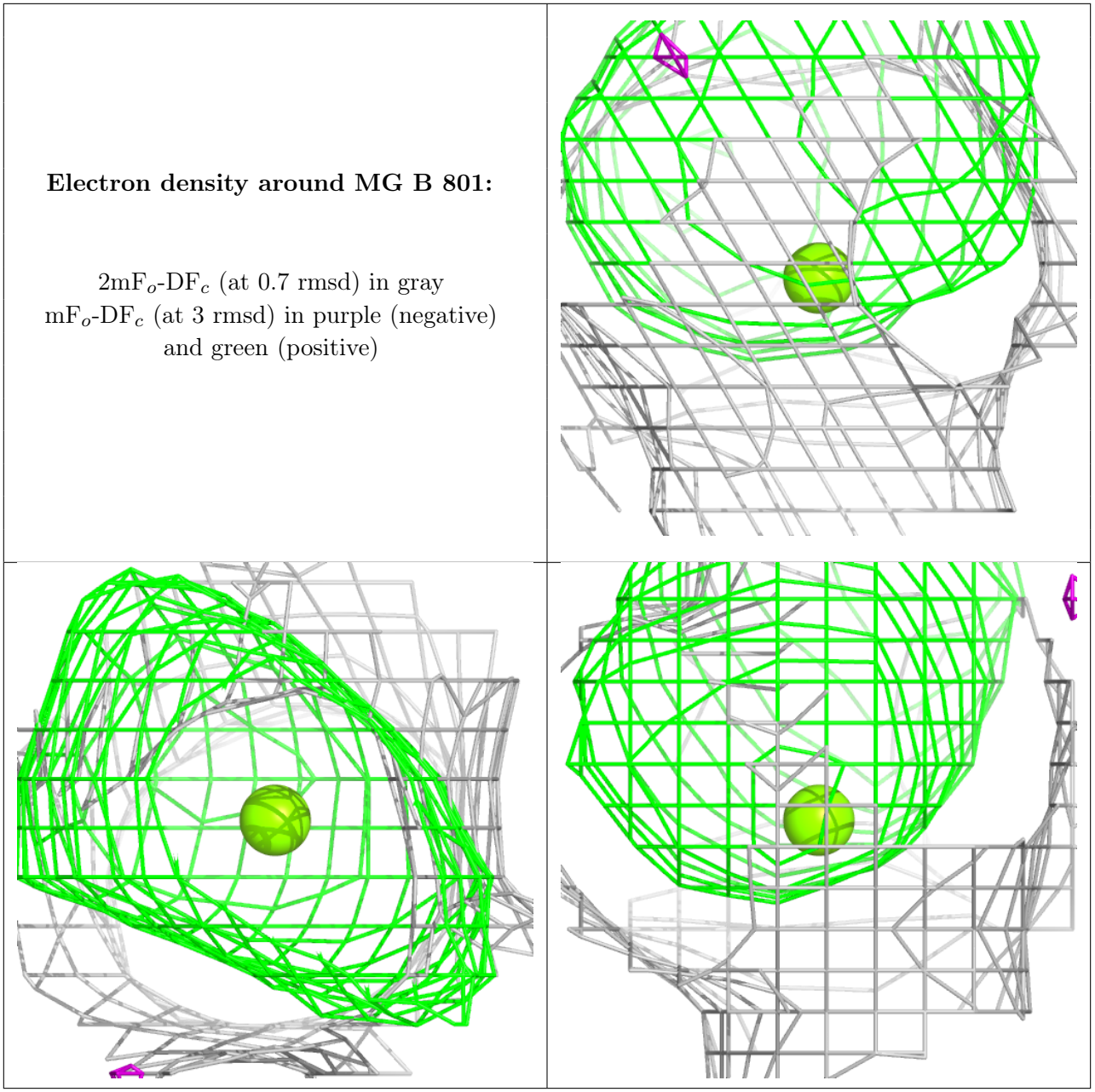
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	B	801	1/1	0.78	0.21	42,42,42,42	0
3	SO4	C	803	5/5	0.79	0.10	76,88,88,89	0
2	MG	C	802	1/1	0.81	0.10	90,90,90,90	0
2	MG	A	802	1/1	0.82	0.11	62,62,62,62	0
2	MG	C	801	1/1	0.86	0.16	61,61,61,61	0
3	SO4	B	804	5/5	0.87	0.14	76,78,80,86	0
3	SO4	C	804	5/5	0.88	0.11	71,82,85,91	0
3	SO4	A	805	5/5	0.90	0.07	62,66,71,71	0
2	MG	A	801	1/1	0.90	0.19	39,39,39,39	0
3	SO4	B	803	5/5	0.92	0.08	72,76,86,89	0
3	SO4	B	805	5/5	0.92	0.08	63,63,68,72	0
2	MG	B	802	1/1	0.93	0.08	60,60,60,60	0
3	SO4	A	803	5/5	0.93	0.07	57,60,69,71	0
3	SO4	C	805	5/5	0.94	0.07	55,57,62,71	0
3	SO4	A	804	5/5	0.97	0.10	51,53,59,60	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.

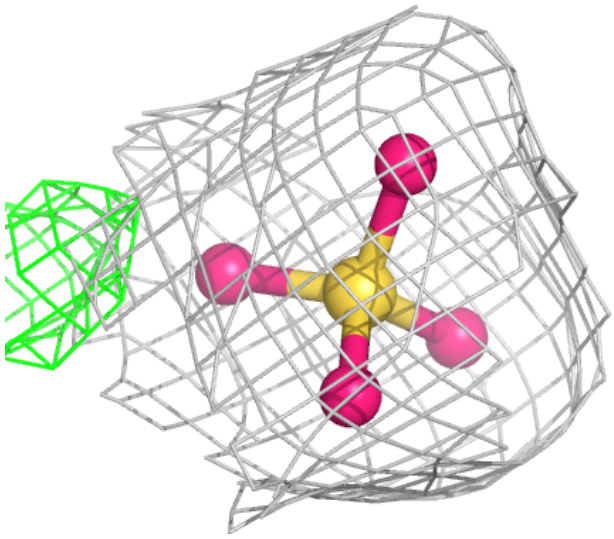
Electron density around MG B 801:

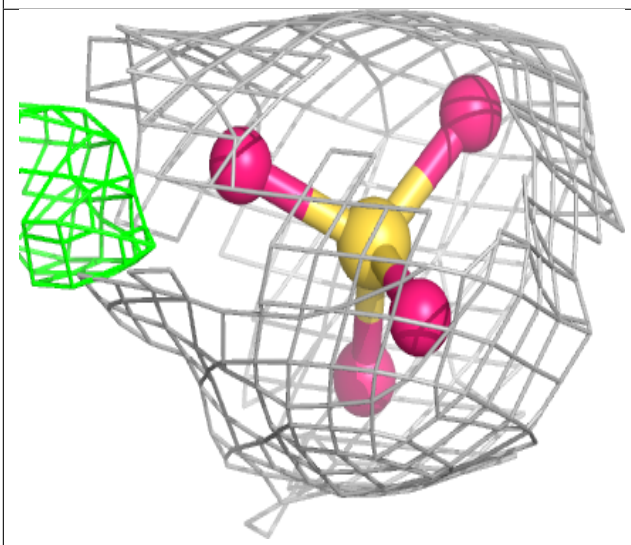
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

