



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2020 – 02:20 PM EDT

PDB ID : 6X5K
Title : Crystal structure of CODH/ACS with carbon monoxide bound to the A-cluster
Authors : Cohen, S.E.; Wittenborn, E.C.; Hendrickson, R.; Drennan, C.L.
Deposited on : 2020-05-26
Resolution : 2.47 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 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) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

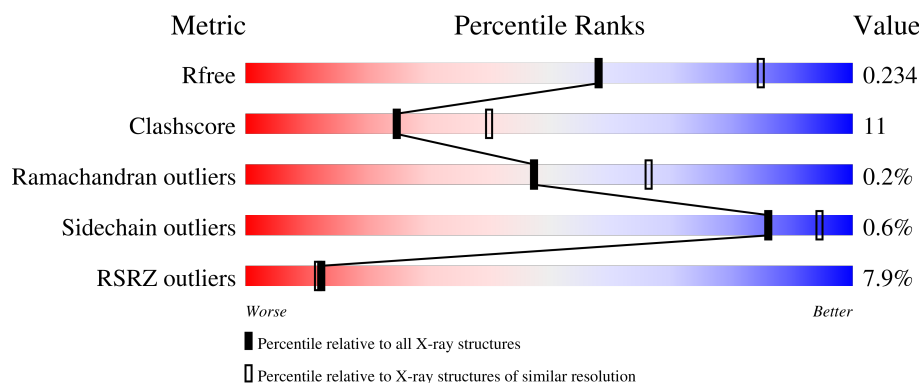
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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.



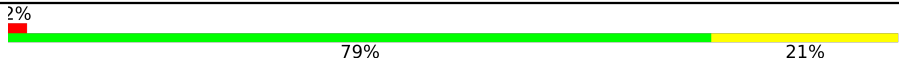
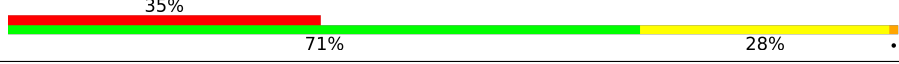
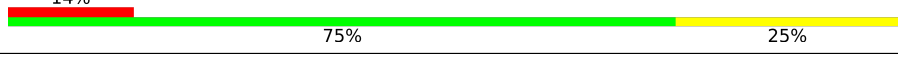
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 on 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	674	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>22%</div> </div> </div>
1	B	674	<div> <div></div> <div> <div>78%</div> <div>21%</div> </div> </div>
1	C	674	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>20%</div> </div> </div>
1	D	674	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>22%</div> </div> </div>
2	M	729	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	N	729	
2	O	729	
2	P	729	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	XCC	A	703	-	-	X	-
4	XCC	B	702	-	-	X	-
4	XCC	C	703	-	-	X	-
4	XCC	D	702	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 44026 atoms, of which 32 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 Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	3	0
			5109	3209	895	961	44			
1	B	672	Total	C	N	O	S	0	3	0
			5109	3209	895	961	44			
1	C	672	Total	C	N	O	S	0	3	0
			5109	3209	895	961	44			
1	D	672	Total	C	N	O	S	0	2	0
			5103	3206	894	960	43			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha.

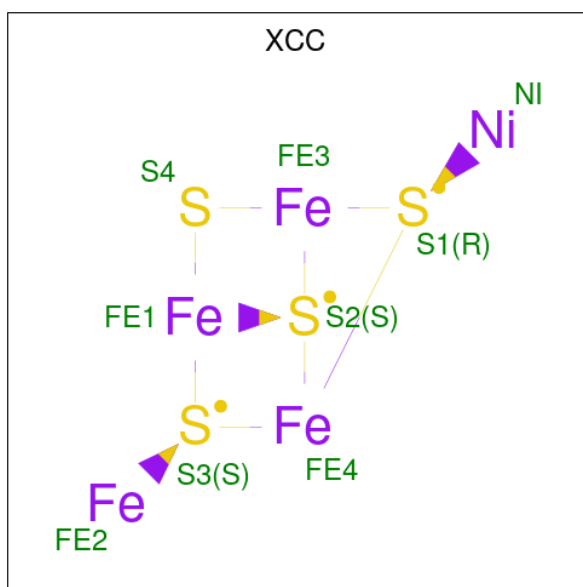
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	0	0
			5740	3681	956	1068	35			
2	N	728	Total	C	N	O	S	0	0	0
			5740	3681	956	1068	35			
2	O	726	Total	C	N	O	S	0	0	0
			5723	3670	954	1065	34			
2	P	728	Total	C	N	O	S	0	0	0
			5740	3681	956	1068	35			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by author).



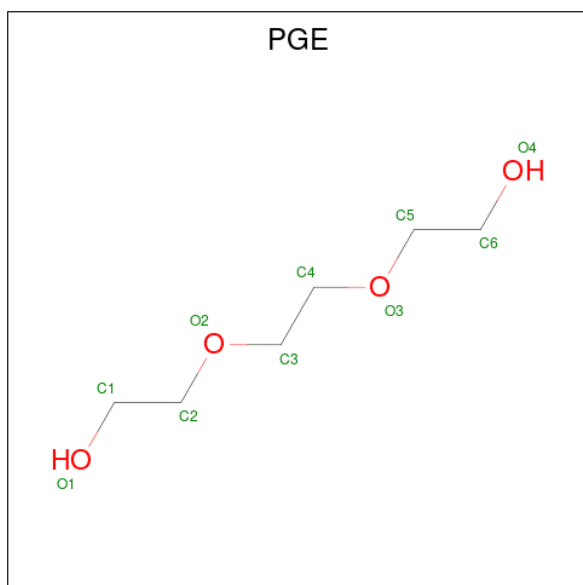
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		
3	P	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe₄NiS₄).



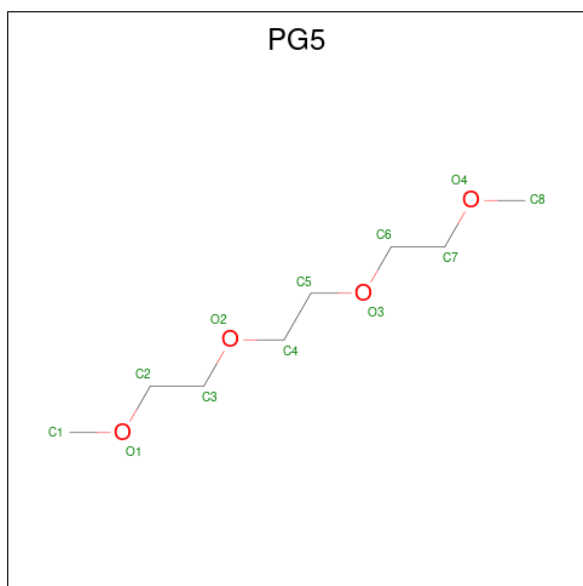
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 6 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)-ETHANE (three-letter code: PG5) (formula: C₈H₁₈O₄).

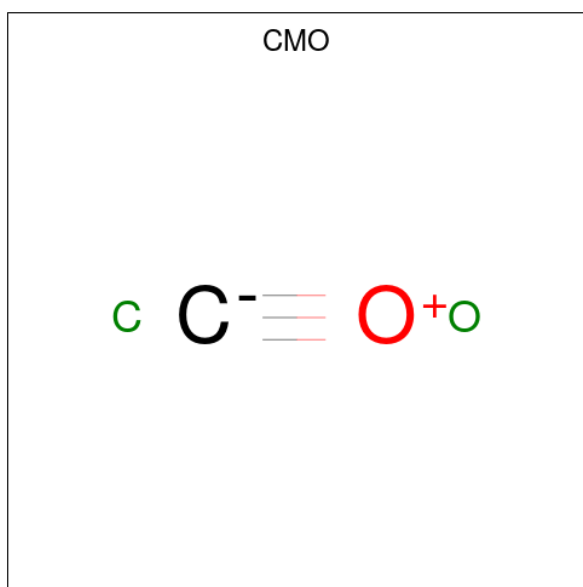


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			30	8	18	4		

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	2	Total	Ni	0	0
			2	2		
7	O	2	Total	Ni	0	0
			2	2		
7	N	2	Total	Ni	0	0
			2	2		
7	M	2	Total	Ni	0	0
			2	2		

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			2	1	1		
8	N	1	Total	C	O	0	0
			2	1	1		
8	P	1	Total	C	O	0	0
			2	1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	N	1	Total	Mg	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	84	Total	O	0	0
			84	84		
10	B	77	Total	O	0	0
			77	77		
10	C	44	Total	O	0	0
			44	44		
10	D	51	Total	O	0	0
			51	51		
10	M	76	Total	O	0	0
			76	76		

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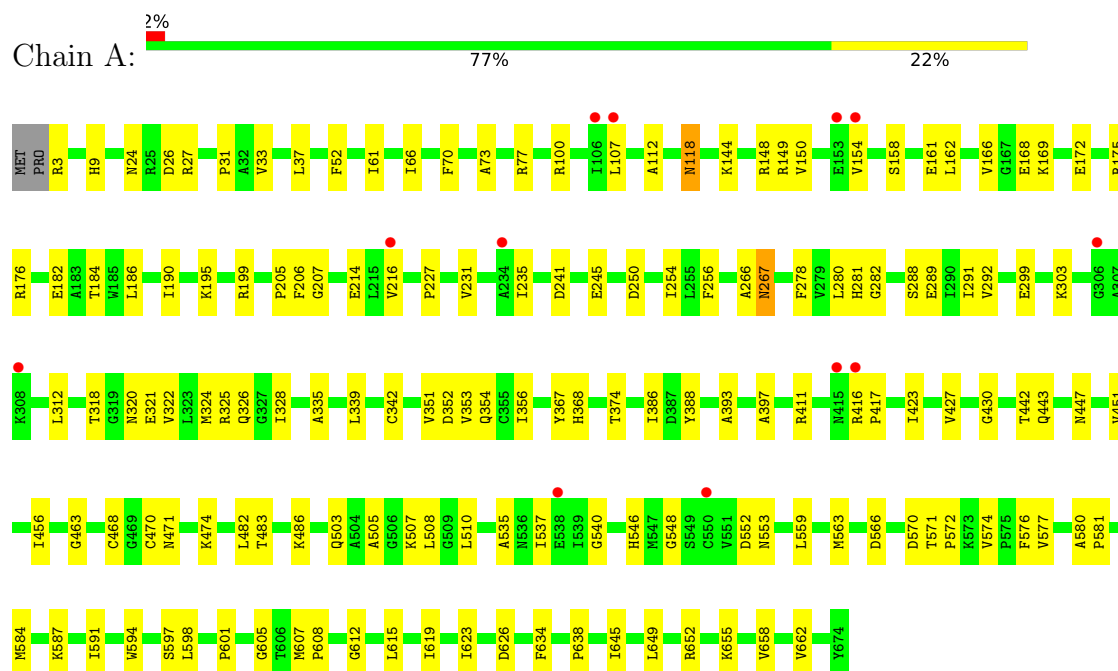
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	N	79	Total 79	O 79	0	0
10	O	12	Total 12	O 12	0	0
10	P	45	Total 45	O 45	0	0