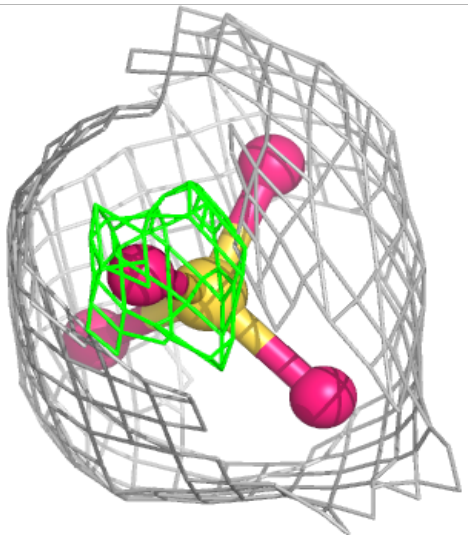


Electron density around SO4 C 803:

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

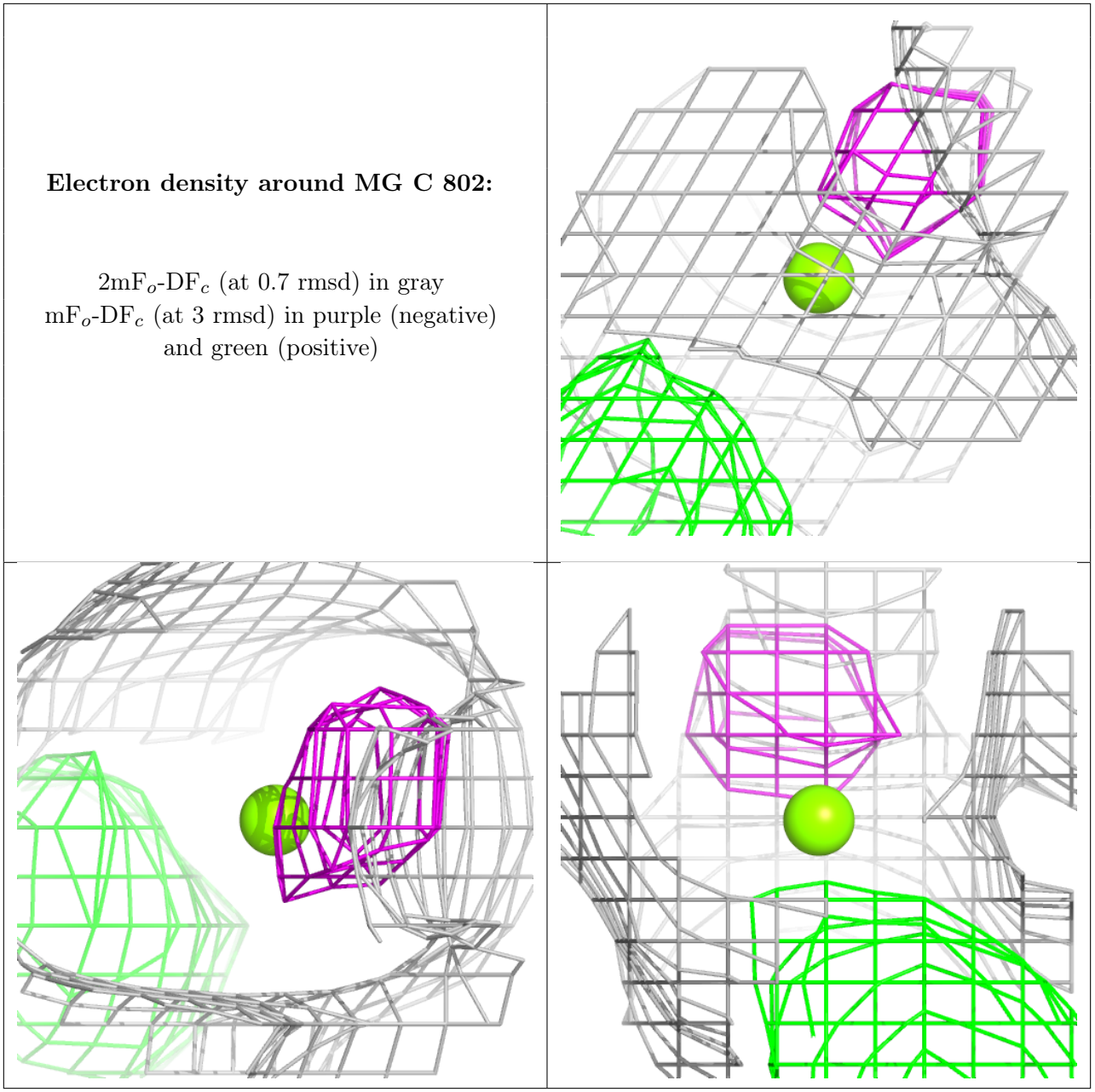