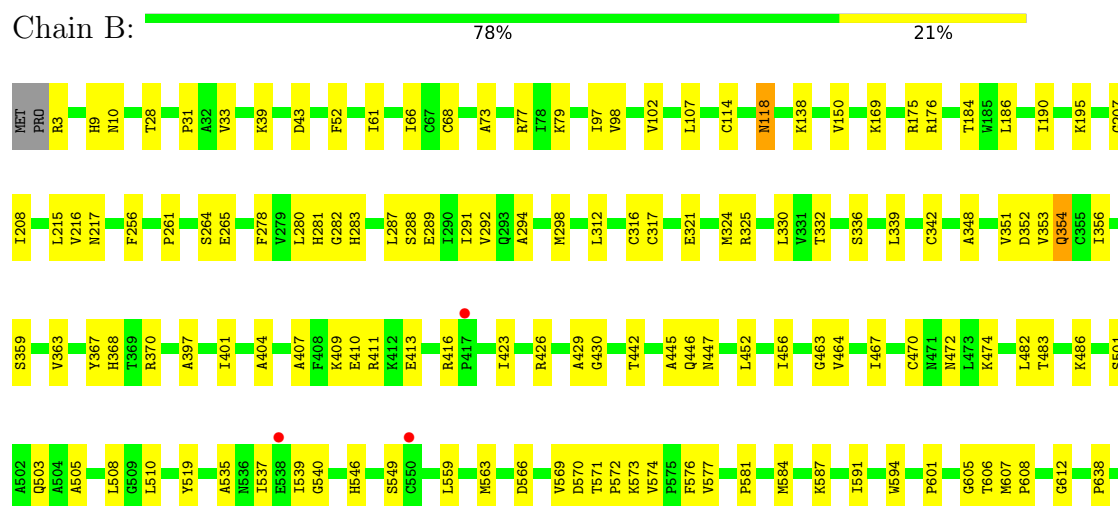
3 Residue-property plots

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

- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

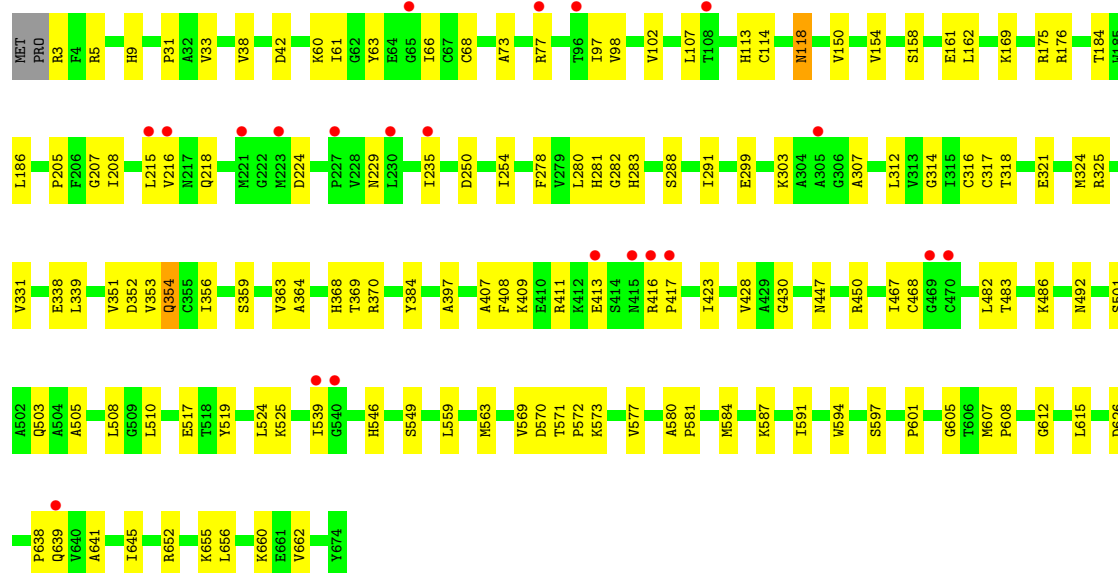
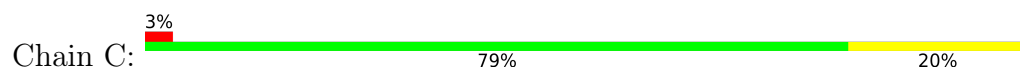


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

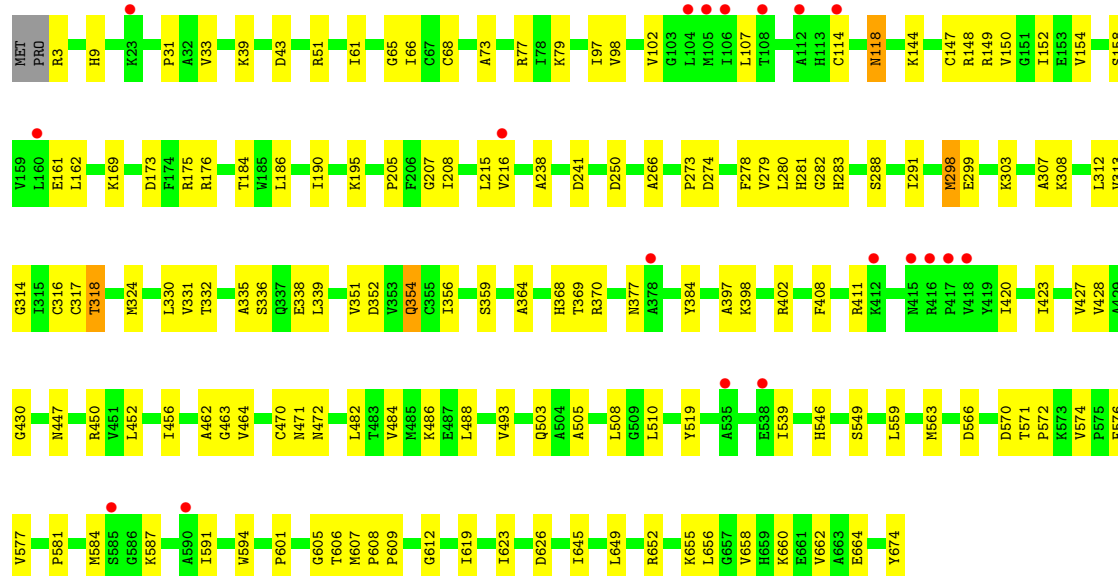
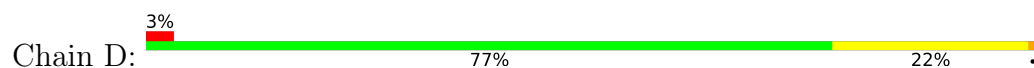




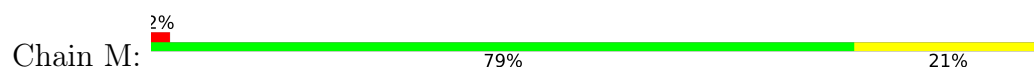
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

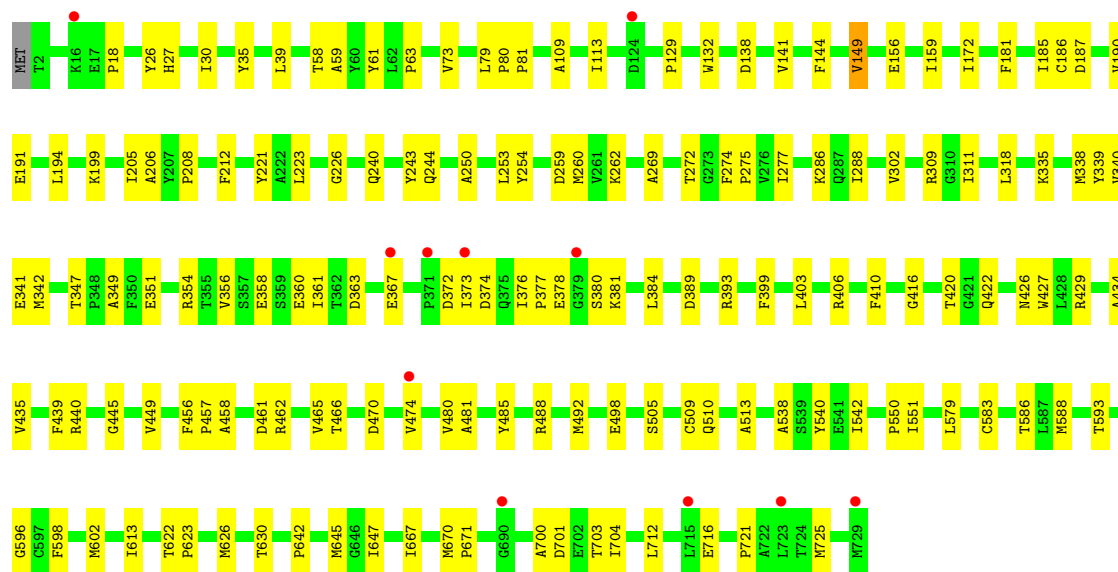


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

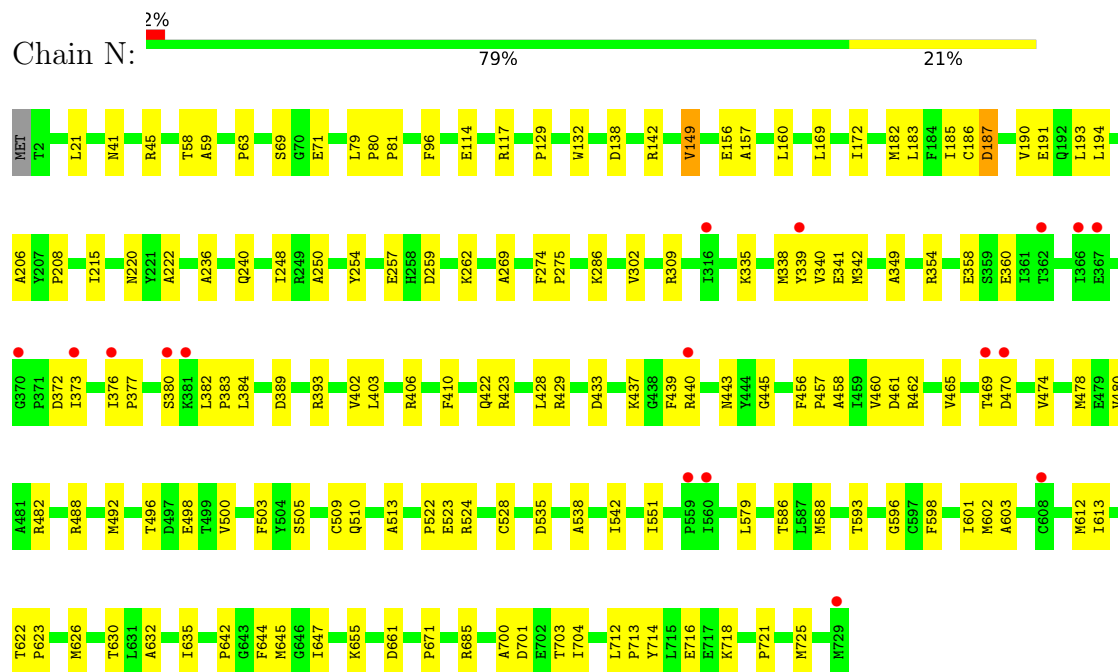


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

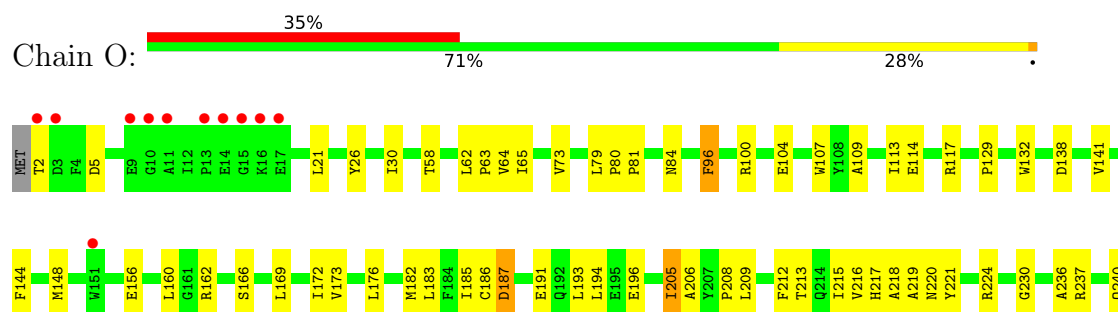


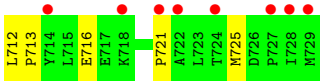


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.73Å 137.38Å 141.87Å 101.82° 109.08° 103.66°	Depositor
Resolution (Å)	49.63 – 2.47 49.63 – 2.47	Depositor EDS
% Data completeness (in resolution range)	86.9 (49.63-2.47) 79.3 (49.63-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.203 , 0.234 0.204 , 0.234	Depositor DCC
R_{free} test set	10245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	44026	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, XCC, MG, PGE, NI, SF4, PG5