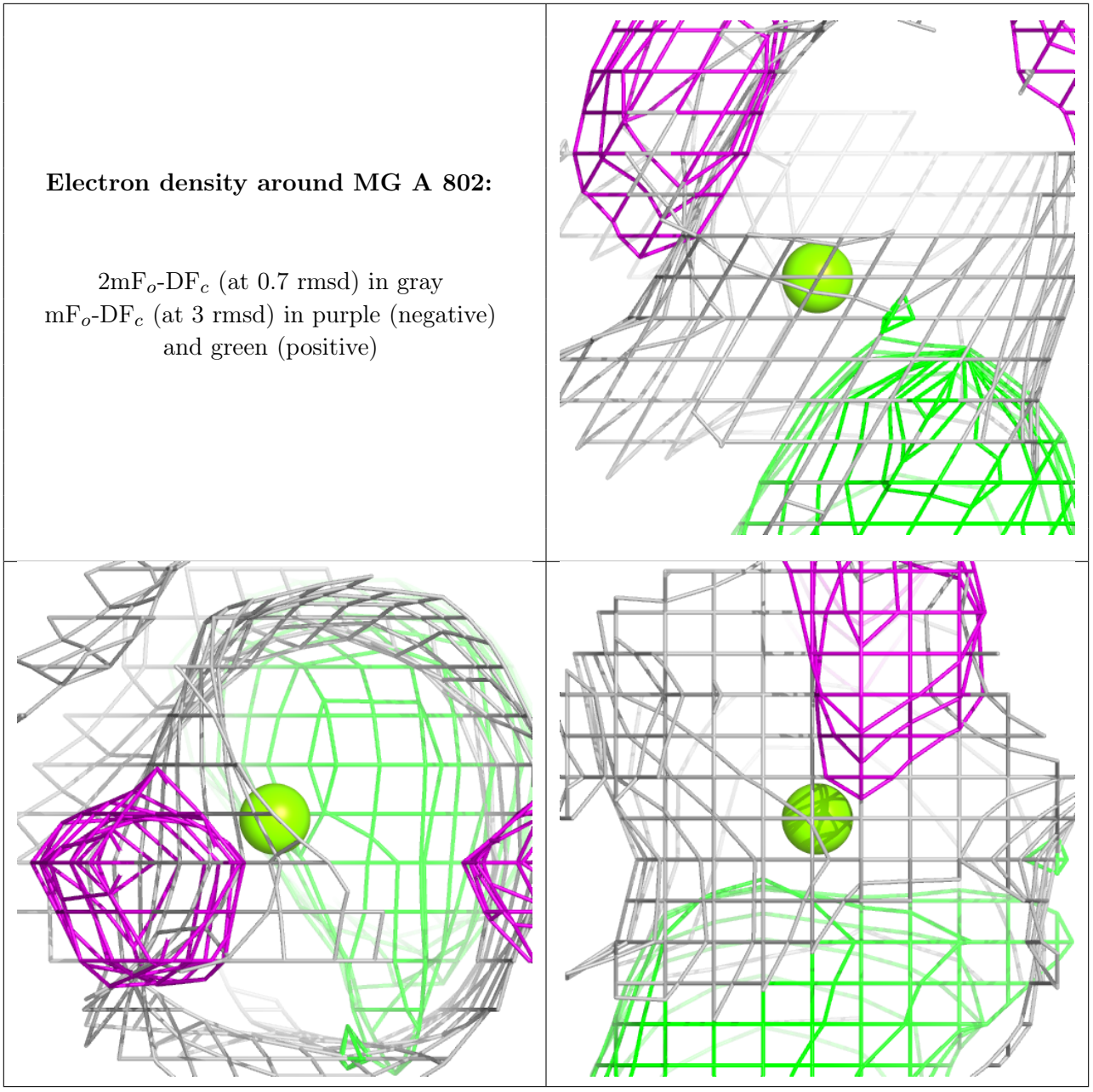
Electron density around MG C 802:

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



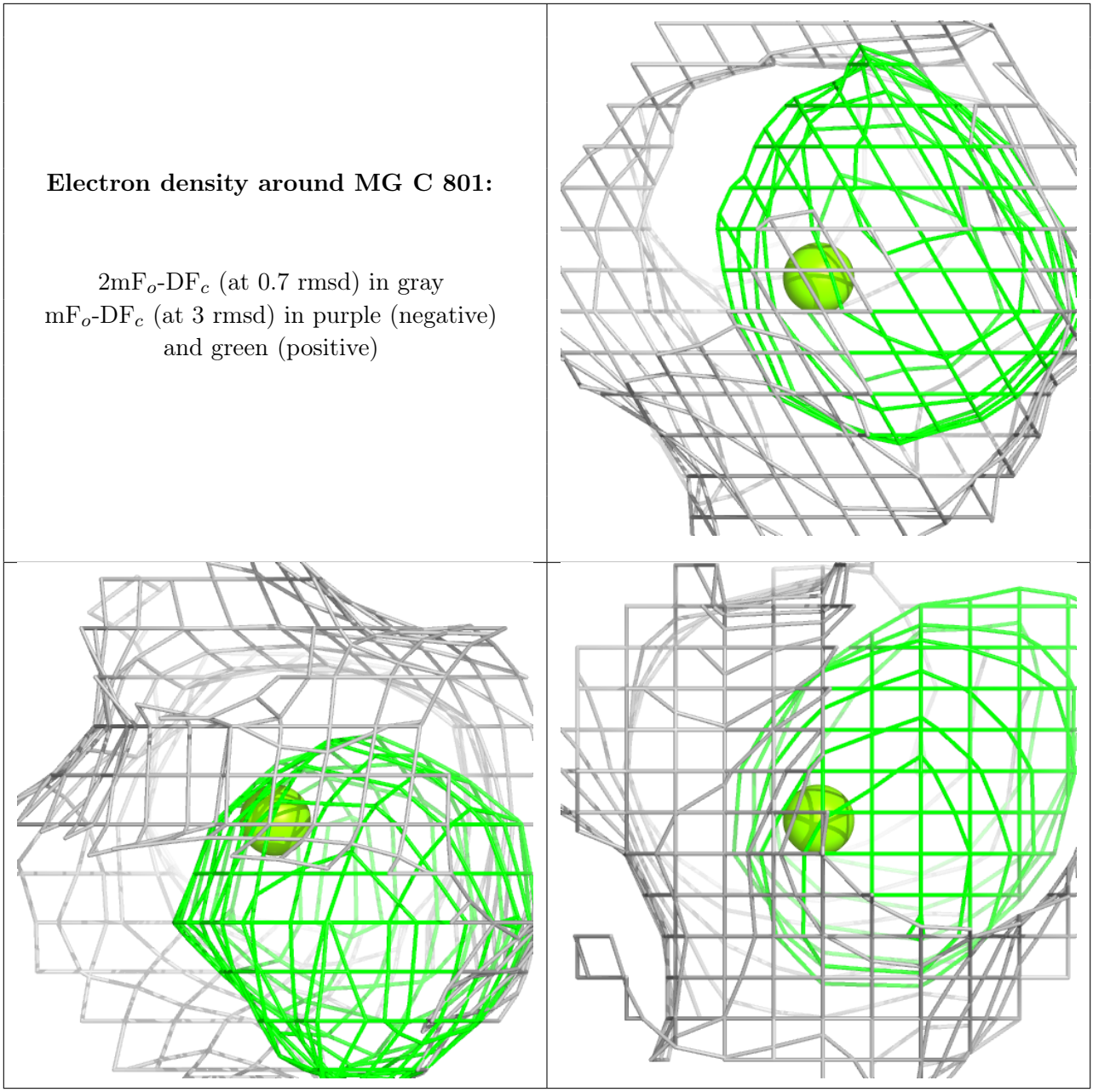
Electron density around MG A 802:

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



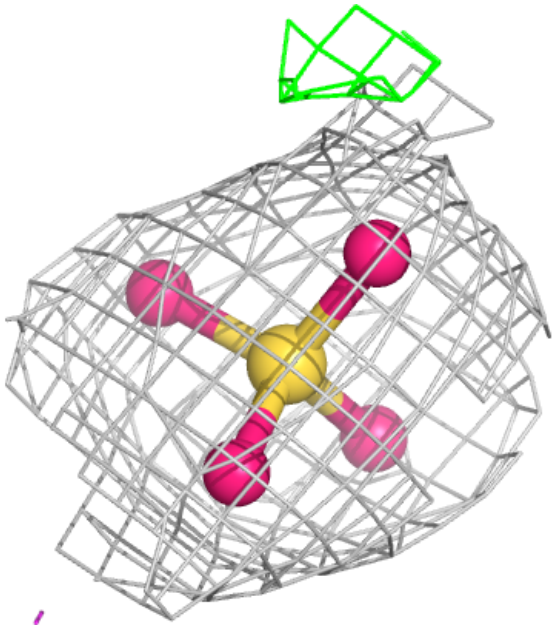
Electron density around MG C 801:

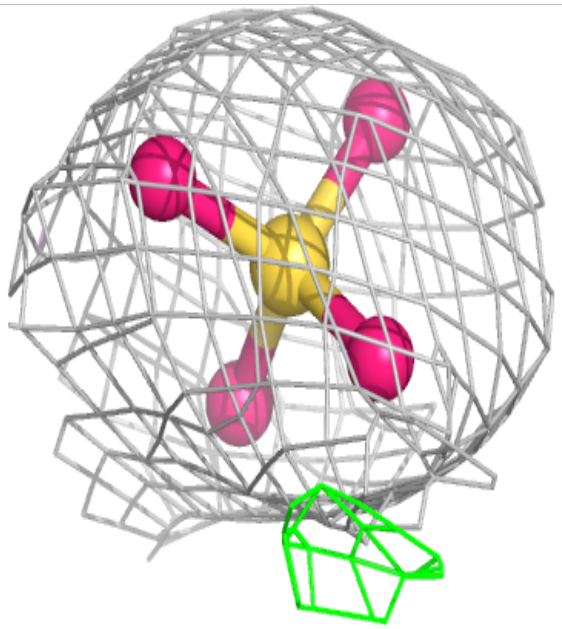
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

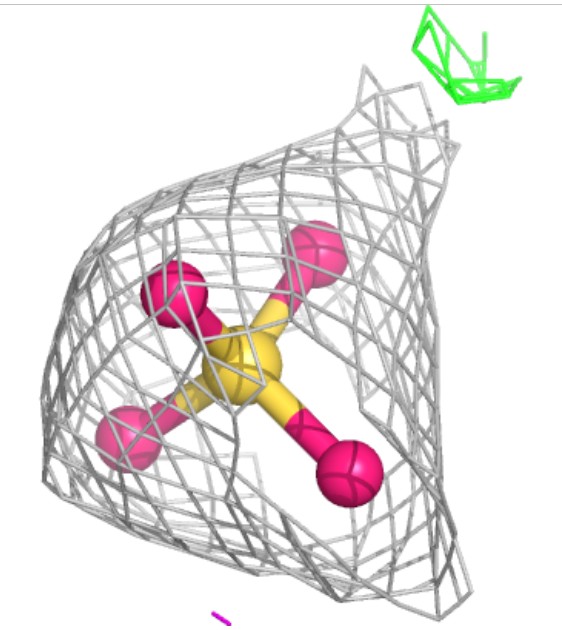


Electron density around SO4 B 804:

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

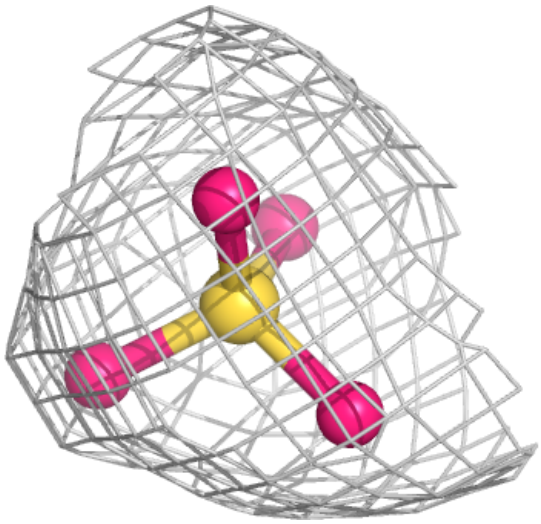


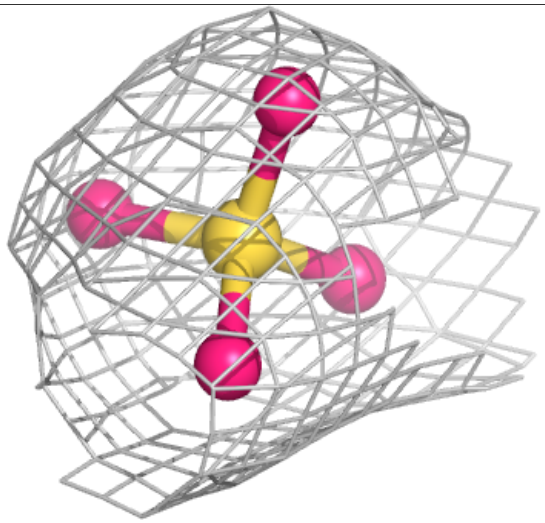


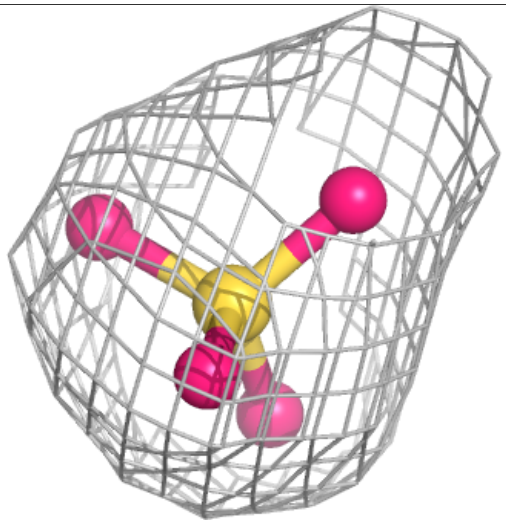


Electron density around SO4 C 804:

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







Electron density around SO4 A 805:

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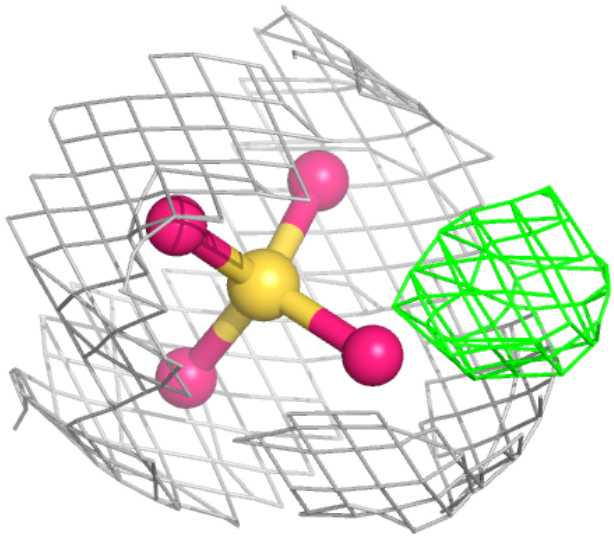
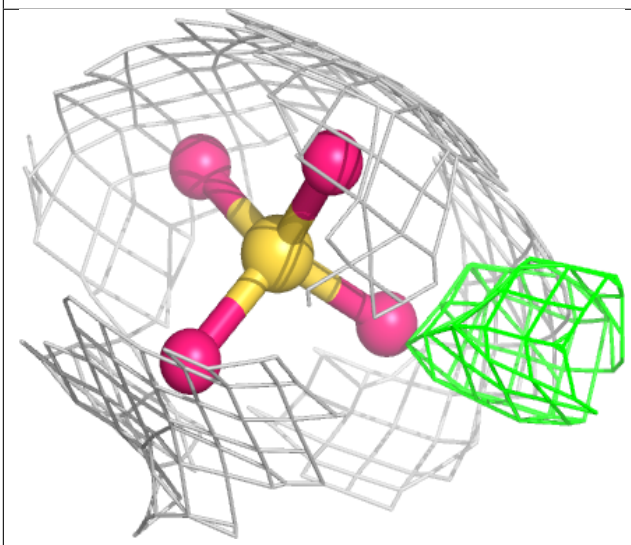
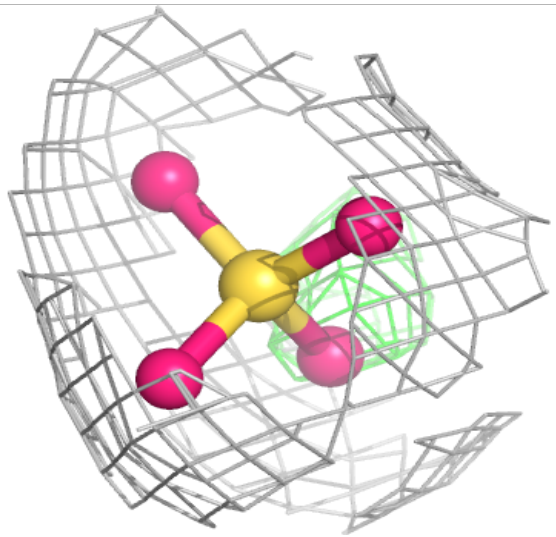
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

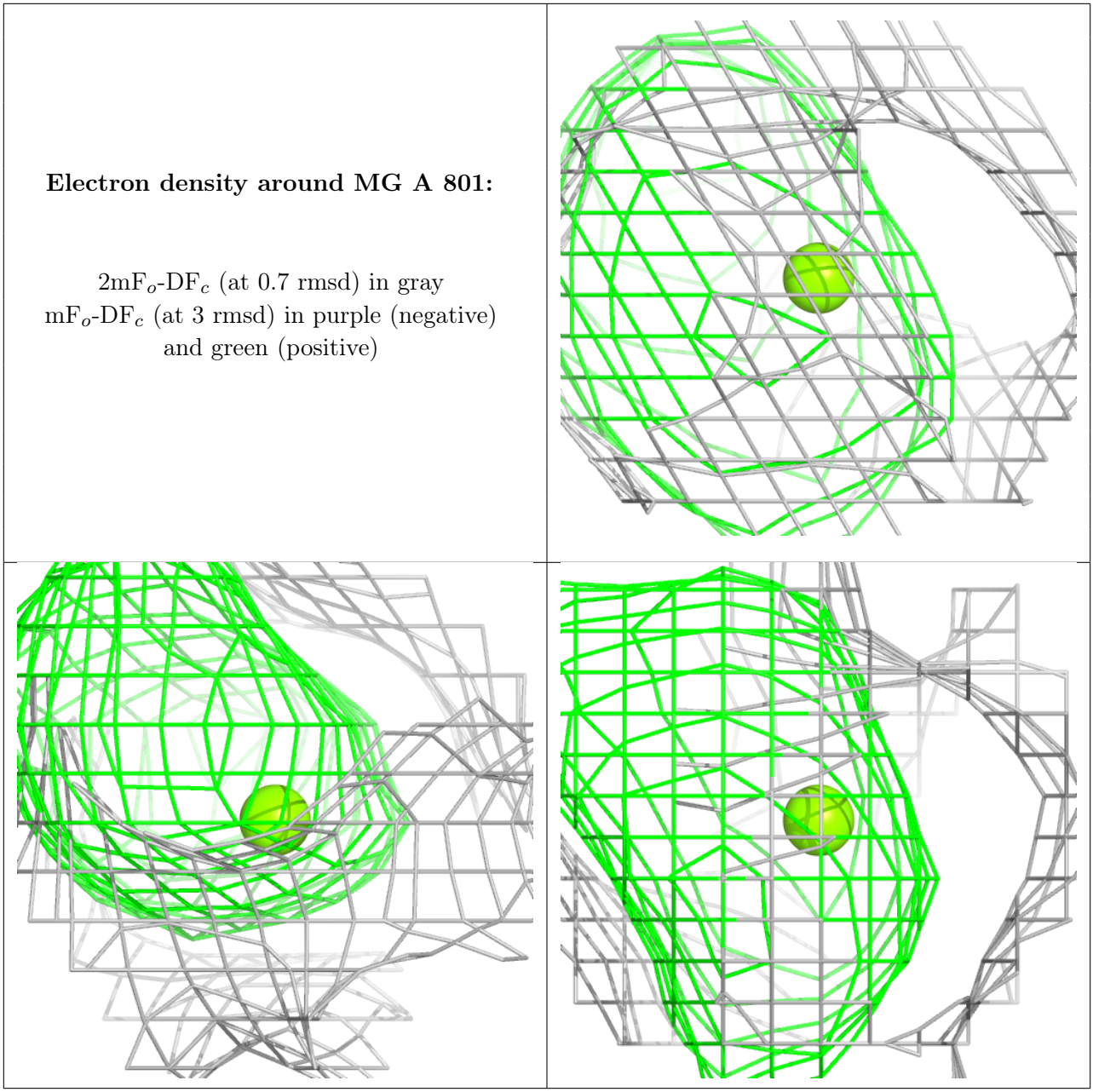






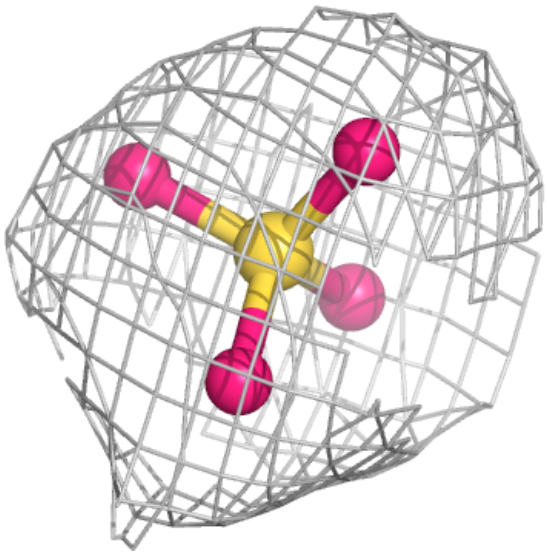
Electron density around MG A 801:

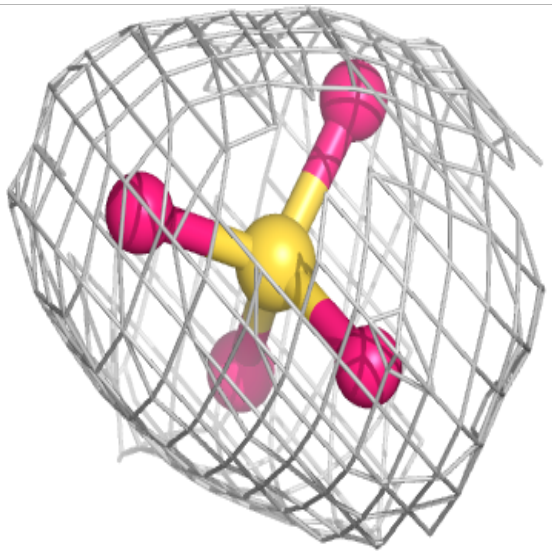
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

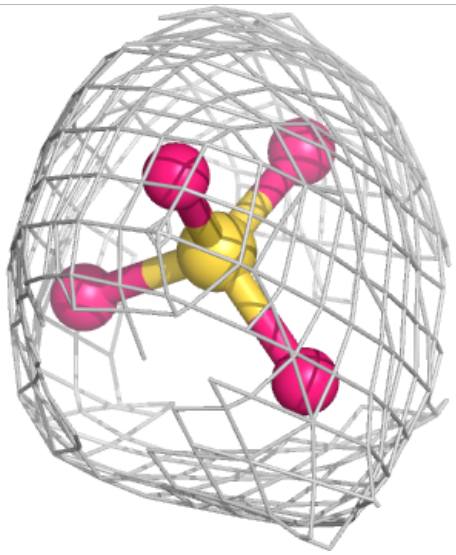


Electron density around SO4 B 803:

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

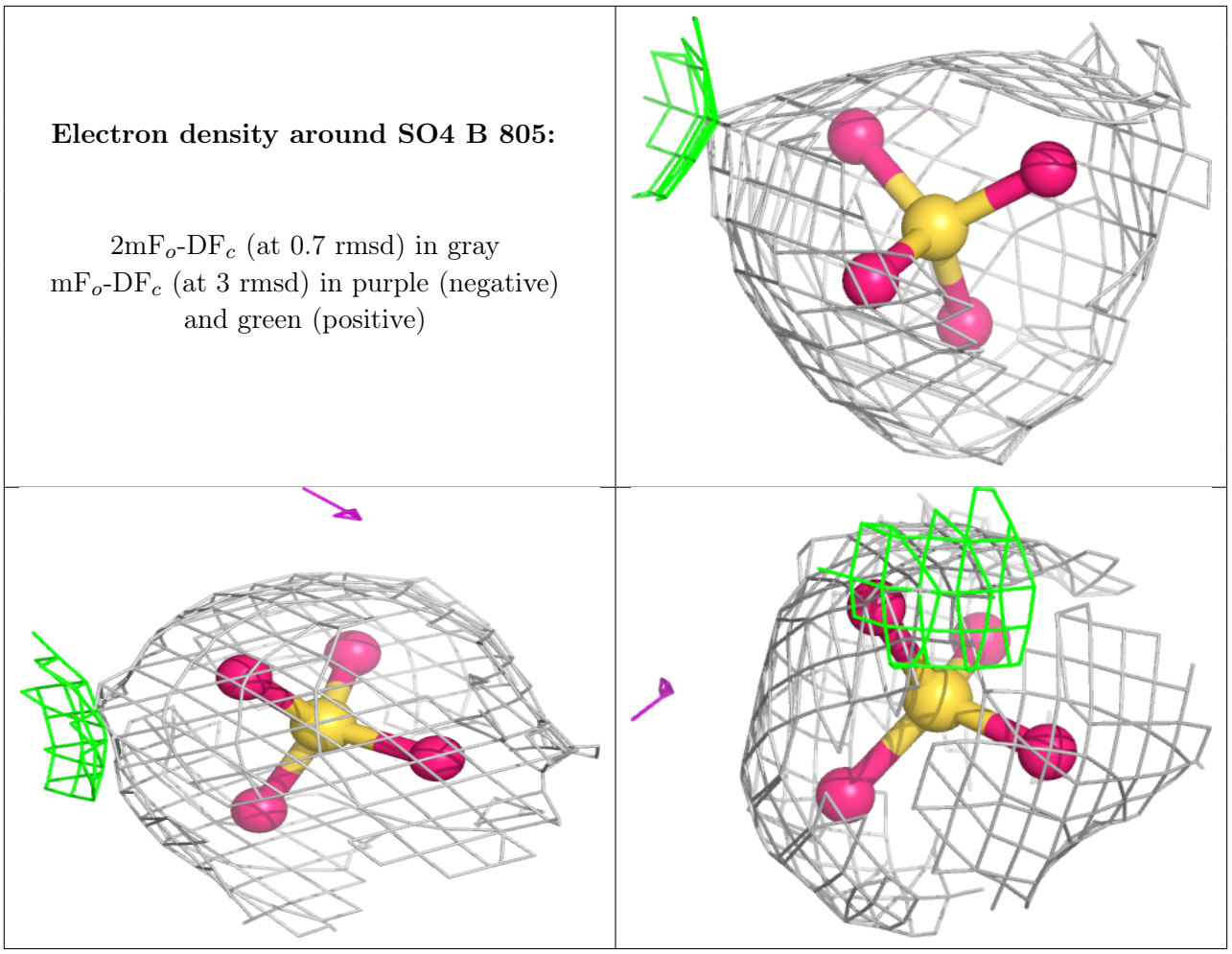






Electron density around SO4 B 805:

$2mF_o$-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 802:

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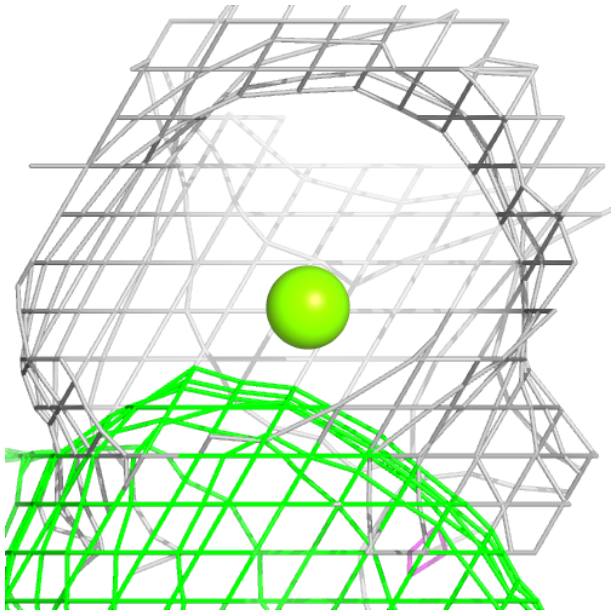
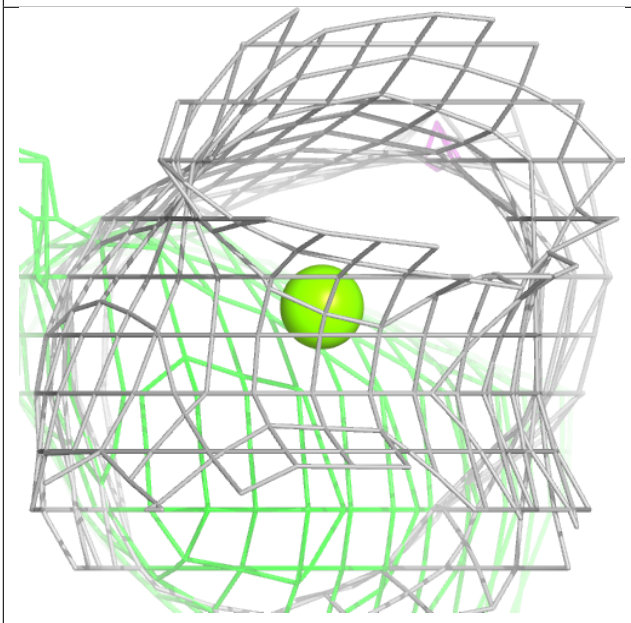
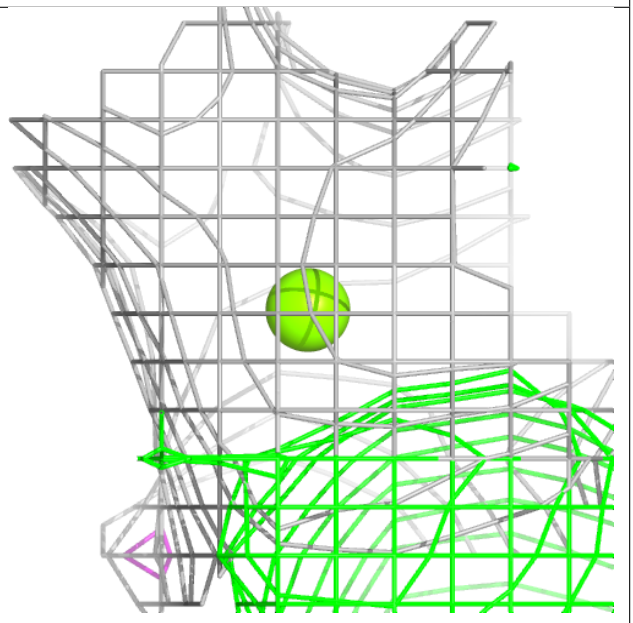
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

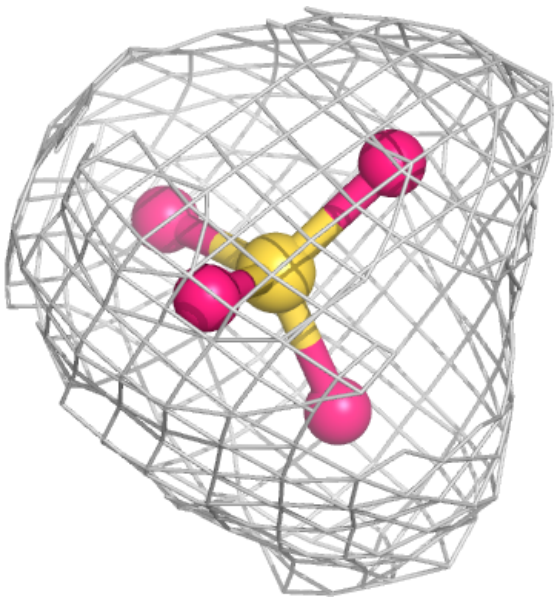


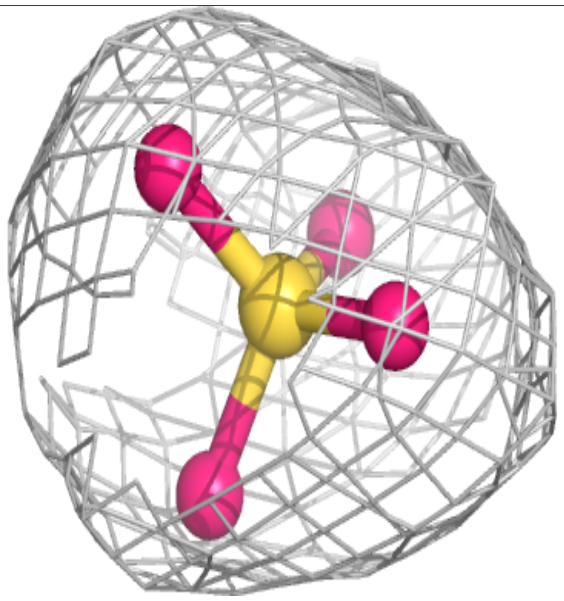


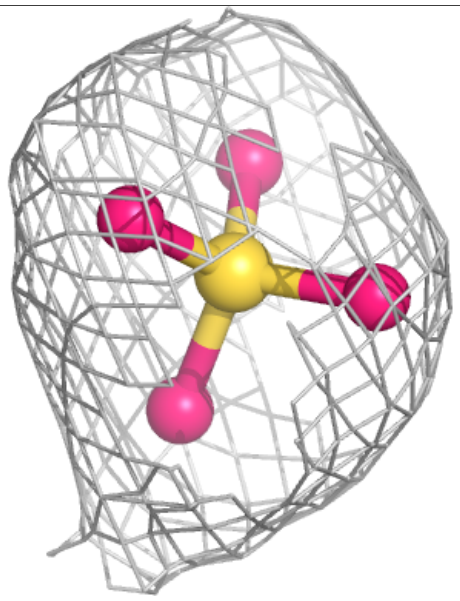


Electron density around SO4 A 803:

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

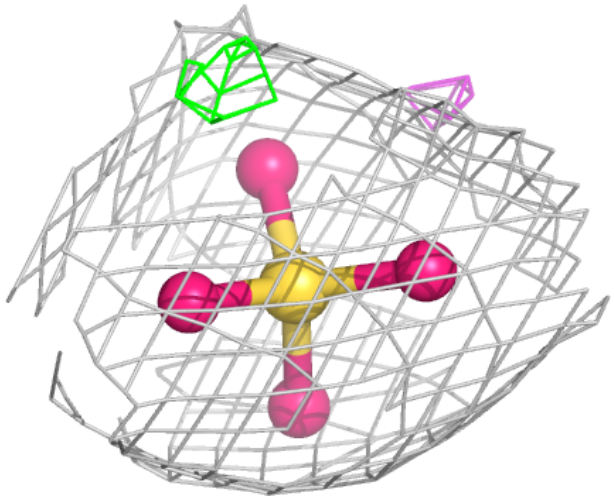


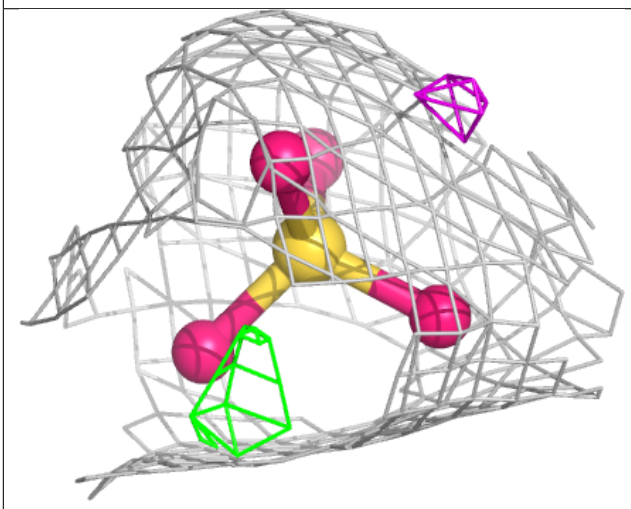


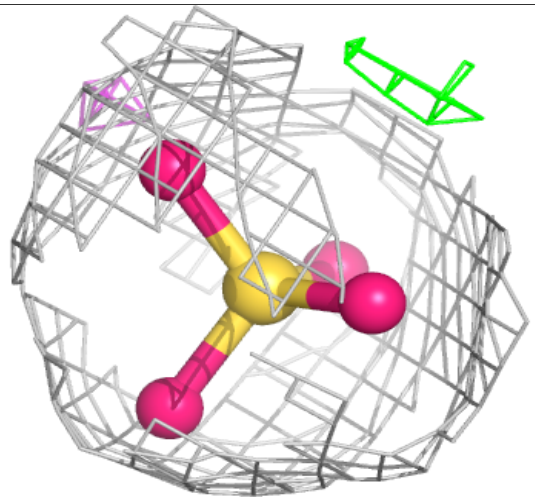


Electron density around SO4 C 805:

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

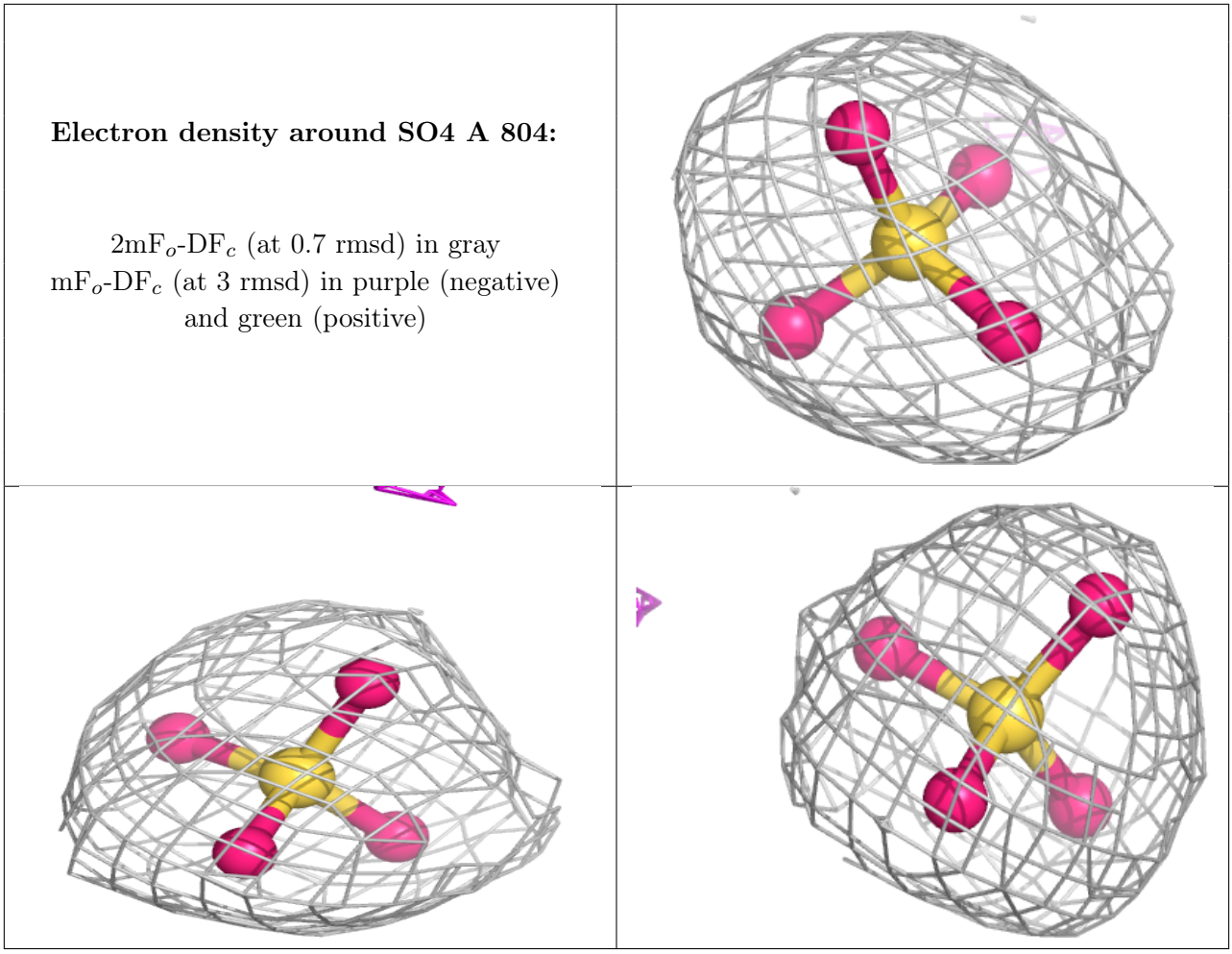






Electron density around SO4 A 804:

$2mF_o$-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.