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	0.24	0/5202	0.41	0/7048
1	B	0.24	0/5202	0.41	0/7048
1	C	0.24	0/5202	0.41	0/7048
1	D	0.24	0/5196	0.40	0/7040
2	M	0.24	0/5874	0.40	0/7954
2	N	0.24	0/5874	0.41	0/7954
2	O	0.24	0/5857	0.40	0/7933
2	P	0.24	0/5874	0.40	0/7954
All	All	0.24	0/44281	0.40	0/59979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5109	0	5103	118	0
1	B	5109	0	5103	114	0
1	C	5109	0	5103	111	0
1	D	5103	0	5099	121	0
2	M	5740	0	5701	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	5740	0	5701	101	0
2	O	5723	0	5681	153	0
2	P	5740	0	5701	138	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	1	0
3	O	8	0	0	0	0
3	P	8	0	0	1	0
4	A	9	0	0	2	0
4	B	9	0	0	2	0
4	C	9	0	0	2	0
4	D	9	0	0	3	0
5	A	10	14	14	0	0
6	C	12	18	18	1	0
7	M	2	0	0	0	0
7	N	2	0	0	0	0
7	O	2	0	0	0	0
7	P	2	0	0	0	0
8	M	2	0	0	0	0
8	N	2	0	0	0	0
8	P	2	0	0	0	0
9	N	1	0	0	0	0
10	A	84	0	0	2	0
10	B	77	0	0	0	0
10	C	44	0	0	1	0
10	D	51	0	0	1	0
10	M	76	0	0	1	0
10	N	79	0	0	1	0
10	O	12	0	0	0	0
10	P	45	0	0	0	0
All	All	43994	32	43224	939	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (939) 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:D:482:LEU:HD21	1:D:508:LEU:HD12	1.53	0.90
1:A:281:HIS:HB3	1:A:351:VAL:HG12	1.51	0.90
1:A:150:VAL:HG11	1:A:169:LYS:HG2	1.56	0.87
2:P:497:ASP:O	2:P:553:LYS:NZ	2.07	0.86
1:B:535:ALA:HB3	1:B:537:ILE:HD11	1.58	0.85
1:A:442:THR:HG21	1:A:535:ALA:HB2	1.59	0.84
2:M:339:TYR:HD2	2:M:340:VAL:HG23	1.42	0.84
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.59	0.83
1:B:482:LEU:HD21	1:B:508:LEU:HD12	1.60	0.82
2:M:149:VAL:HG11	2:M:509:CYS:HA	1.62	0.81
1:B:150:VAL:HG11	1:B:169:LYS:HG2	1.61	0.80
2:N:339:TYR:HD2	2:N:340:VAL:HG23	1.46	0.80
2:P:655:LYS:HG2	2:P:685:ARG:HH12	1.46	0.80
1:D:61:ILE:HD13	1:D:77:ARG:HE	1.48	0.79
2:O:479:GLU:HA	2:O:482:ARG:HD3	1.62	0.78
1:A:368[A]:HIS:CE1	1:A:411:ARG:HD3	2.18	0.78
1:B:559:LEU:HG	1:B:563:MET:HE3	1.66	0.78
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.65	0.77
1:D:150:VAL:HG11	1:D:169:LYS:HG2	1.66	0.76
1:C:482:LEU:HD21	1:C:508:LEU:HD12	1.67	0.76
2:P:149:VAL:HG11	2:P:509:CYS:HA	1.68	0.76
2:O:377:PRO:HG2	2:O:380:SER:HB3	1.68	0.75
1:B:662:VAL:HG21	2:N:194:LEU:HD13	1.69	0.75
1:A:559:LEU:HG	1:A:563:MET:HE3	1.66	0.74
1:A:535:ALA:HB3	1:A:537:ILE:HD11	1.68	0.74
1:C:66:ILE:HG23	1:C:612:GLY:HA3	1.68	0.74
1:C:291:ILE:HD13	1:C:397:ALA:HB1	1.69	0.74
2:P:338:MET:SD	2:P:341:GLU:HB2	2.27	0.74
2:M:335:LYS:HE3	2:M:429:ARG:HH22	1.51	0.74
1:C:368[B]:HIS:CE1	1:C:411:ARG:HD3	2.23	0.74
2:O:478:MET:O	2:O:482:ARG:HG3	1.87	0.74
1:A:282:GLY:HA3	1:A:352:ASP:OD1	1.88	0.74
1:B:61:ILE:HD13	1:B:77:ARG:HE	1.53	0.73
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.70	0.73
1:D:368[A]:HIS:CE1	1:D:411:ARG:HD3	2.23	0.73
1:B:281:HIS:HB3	1:B:351:VAL:HG12	1.70	0.73
1:C:61:ILE:HD13	1:C:77:ARG:NE	2.04	0.73
2:M:339:TYR:CE1	2:M:378:GLU:HG2	2.24	0.73
1:D:281:HIS:HB3	1:D:351:VAL:HG12	1.71	0.73
1:C:150:VAL:HG11	1:C:169:LYS:HG2	1.71	0.72
2:P:721:PRO:O	2:P:725:MET:HG3	1.89	0.71
1:A:442:THR:HG21	1:A:535:ALA:CB	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ILE:HD13	1:D:397:ALA:HB1	1.71	0.71
1:A:537:ILE:HG22	1:A:540:GLY:H	1.55	0.70
2:M:721:PRO:O	2:M:725:MET:HG3	1.91	0.70
2:P:339:TYR:CD2	2:P:340:VAL:HG23	2.26	0.70
2:O:58:THR:HA	2:O:138:ASP:OD1	1.91	0.70
1:D:482:LEU:CD2	1:D:508:LEU:HD12	2.21	0.70
1:A:535:ALA:HB3	1:A:537:ILE:CD1	2.22	0.70
2:O:2:THR:OG1	2:O:5:ASP:OD1	2.07	0.70
2:N:149:VAL:HG11	2:N:509:CYS:HA	1.73	0.69
1:C:559:LEU:HG	1:C:563:MET:HE3	1.73	0.69
1:B:281:HIS:O	1:B:351:VAL:HA	1.92	0.69
2:O:338:MET:SD	2:O:341:GLU:HB2	2.33	0.69
2:P:498:GLU:OE1	2:P:498:GLU:N	2.26	0.69
1:B:537:ILE:HG22	1:B:540:GLY:H	1.56	0.69
1:A:149:ARG:NH2	1:A:250:ASP:OD2	2.24	0.69
1:B:33:VAL:HG13	1:B:339:LEU:HD12	1.74	0.69
2:O:269:ALA:HB1	2:O:274:PHE:HB2	1.73	0.69
1:B:368[B]:HIS:CE1	1:B:411:ARG:HD3	2.27	0.68
1:C:482:LEU:CD2	1:C:508:LEU:HD12	2.23	0.68
1:A:33:VAL:HG13	1:A:339:LEU:HD12	1.76	0.68
1:C:281:HIS:HB3	1:C:351:VAL:HG12	1.75	0.68
2:M:613:ILE:HB	2:M:670:MET:HG2	1.75	0.68
1:C:282:GLY:HA3	1:C:352:ASP:OD1	1.94	0.68
2:P:339:TYR:HD2	2:P:340:VAL:HG23	1.57	0.67
1:D:282:GLY:HA3	1:D:352:ASP:OD1	1.95	0.67
2:O:498:GLU:N	2:O:498:GLU:OE1	2.27	0.67
1:D:559:LEU:HG	1:D:563:MET:HE3	1.77	0.67
1:A:281:HIS:O	1:A:351:VAL:HA	1.95	0.67
1:A:615:LEU:HD23	2:M:27:HIS:HB3	1.75	0.67
1:D:66:ILE:HG23	1:D:612:GLY:HA3	1.76	0.67
2:M:498:GLU:N	2:M:498:GLU:OE2	2.28	0.67
2:P:488:ARG:O	2:P:492:MET:HG2	1.94	0.67
1:B:66:ILE:HG23	1:B:612:GLY:HA3	1.76	0.67
2:O:488:ARG:O	2:O:492:MET:HG2	1.96	0.66
1:A:280:LEU:HD13	1:A:288:SER:HB2	1.77	0.66
1:A:291:ILE:HD13	1:A:397:ALA:HB1	1.75	0.66
1:B:607:MET:CE	1:B:608:PRO:HD2	2.25	0.66
2:O:553:LYS:HE2	2:O:564:TRP:CZ2	2.31	0.66
1:B:442:THR:HG21	1:B:535:ALA:HB2	1.77	0.66
1:B:482:LEU:CD2	1:B:508:LEU:HD12	2.26	0.66
2:N:377:PRO:HG2	2:N:380:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:439:PHE:O	2:M:440:ARG:HD2	1.96	0.65
1:D:144:LYS:O	1:D:148:ARG:HG3	1.96	0.65
1:D:299:GLU:HG2	1:D:303:LYS:HE2	1.78	0.65
2:M:340:VAL:HG21	2:M:376:ILE:HD11	1.79	0.65
2:O:602:MET:HE2	2:O:647:ILE:HD13	1.77	0.65
1:C:416:ARG:CD	1:C:417:PRO:HD2	2.27	0.65
1:C:31:PRO:HB2	1:C:423:ILE:HD13	1.77	0.65
2:P:613:ILE:O	2:P:671:PRO:HD3	1.95	0.65
2:P:363:ASP:OD1	2:P:462:ARG:HA	1.97	0.65
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.27	0.65
1:D:274:ASP:CB	1:D:308:LYS:HE2	2.26	0.65
1:D:470:CYS:HB3	4:D:702:XCC:S2	2.36	0.64
2:N:700:ALA:HA	2:N:704:ILE:HD12	1.78	0.64
1:B:176:ARG:O	1:B:207:GLY:HA3	1.97	0.64
1:D:591:ILE:HA	1:D:594:TRP:NE1	2.12	0.64
2:O:721:PRO:O	2:O:725:MET:HG3	1.98	0.64
1:B:288:SER:O	1:B:292:VAL:HG23	1.96	0.64
1:A:66:ILE:HG23	1:A:612:GLY:HA3	1.78	0.64
1:D:368[A]:HIS:CD2	1:D:411:ARG:HB2	2.33	0.64
2:P:346:ARG:HB3	2:P:381:LYS:HD2	1.80	0.64
2:P:579:LEU:HD11	2:P:593:THR:HG21	1.80	0.64
1:B:282:GLY:HA3	1:B:352:ASP:OD1	1.98	0.63
2:N:602:MET:HE2	2:N:647:ILE:HD13	1.80	0.63
1:C:591:ILE:HA	1:C:594:TRP:NE1	2.13	0.63
1:C:607:MET:CE	1:C:608:PRO:HD2	2.29	0.63
1:A:482:LEU:HD21	1:A:508:LEU:HD12	1.80	0.63
1:B:535:ALA:HB3	1:B:537:ILE:CD1	2.28	0.63
1:C:468:CYS:HB2	10:C:840:HOH:O	1.98	0.63
2:N:338:MET:SD	2:N:341:GLU:HB2	2.39	0.63
2:N:433:ASP:OD2	2:N:437:LYS:HE2	1.98	0.63
2:M:73:VAL:HG11	2:M:79:LEU:HD21	1.80	0.63
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.34	0.62
2:P:422:GLN:OE1	2:P:422:GLN:N	2.32	0.62
2:P:50:ASP:HA	2:P:75:LYS:HD2	1.79	0.62
1:A:591:ILE:HA	1:A:594:TRP:NE1	2.15	0.62
1:B:482:LEU:HD12	1:B:486:LYS:HE3	1.80	0.62
2:M:422:GLN:OE1	2:M:422:GLN:N	2.32	0.62
2:O:339:TYR:CD2	2:O:340:VAL:HG23	2.34	0.62
2:M:349:ALA:HA	2:M:384:LEU:O	2.00	0.62
2:O:339:TYR:CD2	2:O:435:VAL:HG21	2.35	0.62
2:P:510:GLN:HA	2:P:513:ALA:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:GLU:OE2	1:D:359:SER:OG	2.18	0.62
2:O:510:GLN:HA	2:O:513:ALA:O	1.99	0.62
1:A:482:LEU:HD12	1:A:486:LYS:HE3	1.80	0.61
1:D:607:MET:CE	1:D:608:PRO:HD2	2.30	0.61
2:M:505:SER:HB3	2:M:551:ILE:HD11	1.82	0.61
2:O:340:VAL:HG12	2:O:342:MET:SD	2.40	0.61
2:O:423:ARG:HB3	2:O:485:TYR:CZ	2.34	0.61
2:O:372:ASP:OD1	2:O:373:ILE:N	2.31	0.61
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.33	0.61
2:P:382:LEU:HD23	2:P:383:PRO:O	2.00	0.61
2:M:367:GLU:HG3	2:M:466:THR:HG23	1.82	0.61
2:O:349:ALA:HA	2:O:384:LEU:O	2.00	0.61
1:C:351:VAL:HB	1:C:356:ILE:HD13	1.82	0.61
2:N:358:GLU:HG3	2:N:462:ARG:NH1	2.15	0.61
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.83	0.61
2:N:63:PRO:HB2	2:N:220:ASN:HB2	1.83	0.61
2:P:58:THR:HA	2:P:138:ASP:OD1	1.99	0.61
1:A:3:ARG:HG2	10:M:939:HOH:O	2.01	0.61
1:B:107:LEU:HD21	1:B:215:LEU:HB3	1.82	0.61
2:O:572:TYR:CE2	2:O:577:ARG:HG2	2.36	0.61
1:A:33:VAL:HG13	1:A:339:LEU:CD1	2.31	0.61
1:D:281:HIS:O	1:D:351:VAL:HA	2.01	0.61
2:N:586:THR:HG22	2:N:588:MET:H	1.66	0.61
1:C:281:HIS:O	1:C:351:VAL:HA	2.00	0.61
2:O:382:LEU:HD23	2:O:383:PRO:O	2.01	0.61
2:P:701:ASP:OD1	2:P:703:THR:OG1	2.10	0.61
1:B:591:ILE:HA	1:B:594:TRP:NE1	2.15	0.60
1:C:154:VAL:HG13	1:C:162:LEU:HD11	1.83	0.60
2:O:348:PRO:HG2	2:O:383:PRO:HB3	1.83	0.60
1:C:601:PRO:HD3	1:C:652:ARG:NH2	2.17	0.60
1:D:176:ARG:O	1:D:207:GLY:HA3	2.01	0.60
2:O:186:CYS:O	2:O:187:ASP:HB2	2.01	0.60
1:D:447:ASN:ND2	1:D:450:ARG:HB2	2.17	0.60
1:A:570:ASP:OD2	1:A:571:THR:N	2.33	0.60
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.31	0.60
2:P:358:GLU:HG3	2:P:462:ARG:NH1	2.16	0.60
1:C:291:ILE:HD13	1:C:397:ALA:CB	2.31	0.59
1:D:601:PRO:HD3	1:D:652:ARG:CZ	2.32	0.59
2:N:354:ARG:NH2	2:N:480:VAL:HG11	2.16	0.59
2:N:602:MET:HE2	2:N:647:ILE:HG21	1.84	0.59
2:O:358:GLU:HG3	2:O:462:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HG23	1:A:597:SER:OG	2.03	0.59
1:A:607:MET:CE	1:A:608:PRO:HD2	2.33	0.59
2:N:187:ASP:OD2	2:N:262:LYS:HE3	2.02	0.59
2:N:349:ALA:HA	2:N:384:LEU:O	2.02	0.59
2:N:58:THR:HA	2:N:138:ASP:OD1	2.01	0.59
2:O:626:MET:HB3	2:O:630:THR:HB	1.84	0.59
2:P:372:ASP:OD1	2:P:373:ILE:N	2.32	0.59
1:B:655:LYS:HG3	2:N:191:GLU:HG2	1.85	0.59
1:C:584:MET:HG3	1:D:73:ALA:HB2	1.85	0.59
1:B:442:THR:HG21	1:B:535:ALA:CB	2.33	0.59
1:D:33:VAL:HG13	1:D:339:LEU:HD12	1.85	0.59
1:D:559:LEU:HG	1:D:563:MET:CE	2.32	0.59
2:M:339:TYR:CD2	2:M:340:VAL:HG23	2.31	0.59
1:A:581:PRO:O	1:A:605:GLY:HA3	2.03	0.59
1:A:615:LEU:CD2	2:M:27:HIS:HB3	2.33	0.59
1:C:235:ILE:HG23	1:C:597:SER:OG	2.02	0.59
2:N:721:PRO:O	2:N:725:MET:HG3	2.02	0.59
2:P:356:VAL:HG21	2:P:361:ILE:HB	1.85	0.59
2:P:354:ARG:HD2	2:P:389:ASP:OD2	2.03	0.58
2:P:479:GLU:OE1	2:P:482:ARG:HD2	2.03	0.58
1:B:31:PRO:HB2	1:B:423:ILE:HD13	1.86	0.58
1:A:154:VAL:HG13	1:A:162:LEU:HD11	1.85	0.58
1:B:447:ASN:ND2	1:B:566:ASP:OD2	2.24	0.58
2:M:338:MET:SD	2:M:341:GLU:HB2	2.43	0.58
2:P:269:ALA:HB1	2:P:274:PHE:HB2	1.85	0.58
1:D:607:MET:HE2	1:D:608:PRO:HD2	1.85	0.58
1:A:351:VAL:HB	1:A:356:ILE:HD13	1.84	0.58
1:A:150:VAL:HG13	1:A:184:THR:HG21	1.85	0.58
2:P:199:LYS:HE2	2:P:199:LYS:HA	1.85	0.58
1:B:577:VAL:HG21	1:B:645:ILE:HG23	1.86	0.58
2:O:423:ARG:HD3	2:O:485:TYR:CD2	2.39	0.58
2:M:351:GLU:HB3	2:M:426:ASN:HD21	1.69	0.57
2:M:602:MET:HE2	2:M:647:ILE:HG21	1.86	0.57
1:C:33:VAL:HG13	1:C:339:LEU:HD12	1.85	0.57
2:O:172:ILE:HG23	2:O:302:VAL:CG2	2.34	0.57
1:A:587:LYS:HE3	4:A:703:XCC:S4	2.44	0.57
1:C:61:ILE:HG21	1:C:77:ARG:HE	1.69	0.57
2:N:422:GLN:HG2	2:N:423:ARG:HG3	1.86	0.57
2:N:335:LYS:HE3	2:N:429:ARG:HH22	1.68	0.57
2:P:433:ASP:OD1	2:P:437:LYS:HE2	2.03	0.57
1:C:176:ARG:O	1:C:207:GLY:HA3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:LYS:HE3	4:D:702:XCC:S4	2.45	0.57
2:N:393:ARG:HG2	2:N:461:ASP:OD2	2.05	0.57
1:A:416:ARG:HG3	1:A:417:PRO:HD2	1.86	0.57
1:D:398:LYS:O	1:D:402:ARG:HG3	2.03	0.57
2:N:186:CYS:O	2:N:187:ASP:HB2	2.05	0.57
2:O:399:PHE:HZ	2:O:541:GLU:HG3	1.69	0.57
2:O:433:ASP:OD2	2:O:437:LYS:HE2	2.04	0.57
1:D:150:VAL:HG13	1:D:184:THR:HG21	1.86	0.57
1:D:317:CYS:HB3	1:D:549:SER:HB2	1.87	0.57
2:M:141:VAL:HG22	2:M:221:TYR:CE2	2.39	0.57
2:N:114:GLU:OE1	2:N:117:ARG:NH1	2.38	0.57
1:A:175:ARG:HB3	1:B:175:ARG:HB3	1.87	0.56
1:B:278:PHE:HB3	1:B:312:LEU:HD23	1.87	0.56
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.86	0.56
1:C:61:ILE:HD13	1:C:77:ARG:HE	1.69	0.56
1:C:303:LYS:HA	1:C:307:ALA:O	2.04	0.56
1:D:291:ILE:HD13	1:D:397:ALA:CB	2.34	0.56
1:C:559:LEU:HG	1:C:563:MET:CE	2.35	0.56
1:A:144:LYS:O	1:A:148:ARG:HG3	2.06	0.56
1:B:351:VAL:HB	1:B:356:ILE:HD13	1.87	0.56
2:M:579:LEU:HD11	2:M:593:THR:HG21	1.88	0.56
2:P:583:CYS:HB2	2:P:586:THR:HG22	1.87	0.56
1:B:587:LYS:HE3	4:B:702:XCC:S4	2.46	0.56
1:B:470:CYS:HB3	4:B:702:XCC:S2	2.46	0.56
1:A:615:LEU:HD23	2:M:27:HIS:CB	2.36	0.56
2:M:358:GLU:HG3	2:M:462:ARG:NH1	2.21	0.56
2:O:26:TYR:CZ	2:O:30:ILE:HD11	2.40	0.56
2:O:679:HIS:O	2:O:683:VAL:HG23	2.06	0.56
2:P:376:ILE:HG21	2:P:382:LEU:HD12	1.87	0.56
2:P:583:CYS:CB	2:P:586:THR:HG22	2.36	0.56
1:C:60:LYS:H	6:C:704:PG5:H83	1.71	0.56
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.86	0.56
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.05	0.56
2:N:478:MET:O	2:N:482:ARG:HG3	2.06	0.56
2:O:433:ASP:O	2:O:437:LYS:HG3	2.05	0.56
1:A:470:CYS:HB3	4:A:703:XCC:S2	2.46	0.55
2:N:498:GLU:OE2	2:N:498:GLU:N	2.38	0.55
1:B:370:ARG:HD3	1:B:407:ALA:HB2	1.87	0.55
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.88	0.55
1:A:456:ILE:HD13	1:A:463:GLY:HA2	1.88	0.55
2:P:602:MET:HE3	2:P:645:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:PRO:O	1:C:605:GLY:HA3	2.06	0.55
2:O:422:GLN:N	2:O:422:GLN:OE1	2.39	0.55
2:P:342:MET:HE2	2:P:384:LEU:HD22	1.89	0.55
1:A:150:VAL:CG1	1:A:169:LYS:HG2	2.32	0.55
1:A:292:VAL:HB	10:A:838:HOH:O	2.07	0.55
1:A:61:ILE:HD13	1:A:77:ARG:HD2	1.87	0.55
1:B:559:LEU:HG	1:B:563:MET:CE	2.36	0.55
1:B:77:ARG:NH1	1:B:79:LYS:HE2	2.22	0.55
1:C:587:LYS:HE3	4:C:703:XCC:S4	2.46	0.55
1:B:607:MET:HE3	1:B:608:PRO:HD2	1.87	0.55
2:M:416:GLY:HA3	2:M:434:ALA:HB2	1.88	0.55
2:P:700:ALA:HA	2:P:704:ILE:HD12	1.87	0.55
2:M:583:CYS:CB	2:M:586:THR:HG22	2.37	0.55
1:C:447:ASN:ND2	1:C:450:ARG:HB2	2.22	0.55
1:D:335:ALA:HB2	1:D:471:ASN:HB3	1.89	0.55
2:P:342:MET:HG3	2:P:382:LEU:O	2.07	0.55
1:C:150:VAL:HG13	1:C:184:THR:HG21	1.88	0.54
1:D:601:PRO:HD3	1:D:652:ARG:NH2	2.22	0.54
1:A:559:LEU:HG	1:A:563:MET:CE	2.36	0.54
2:M:144:PHE:CE1	2:M:205:ILE:HG12	2.43	0.54
2:O:278:THR:HG21	2:O:282:LEU:HD11	1.89	0.54
1:C:158:SER:OG	1:C:161:GLU:HG3	2.07	0.54
2:O:317:LYS:HB3	2:O:317:LYS:NZ	2.22	0.54
1:D:158:SER:OG	1:D:161:GLU:HG3	2.07	0.54
1:C:107:LEU:HD13	1:C:216:VAL:HG22	1.89	0.54
2:M:206:ALA:O	2:M:208:PRO:HD3	2.08	0.54
2:O:503:PHE:O	2:O:551:ILE:N	2.36	0.54
2:O:686:SER:HB3	2:O:692:GLY:O	2.08	0.54
2:P:186:CYS:O	2:P:187:ASP:HB2	2.07	0.54
1:A:321:GLU:OE1	1:A:325:ARG:NH1	2.34	0.54
2:P:114:GLU:OE1	2:P:117:ARG:NH1	2.41	0.54
1:D:577:VAL:HG13	1:D:649:LEU:CD2	2.38	0.54
2:O:114:GLU:OE1	2:O:117:ARG:NH1	2.41	0.54
2:O:182:MET:HA	2:O:205:ILE:HG22	1.90	0.54
1:A:176:ARG:O	1:A:207:GLY:HA3	2.08	0.54
2:N:712:LEU:O	2:N:716:GLU:HG3	2.08	0.54
2:O:156:GLU:HG3	2:O:182:MET:HB3	1.89	0.54
2:O:333:ILE:HD12	2:O:429:ARG:HB2	1.91	0.54
1:D:314:GLY:O	1:D:331:VAL:HG12	2.09	0.53
1:D:581:PRO:O	1:D:605:GLY:HA3	2.08	0.53
2:M:470:ASP:O	2:M:474:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:700:ALA:HA	2:M:704:ILE:HD12	1.89	0.53
2:O:602:MET:CE	2:O:647:ILE:HD13	2.38	0.53
2:P:199:LYS:HD3	2:P:204:TYR:OH	2.08	0.53
1:D:656:LEU:O	1:D:660:LYS:HG3	2.09	0.53
2:M:399:PHE:O	2:M:403:LEU:HD13	2.07	0.53
1:D:486:LYS:HE2	1:D:519:TYR:CE2	2.43	0.53
1:D:570:ASP:OD2	1:D:571:THR:N	2.40	0.53
2:O:316:ILE:N	2:O:316:ILE:HD12	2.24	0.53
2:O:456:PHE:HB3	2:O:459:ILE:CG2	2.38	0.53
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.90	0.53
2:O:585:TYR:CE1	2:O:656:LYS:HB3	2.44	0.53
2:O:141:VAL:HG22	2:O:221:TYR:CE2	2.43	0.53
2:M:372:ASP:OD1	2:M:373:ILE:N	2.39	0.53
2:P:187:ASP:OD2	2:P:262:LYS:HE3	2.09	0.53
2:P:439:PHE:O	2:P:440:ARG:HD2	2.08	0.53
1:A:291:ILE:HD13	1:A:397:ALA:CB	2.37	0.53
2:M:356:VAL:HG21	2:M:361:ILE:HB	1.91	0.53
2:M:340:VAL:CG2	2:M:376:ILE:HD11	2.38	0.53
2:N:439:PHE:O	2:N:440:ARG:HD2	2.09	0.53
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.39	0.53
1:C:607:MET:HE2	1:C:608:PRO:HD2	1.90	0.53
2:M:187:ASP:OD2	2:M:262:LYS:HE3	2.09	0.53
2:O:404:GLU:OE1	2:O:423:ARG:HG2	2.08	0.53
1:A:505:ALA:HB1	1:A:510:LEU:HB2	1.89	0.53
2:N:354:ARG:HD2	2:N:389:ASP:OD2	2.08	0.53
2:N:402:VAL:HG13	2:N:535:ASP:OD1	2.09	0.53
2:O:21:LEU:HB2	2:O:286:LYS:HA	1.90	0.53
1:B:570:ASP:OD2	1:B:571:THR:N	2.41	0.53
1:C:338:GLU:OE2	1:C:359:SER:OG	2.20	0.53
2:P:588:MET:O	2:P:642:PRO:HB3	2.08	0.53
1:C:33:VAL:HG13	1:C:339:LEU:CD1	2.38	0.52
1:C:428:VAL:HG22	1:C:539:ILE:HD11	1.91	0.52
2:O:376:ILE:HG21	2:O:382:LEU:HD12	1.91	0.52
1:A:368[A]:HIS:CD2	1:A:411:ARG:HB2	2.45	0.52
1:C:370:ARG:HD2	1:C:384:TYR:CE2	2.44	0.52
1:B:482:LEU:HD13	1:B:510:LEU:HD11	1.92	0.52
1:A:577:VAL:HG13	1:A:649:LEU:CD2	2.40	0.52
2:O:524:ARG:NH1	2:O:584:LEU:O	2.41	0.52
2:P:141:VAL:HG22	2:P:221:TYR:CE2	2.44	0.52
1:A:577:VAL:HG21	1:A:645:ILE:CG2	2.40	0.52
2:N:21:LEU:HB2	2:N:286:LYS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:438:GLY:HA2	2:P:440:ARG:NH1	2.24	0.52
1:A:107:LEU:HD13	1:A:216:VAL:HG22	1.92	0.52
1:D:107:LEU:HD13	1:D:216:VAL:HG22	1.91	0.52
2:M:58:THR:HA	2:M:138:ASP:OD1	2.10	0.52
2:N:206:ALA:O	2:N:208:PRO:HD3	2.09	0.52
2:N:422:GLN:N	2:N:422:GLN:OE1	2.43	0.52
2:P:350:PHE:HA	2:P:426:ASN:HD22	1.75	0.52
1:A:607:MET:HE2	1:A:608:PRO:HD2	1.91	0.52
1:B:10:ASN:HB2	2:N:257:GLU:OE2	2.09	0.52
2:P:384:LEU:CD2	2:P:428:LEU:HD22	2.39	0.52
1:B:446:GLN:NE2	1:C:42:ASP:OD2	2.43	0.52
2:O:445:GLY:O	2:O:449:VAL:HG23	2.10	0.52
1:C:224:ASP:OD1	1:C:229:ASN:ND2	2.40	0.51
1:C:368[B]:HIS:CD2	1:C:407:ALA:HB1	2.45	0.51
1:D:447:ASN:ND2	1:D:566:ASP:OD2	2.25	0.51
1:C:324:MET:HE3	1:C:430:GLY:HA2	1.92	0.51
2:M:156:GLU:O	2:M:250:ALA:HA	2.11	0.51
1:B:150:VAL:CG1	1:B:169:LYS:HG2	2.34	0.51
1:D:77:ARG:NH1	1:D:79:LYS:HE2	2.24	0.51
2:O:187:ASP:OD2	2:O:262:LYS:HE3	2.11	0.51
1:A:468:CYS:HB2	10:A:857:HOH:O	2.10	0.51
1:B:607:MET:HE2	1:B:608:PRO:HD2	1.92	0.51
1:C:577:VAL:HG21	1:C:645:ILE:HG23	1.91	0.51
1:D:77:ARG:HH11	1:D:79:LYS:HE2	1.75	0.51
2:N:510:GLN:HA	2:N:513:ALA:O	2.11	0.51
2:O:701:ASP:OD1	2:O:703:THR:OG1	2.19	0.51
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.41	0.51
1:C:587:LYS:O	1:C:591:ILE:HG13	2.10	0.51
1:D:571:THR:OG1	1:D:572:PRO:HD3	2.10	0.51
2:M:186:CYS:O	2:M:187:ASP:HB2	2.10	0.51
2:N:156:GLU:HG3	2:N:182:MET:HB3	1.93	0.51
2:N:406:ARG:HB3	2:N:410:PHE:CZ	2.46	0.51
2:P:373:ILE:HD13	2:P:435:VAL:HG22	1.93	0.51
1:D:370:ARG:HD2	1:D:384:TYR:CE2	2.46	0.51
1:D:456:ILE:HD13	1:D:463:GLY:HA2	1.93	0.51
2:M:377:PRO:HG2	2:M:380:SER:HB3	1.92	0.51
1:B:601:PRO:HD3	1:B:652:ARG:NH2	2.25	0.50
2:P:346:ARG:HB3	2:P:381:LYS:CD	2.41	0.50
2:P:423:ARG:O	2:P:426:ASN:ND2	2.44	0.50
1:D:577:VAL:HG21	1:D:645:ILE:HG23	1.92	0.50
2:P:655:LYS:HA	2:P:685:ARG:NH2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TYR:OH	1:A:393:ALA:HB1	2.12	0.50
1:B:61:ILE:HD13	1:B:77:ARG:NE	2.22	0.50
1:C:368[B]:HIS:HD2	1:C:407:ALA:HB1	1.77	0.50
1:D:298:MET:HE1	1:D:402:ARG:HG2	1.94	0.50
1:D:330:LEU:HD11	1:D:503:GLN:CG	2.42	0.50
2:P:338:MET:O	2:P:432:LYS:HE3	2.11	0.50
1:B:656:LEU:O	1:B:660:LYS:HG3	2.11	0.50
1:C:317:CYS:HB3	1:C:549:SER:HB2	1.93	0.50
1:B:291:ILE:HD13	1:B:397:ALA:HB1	1.93	0.50
1:B:316:CYS:N	1:B:503:GLN:HE22	2.09	0.50
1:C:5:ARG:HB2	2:O:162:ARG:NH2	2.26	0.50
2:M:613:ILE:O	2:M:671:PRO:HD3	2.11	0.50
2:N:384:LEU:CD2	2:N:428:LEU:HD22	2.41	0.50
2:O:156:GLU:HB2	2:O:250:ALA:HB2	1.94	0.50
2:O:470:ASP:HB3	2:O:473:LYS:CG	2.42	0.50
2:P:316:ILE:HG13	2:P:454:GLU:OE2	2.12	0.50
2:M:172:ILE:HG23	2:M:302:VAL:CG2	2.42	0.50
2:N:505:SER:HB3	2:N:551:ILE:HD11	1.94	0.50
2:O:354:ARG:HD2	2:O:389:ASP:OD2	2.12	0.50
2:P:335:LYS:HD2	2:P:335:LYS:H	1.76	0.50
2:P:342:MET:HG2	2:P:384:LEU:HB2	1.92	0.50
2:P:393:ARG:HG2	2:P:461:ASP:OD2	2.12	0.50
1:A:548:GLY:HA3	1:A:552:ASP:OD2	2.12	0.50
2:M:354:ARG:NH2	2:M:480:VAL:HG11	2.27	0.50
2:M:583:CYS:HB2	2:M:586:THR:HG22	1.92	0.50
2:O:562:GLY:HA3	2:O:585:TYR:CD2	2.47	0.50
2:P:356:VAL:CG2	2:P:361:ILE:HB	2.40	0.50
2:P:478:MET:O	2:P:482:ARG:HG3	2.11	0.50
1:A:447:ASN:ND2	1:A:566:ASP:OD2	2.30	0.49
1:B:33:VAL:HG13	1:B:339:LEU:CD1	2.40	0.49
1:B:77:ARG:HH11	1:B:79:LYS:HE2	1.76	0.49
1:D:384:TYR:CD1	2:O:84:ASN:HB3	2.46	0.49
1:A:626:ASP:HB3	2:M:212:PHE:CG	2.47	0.49
2:P:206:ALA:O	2:P:208:PRO:HD3	2.11	0.49
2:P:602:MET:CE	2:P:647:ILE:HG21	2.42	0.49
1:C:316:CYS:N	1:C:503:GLN:HE22	2.11	0.49
1:D:505:ALA:HB1	1:D:510:LEU:HB2	1.94	0.49
2:P:173:VAL:HG21	2:P:193:LEU:HD21	1.93	0.49
2:M:701:ASP:OD1	2:M:703:THR:OG1	2.14	0.49
2:N:456:PHE:HA	2:N:542:ILE:HD13	1.95	0.49
1:C:505:ALA:HB1	1:C:510:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:VAL:HB	1:C:573:LYS:HD3	1.94	0.49
1:D:190:ILE:HG13	1:D:195:LYS:HG3	1.94	0.49
2:O:73:VAL:HG11	2:O:79:LEU:HD21	1.94	0.49
2:M:393:ARG:HG2	2:M:461:ASP:OD2	2.12	0.49
1:D:662:VAL:HG21	2:P:194:LEU:HD13	1.94	0.49
2:P:340:VAL:HG12	2:P:342:MET:SD	2.53	0.49
1:B:581:PRO:O	1:B:605:GLY:HA3	2.12	0.49
2:M:156:GLU:HB2	2:M:250:ALA:HB2	1.95	0.49
2:M:456:PHE:HA	2:M:542:ILE:HD13	1.94	0.49
2:O:335:LYS:NZ	2:O:429:ARG:HH22	2.10	0.49
2:O:583:CYS:HB2	2:O:586:THR:HG22	1.94	0.49
2:M:363:ASP:OD1	2:M:462:ARG:HA	2.13	0.49
2:N:602:MET:CE	2:N:647:ILE:HG21	2.42	0.49
2:O:524:ARG:NH2	2:O:645:MET:SD	2.85	0.49
1:A:443:GLN:HB2	1:A:451:VAL:HG21	1.93	0.49
1:C:280:LEU:HD13	1:C:288:SER:HB2	1.95	0.49
2:O:626:MET:HG2	2:O:630:THR:HG21	1.95	0.49
1:B:150:VAL:HG13	1:B:184:THR:HG21	1.94	0.49
1:B:321:GLU:OE1	1:B:325:ARG:NH1	2.41	0.49
1:C:150:VAL:HG12	1:C:169:LYS:HE2	1.94	0.49
1:C:482:LEU:HD12	1:C:486:LYS:HE3	1.94	0.49
1:C:63:TYR:OH	1:C:607:MET:HB3	2.13	0.49
2:M:109:ALA:O	2:M:113:ILE:HG13	2.13	0.49
2:O:523:GLU:OE1	2:O:655:LYS:HB2	2.13	0.49
2:M:588:MET:O	2:M:642:PRO:HB3	2.13	0.48
2:O:315:LYS:HA	2:O:454:GLU:OE2	2.13	0.48
2:P:259:ASP:OD1	2:P:262:LYS:HD2	2.12	0.48
1:B:39:LYS:NZ	1:B:43:ASP:OD2	2.42	0.48
1:D:587:LYS:O	1:D:591:ILE:HG13	2.12	0.48
2:P:602:MET:CE	2:P:647:ILE:HD13	2.38	0.48
1:D:98:VAL:O	1:D:102:VAL:HG12	2.13	0.48
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.48	0.48
2:O:470:ASP:O	2:O:474:VAL:HG23	2.14	0.48
1:A:615:LEU:HD22	2:M:260:MET:SD	2.54	0.48
1:A:658:VAL:O	1:A:662:VAL:HG23	2.14	0.48
1:B:483:THR:HB	1:B:638:PRO:HB2	1.95	0.48
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.95	0.48
1:C:482:LEU:HD13	1:C:510:LEU:HD11	1.96	0.48
1:D:107:LEU:HD21	1:D:215:LEU:HB3	1.96	0.48
2:M:540:TYR:CD1	2:M:550:PRO:HD3	2.49	0.48
2:P:199:LYS:HD3	2:P:204:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ALA:HB1	1:B:510:LEU:HB2	1.96	0.48
1:C:570:ASP:HB3	1:C:572:PRO:HD2	1.96	0.48
1:D:279:VAL:HG22	1:D:313:VAL:CG2	2.43	0.48
2:N:259:ASP:OD1	2:N:262:LYS:HD2	2.13	0.48
2:O:376:ILE:HD12	2:O:376:ILE:O	2.14	0.48
2:P:360:GLU:O	2:P:360:GLU:HG2	2.13	0.48
1:A:482:LEU:CD2	1:A:508:LEU:HD12	2.44	0.48
1:B:577:VAL:HG21	1:B:645:ILE:CG2	2.43	0.48
1:C:607:MET:HE3	1:C:608:PRO:HD2	1.95	0.48
2:N:603:ALA:HB3	2:N:612:MET:HG3	1.96	0.48
2:O:393:ARG:HG2	2:O:461:ASP:OD2	2.14	0.48
1:A:31:PRO:HB2	1:A:423:ILE:HD13	1.96	0.48
1:B:186:LEU:O	1:B:190:ILE:HG12	2.14	0.48
1:B:464:VAL:HG21	1:B:563:MET:HE1	1.96	0.48
2:N:622:THR:HB	2:N:623:PRO:HD2	1.96	0.48
1:A:299:GLU:HG2	1:A:303:LYS:HE2	1.96	0.48
1:B:118:ASN:C	1:B:118:ASN:HD22	2.17	0.48
1:B:368[B]:HIS:CD2	1:B:411:ARG:HB2	2.48	0.48
2:O:206:ALA:O	2:O:208:PRO:HD3	2.14	0.48
2:O:236:ALA:O	2:O:240:GLN:HG2	2.14	0.48
1:D:274:ASP:HB2	1:D:308:LYS:HE2	1.95	0.47
1:D:33:VAL:HG13	1:D:339:LEU:CD1	2.44	0.47
2:O:377:PRO:HG2	2:O:380:SER:CB	2.42	0.47
2:O:321:PRO:HG3	2:O:438:GLY:O	2.14	0.47
2:O:527:LEU:HD12	2:O:528:CYS:N	2.29	0.47
2:P:156:GLU:HG3	2:P:182:MET:HB3	1.95	0.47
1:A:150:VAL:HG12	1:A:169:LYS:HE2	1.95	0.47
1:A:186:LEU:O	1:A:190:ILE:HG12	2.14	0.47
1:B:409:LYS:O	1:B:413:GLU:HG3	2.14	0.47
1:C:517:GLU:OE2	1:C:525:LYS:HD2	2.14	0.47
1:C:113:HIS:NE2	1:C:587:LYS:HD2	2.29	0.47
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.48	0.47
2:M:59:ALA:HB2	2:M:630:THR:HA	1.96	0.47
1:A:278:PHE:HB3	1:A:312:LEU:HD23	1.96	0.47
2:M:602:MET:HE3	2:M:645:MET:HE2	1.95	0.47
2:N:579:LEU:HD11	2:N:593:THR:HG21	1.97	0.47
1:C:571:THR:OG1	1:C:572:PRO:HD3	2.13	0.47
1:D:283:HIS:CE1	4:D:702:XCC:S3	3.07	0.47
2:N:129:PRO:O	2:N:132:TRP:HB2	2.15	0.47
2:N:360:GLU:O	2:N:360:GLU:HG2	2.14	0.47
2:O:470:ASP:HB3	2:O:473:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:505:SER:HB3	2:P:551:ILE:HD11	1.95	0.47
1:C:483:THR:CG2	1:C:638:PRO:HB2	2.44	0.47
2:O:538:ALA:O	2:O:542:ILE:HG13	2.14	0.47
2:P:315:LYS:HA	2:P:454:GLU:OE1	2.15	0.47
1:A:118:ASN:HD22	1:A:118:ASN:C	2.18	0.47
1:B:107:LEU:HD13	1:B:216:VAL:HG22	1.96	0.47
2:M:199:LYS:HA	2:M:199:LYS:HD2	1.59	0.47
2:N:340:VAL:HG12	2:N:342:MET:SD	2.55	0.47
2:N:372:ASP:OD1	2:N:373:ILE:N	2.42	0.47
2:P:354:ARG:NH2	2:P:480:VAL:HG11	2.29	0.47
1:D:150:VAL:CG1	1:D:169:LYS:HG2	2.40	0.47
2:M:373:ILE:CD1	2:M:435:VAL:HG22	2.44	0.47
2:M:510:GLN:HA	2:M:513:ALA:O	2.14	0.47
1:B:332:THR:OG1	1:B:336:SER:OG	2.20	0.47
1:C:250:ASP:O	1:C:254:ILE:HG13	2.15	0.47
1:D:655:LYS:HG2	2:P:191:GLU:HG2	1.97	0.47
2:M:457:PRO:O	2:M:458:ALA:HB3	2.15	0.47
2:O:144:PHE:O	2:O:148:MET:HG3	2.14	0.47
2:O:572:TYR:HA	2:O:579:LEU:O	2.14	0.47
2:O:585:TYR:CD1	2:O:656:LYS:HB3	2.50	0.47
2:P:73:VAL:HG11	2:P:79:LEU:HD21	1.97	0.47
1:A:182:GLU:OE2	1:A:199:ARG:HD3	2.14	0.47
1:B:452:LEU:HD21	1:B:464:VAL:HG21	1.96	0.47
1:C:150:VAL:CG1	1:C:169:LYS:HE2	2.44	0.47
1:C:468:CYS:O	1:C:580:ALA:HA	2.15	0.47
1:D:655:LYS:NZ	1:D:674:TYR:O	2.36	0.47
2:O:144:PHE:CE1	2:O:205:ILE:HG12	2.49	0.47
2:O:479:GLU:HA	2:O:482:ARG:CD	2.37	0.47
2:P:185:ILE:HD12	2:P:185:ILE:N	2.30	0.47
2:P:445:GLY:O	2:P:449:VAL:HG23	2.15	0.47
1:C:73:ALA:HB2	1:D:584:MET:HG3	1.97	0.47
1:D:282:GLY:C	1:D:318:THR:HB	2.35	0.47
2:O:96:PHE:O	2:O:100:ARG:HG3	2.15	0.47
2:O:373:ILE:CD1	2:O:435:VAL:HG22	2.45	0.47
2:P:712:LEU:O	2:P:716:GLU:HG3	2.15	0.47
1:B:190:ILE:HG13	1:B:195:LYS:HG3	1.96	0.46
2:M:335:LYS:H	2:M:335:LYS:HD2	1.81	0.46
2:P:283:PRO:HD2	2:P:286:LYS:HD3	1.96	0.46
2:P:342:MET:CE	2:P:384:LEU:HD22	2.45	0.46
1:D:154:VAL:HG13	1:D:162:LEU:HD11	1.98	0.46
2:N:500:VAL:HG21	2:N:522:PRO:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:701:ASP:OD1	2:N:703:THR:OG1	2.22	0.46
2:O:166:SER:OG	2:O:196:GLU:HG2	2.14	0.46
1:A:190:ILE:HG13	1:A:195:LYS:HG3	1.97	0.46
1:A:468:CYS:O	1:A:580:ALA:HA	2.14	0.46
1:C:314:GLY:O	1:C:331:VAL:HG12	2.15	0.46
2:O:26:TYR:CE2	2:O:30:ILE:HD11	2.51	0.46
2:P:377:PRO:HG2	2:P:380:SER:HB3	1.98	0.46
1:A:607:MET:HE3	1:A:634:PHE:CD2	2.51	0.46
2:M:269:ALA:HB1	2:M:274:PHE:HB2	1.98	0.46
2:N:236:ALA:O	2:N:240:GLN:HG2	2.15	0.46
2:O:185:ILE:HD12	2:O:185:ILE:N	2.31	0.46
2:O:176:LEU:HD21	2:O:302:VAL:HG13	1.98	0.46
1:B:3:ARG:HB2	10:N:954:HOH:O	2.14	0.46
1:C:98:VAL:O	1:C:102:VAL:HG12	2.16	0.46
1:C:416:ARG:CG	1:C:417:PRO:HD2	2.45	0.46
1:D:332:THR:HG1	1:D:336:SER:HG	1.62	0.46
2:M:275:PRO:HD2	2:M:309:ARG:HD3	1.97	0.46
2:P:670:MET:CE	2:P:674:LEU:HG	2.46	0.46
1:B:68:CYS:HB2	1:B:97:ILE:HG23	1.96	0.46
1:C:662:VAL:HG21	2:O:194:LEU:HD13	1.97	0.46
2:M:185:ILE:HG22	2:M:190:VAL:HG23	1.97	0.46
1:D:147:CYS:HB3	1:D:152:ILE:HB	1.96	0.46
2:N:222:ALA:HB1	2:N:248:ILE:HG21	1.98	0.46
2:P:523:GLU:OE1	2:P:655:LYS:HB2	2.16	0.46
1:A:52:PHE:CZ	1:A:474:LYS:HA	2.51	0.46
1:D:273:PRO:HD3	1:D:420:ILE:HD12	1.97	0.46
1:D:559:LEU:O	1:D:563:MET:HG3	2.16	0.46
2:N:503:PHE:O	2:N:551:ILE:N	2.46	0.46
2:O:277:ILE:N	2:O:277:ILE:HD12	2.31	0.46
2:P:80:PRO:N	2:P:81:PRO:HD2	2.31	0.46
1:A:577:VAL:HG21	1:A:645:ILE:HG23	1.96	0.46
1:C:416:ARG:HD2	1:C:417:PRO:HD2	1.97	0.46
1:C:570:ASP:OD2	1:C:571:THR:N	2.48	0.46
1:D:452:LEU:HD21	1:D:464:VAL:HG21	1.98	0.46
1:D:354:GLN:HB3	1:D:587:LYS:HZ1	1.81	0.46
2:M:445:GLY:O	2:M:449:VAL:HG23	2.16	0.46
2:M:149:VAL:CG1	2:M:509:CYS:HA	2.41	0.46
2:N:626:MET:HB3	2:N:630:THR:HB	1.98	0.46
2:P:607:GLU:HB2	2:P:708:VAL:HG11	1.97	0.46
1:B:658:VAL:O	1:B:662:VAL:HG23	2.16	0.46
2:N:457:PRO:O	2:N:458:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:160:LEU:HD13	2:O:215:ILE:HD13	1.97	0.46
2:O:605:LEU:HD11	2:O:612:MET:HB3	1.98	0.46
2:O:613:ILE:O	2:O:671:PRO:HD3	2.16	0.46
2:O:525:VAL:HG21	2:O:650:THR:HB	1.97	0.46
1:A:353:VAL:O	1:A:354:GLN:HB2	2.16	0.45
1:A:570:ASP:HB3	1:A:572:PRO:HD2	1.98	0.45
1:B:317:CYS:HB3	1:B:549:SER:HB2	1.98	0.45
1:B:342:CYS:HA	1:B:367:TYR:CZ	2.51	0.45
1:C:656:LEU:O	1:C:660:LYS:HG3	2.16	0.45
1:D:266:ALA:HB2	1:D:427:VAL:HG21	1.98	0.45
1:D:472:ASN:ND2	1:D:606:THR:HG21	2.31	0.45
1:D:51:ARG:HD3	10:D:810:HOH:O	2.15	0.45
2:M:626:MET:HB3	2:M:630:THR:HB	1.98	0.45
1:A:150:VAL:HG12	1:A:150:VAL:O	2.15	0.45
1:A:324:MET:HE3	1:A:430:GLY:HA2	1.98	0.45
1:C:316:CYS:O	1:C:503:GLN:NE2	2.49	0.45
1:D:384:TYR:HD1	2:O:84:ASN:HB3	1.81	0.45
2:M:540:TYR:CE1	2:M:550:PRO:HD3	2.51	0.45
1:C:359:SER:O	1:C:363:VAL:HG23	2.15	0.45
2:M:712:LEU:O	2:M:716:GLU:HG3	2.15	0.45
2:N:269:ALA:HB1	2:N:274:PHE:HB2	1.98	0.45
2:O:333:ILE:HD12	2:O:418:TRP:HB3	1.98	0.45
2:P:335:LYS:HD2	2:P:335:LYS:N	2.31	0.45
2:P:392:GLY:HA3	2:P:459:ILE:O	2.15	0.45
2:P:479:GLU:HA	2:P:482:ARG:HD2	1.98	0.45
2:P:664:ILE:HD13	2:P:685:ARG:HG3	1.97	0.45
1:A:250:ASP:O	1:A:254:ILE:HG13	2.17	0.45
1:B:537:ILE:HD12	1:B:537:ILE:N	2.31	0.45
2:M:602:MET:CE	2:M:647:ILE:HG21	2.46	0.45
2:N:59:ALA:HB2	2:N:630:THR:HA	1.99	0.45
2:O:669:TRP:HA	2:O:700:ALA:O	2.16	0.45
2:O:708:VAL:O	2:O:712:LEU:HB2	2.17	0.45
2:P:439:PHE:C	2:P:440:ARG:HD2	2.37	0.45
1:B:28:THR:HG21	1:B:33:VAL:HG12	1.99	0.45
2:M:356:VAL:CG2	2:M:361:ILE:HB	2.45	0.45
2:O:107:TRP:CZ3	2:O:219:ALA:HB1	2.52	0.45
1:A:266:ALA:HB2	1:A:427:VAL:HG21	1.98	0.45
1:A:607:MET:HE3	1:A:608:PRO:HD2	1.98	0.45
1:A:70:PHE:CE1	1:A:100:ARG:HB3	2.52	0.45
1:C:175:ARG:HB3	1:D:175:ARG:HB3	1.97	0.45
1:D:577:VAL:HG21	1:D:645:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:602:MET:CE	2:N:645:MET:HE3	2.46	0.45
2:P:524:ARG:NH2	2:P:645:MET:SD	2.87	0.45
1:B:280:LEU:HD13	1:B:288:SER:HB2	1.99	0.45
1:B:569:VAL:HB	1:B:573:LYS:HD3	1.99	0.45
1:C:307:ALA:HB2	1:C:408:PHE:CE2	2.52	0.45
2:N:602:MET:HE3	2:N:645:MET:CE	2.47	0.45
2:P:373:ILE:CD1	2:P:435:VAL:HG22	2.46	0.45
1:A:318:THR:O	1:A:322:VAL:HG22	2.15	0.45
1:B:114[A]:CYS:SG	1:B:208:ILE:CG2	3.05	0.45
2:N:185:ILE:HD12	2:N:185:ILE:N	2.32	0.45
2:O:339:TYR:CE2	2:O:376:ILE:HD11	2.52	0.45
2:P:399:PHE:HZ	2:P:541:GLU:HG3	1.82	0.45
2:P:496:THR:OG1	2:P:499:THR:HG23	2.17	0.45
1:B:291:ILE:HD13	1:B:397:ALA:CB	2.47	0.45
1:C:107:LEU:HD21	1:C:215:LEU:HB3	1.98	0.45
1:D:274:ASP:OD2	1:D:308:LYS:HE2	2.17	0.45
2:N:601:ILE:HG23	2:N:635:ILE:HD13	1.98	0.45
2:N:69:SER:OG	2:N:71:GLU:OE1	2.23	0.45
2:O:173:VAL:HG13	2:O:183:LEU:CD1	2.47	0.45
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.52	0.45
1:C:283:HIS:CE1	4:C:703:XCC:S3	3.10	0.44
1:D:324:MET:HE3	1:D:430:GLY:HA2	1.98	0.44
2:M:342:MET:CE	2:M:384:LEU:HD22	2.47	0.44
2:M:159:ILE:HG12	2:M:253:LEU:HD12	1.98	0.44
2:N:354:ARG:HH21	2:N:480:VAL:HG11	1.81	0.44
2:N:80:PRO:N	2:N:81:PRO:HD2	2.32	0.44
2:M:35:TYR:CZ	2:M:39:LEU:HD11	2.52	0.44
2:M:406:ARG:HB3	2:M:410:PHE:CZ	2.52	0.44
2:N:445:GLY:HA2	2:N:465:VAL:HG11	1.99	0.44
2:O:213:THR:O	2:O:216:VAL:HG12	2.18	0.44
2:O:373:ILE:HD11	2:O:435:VAL:HG22	1.98	0.44
1:A:619:ILE:HA	1:A:623:ILE:HB	1.99	0.44
2:N:496:THR:HB	2:N:523:GLU:OE2	2.16	0.44
2:O:80:PRO:N	2:O:81:PRO:HD2	2.33	0.44
2:P:341:GLU:OE2	2:P:427:TRP:NE1	2.39	0.44
2:P:712:LEU:HB3	2:P:713:PRO:HD3	2.00	0.44
1:A:577:VAL:HG13	1:A:649:LEU:HD21	1.99	0.44
1:B:559:LEU:O	1:B:563:MET:HG3	2.17	0.44
1:B:445:ALA:HB3	1:C:38:VAL:HG13	1.99	0.44
1:D:114[A]:CYS:SG	1:D:208:ILE:CG2	3.05	0.44
2:M:439:PHE:C	2:M:440:ARG:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:79:LEU:N	2:M:80:PRO:CD	2.81	0.44
2:O:79:LEU:N	2:O:80:PRO:CD	2.80	0.44
2:P:277:ILE:N	2:P:277:ILE:HD12	2.33	0.44
2:P:365:LYS:HB3	2:P:464:GLN:HG3	1.98	0.44
1:B:397:ALA:O	1:B:401:ILE:HG13	2.18	0.44
1:B:52:PHE:CZ	1:B:474:LYS:HA	2.52	0.44
1:C:351:VAL:HB	1:C:356:ILE:CD1	2.47	0.44
1:C:483:THR:HG23	1:C:639:GLN:OE1	2.17	0.44
1:C:428:VAL:HG13	1:C:539:ILE:HD11	2.00	0.44
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.99	0.44
2:M:80:PRO:N	2:M:81:PRO:HD2	2.33	0.44
2:O:62:LEU:HD12	2:O:65:ILE:HD12	1.99	0.44
2:P:61:TYR:O	2:P:63:PRO:HD3	2.18	0.44
1:B:150:VAL:HG12	1:B:150:VAL:O	2.18	0.44
1:B:256:PHE:CG	1:B:289:GLU:HG3	2.52	0.44
1:B:486:LYS:HE2	1:B:519:TYR:CE2	2.52	0.44
1:D:118:ASN:HD22	1:D:118:ASN:C	2.21	0.44
1:D:619:ILE:HA	1:D:623:ILE:HB	2.00	0.44
1:D:626:ASP:HB3	2:P:212:PHE:CG	2.53	0.44
2:N:157:ALA:HB3	2:N:183:LEU:CD2	2.47	0.44
2:O:205:ILE:O	2:O:205:ILE:HG22	2.18	0.44
2:O:553:LYS:HG2	2:O:553:LYS:O	2.18	0.44
2:P:349:ALA:HA	2:P:384:LEU:O	2.18	0.44
2:P:556:GLU:OE2	2:P:559:PRO:HB3	2.18	0.44
2:P:63:PRO:HB2	2:P:220:ASN:HB2	1.99	0.44
2:M:481:ALA:HB1	2:M:485:TYR:CZ	2.53	0.44
2:M:667:ILE:HG21	2:M:670:MET:SD	2.58	0.44
1:B:294:ALA:O	1:B:298:MET:HG2	2.17	0.44
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.53	0.44
1:D:351:VAL:HB	1:D:356:ILE:HD13	1.99	0.44
2:N:340:VAL:CG2	2:N:376:ILE:HD11	2.48	0.44
2:N:488:ARG:O	2:N:492:MET:HG2	2.18	0.44
2:O:497:ASP:OD1	2:O:522:PRO:HD2	2.18	0.44
2:P:470:ASP:HB3	2:P:473:LYS:CG	2.48	0.44
1:C:467:ILE:HG22	1:C:501:SER:OG	2.17	0.43
1:B:467:ILE:HG22	1:B:501:SER:OG	2.17	0.43
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.54	0.43
2:O:602:MET:CE	2:O:645:MET:HE3	2.48	0.43
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.53	0.43
1:C:118:ASN:HD22	1:C:118:ASN:C	2.20	0.43
1:D:354:GLN:HB3	1:D:587:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:185:ILE:N	2:M:185:ILE:HD12	2.34	0.43
2:M:26:TYR:CZ	2:M:30:ILE:HD11	2.53	0.43
2:M:339:TYR:CG	2:M:435:VAL:HG21	2.53	0.43
2:N:156:GLU:O	2:N:250:ALA:HA	2.18	0.43
2:N:340:VAL:HG21	2:N:376:ILE:HD11	2.00	0.43
2:O:237:ARG:O	2:O:241:ARG:HG3	2.19	0.43
2:P:144:PHE:CE1	2:P:205:ILE:HG12	2.53	0.43
2:N:712:LEU:HB3	2:N:713:PRO:HD3	2.01	0.43
2:M:347:THR:CG2	2:M:381:LYS:HD2	2.48	0.43
2:M:61:TYR:O	2:M:63:PRO:HD3	2.18	0.43
1:A:335:ALA:HB2	1:A:471:ASN:HB3	2.00	0.43
1:D:364:ALA:HB1	1:D:369:THR:HB	2.00	0.43
2:M:335:LYS:N	2:M:335:LYS:HD2	2.33	0.43
2:P:483:GLU:O	2:P:487:GLU:HG3	2.19	0.43
2:O:388:VAL:HG21	2:O:448:LEU:HD13	2.00	0.43
2:P:79:LEU:N	2:P:80:PRO:CD	2.81	0.43
1:A:162:LEU:O	1:A:166:VAL:HG12	2.19	0.43
1:C:3:ARG:O	2:O:162:ARG:NH1	2.49	0.43
2:M:286:LYS:HB3	2:M:286:LYS:HE2	1.87	0.43
2:M:583:CYS:HB3	2:M:586:THR:HG22	2.00	0.43
2:N:335:LYS:HD2	2:N:335:LYS:H	1.83	0.43
2:P:247:ARG:NH2	2:P:514:PRO:HG3	2.34	0.43
2:P:277:ILE:HG13	2:P:293:PHE:CZ	2.54	0.43
2:P:538:ALA:O	2:P:542:ILE:HG13	2.19	0.43
1:A:149:ARG:HH22	1:A:250:ASP:CG	2.21	0.43
1:A:483:THR:HB	1:A:638:PRO:HB2	2.00	0.43
1:A:503:GLN:O	1:A:507:LYS:HG3	2.19	0.43
1:A:73:ALA:HB2	1:B:584:MET:HG3	2.01	0.43
1:C:416:ARG:HG3	1:C:417:PRO:HD2	2.01	0.43
2:N:172:ILE:HG23	2:N:302:VAL:CG2	2.49	0.43
2:N:538:ALA:O	2:N:542:ILE:HG13	2.19	0.43
2:N:613:ILE:O	2:N:671:PRO:HD3	2.19	0.43
2:O:420:THR:CG2	2:O:427:TRP:HB3	2.49	0.43
2:O:456:PHE:HB3	2:O:459:ILE:HG23	2.00	0.43
1:C:409:LYS:O	1:C:413:GLU:HG3	2.19	0.43
1:D:150:VAL:O	1:D:150:VAL:HG12	2.18	0.43
2:M:318:LEU:N	2:M:318:LEU:HD12	2.33	0.43
2:N:275:PRO:HD2	2:N:309:ARG:HD3	2.00	0.43
2:O:63:PRO:HB2	2:O:220:ASN:HB2	2.01	0.43
2:O:408:HIS:O	2:O:412:ASN:ND2	2.51	0.43
2:O:80:PRO:HB2	2:O:81:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:37:GLU:OE1	2:P:41:ASN:ND2	2.42	0.43
1:B:368[A]:HIS:CD2	1:B:416:ARG:HD3	2.54	0.42
2:M:181:PHE:CE2	2:M:311:ILE:HD13	2.54	0.42
2:M:488:ARG:O	2:M:492:MET:HG2	2.18	0.42
2:N:79:LEU:N	2:N:80:PRO:CD	2.82	0.42
2:O:209:LEU:HD22	2:O:217:HIS:HB2	2.01	0.42
2:O:64:VAL:HG23	2:O:220:ASN:HB3	2.01	0.42
2:O:230:GLY:HA2	2:O:512:PHE:O	2.18	0.42
2:O:425:ILE:HG22	2:O:425:ILE:O	2.18	0.42
1:B:348:ALA:CB	1:B:404:ALA:HB2	2.48	0.42
1:B:370:ARG:HH22	1:B:410:GLU:CD	2.22	0.42
1:D:330:LEU:C	1:D:330:LEU:HD23	2.39	0.42
1:D:462:ALA:HB3	1:D:493:VAL:HG22	2.01	0.42
1:D:570:ASP:HB3	1:D:572:PRO:HD2	2.00	0.42
2:M:420:THR:HG22	2:M:427:TRP:HB3	2.01	0.42
2:N:41:ASN:O	2:N:45:ARG:HG3	2.19	0.42
1:C:114[B]:CYS:SG	1:C:208:ILE:CG2	3.08	0.42
1:C:492:ASN:HA	1:C:524:LEU:HB2	2.01	0.42
2:M:342:MET:HE2	2:M:384:LEU:HD22	2.01	0.42
2:N:382:LEU:HD12	2:N:383:PRO:HD2	2.00	0.42
2:N:588:MET:O	2:N:642:PRO:HB3	2.19	0.42
2:O:382:LEU:HD21	2:O:469:THR:HB	2.01	0.42
2:O:651:TYR:CZ	2:O:657:PHE:HA	2.54	0.42
2:P:528:CYS:HB3	3:P:801:SF4:S3	2.58	0.42
2:P:669:TRP:HA	2:P:700:ALA:O	2.19	0.42
1:A:553:ASN:ND2	1:A:591:ILE:HD13	2.34	0.42
1:B:353:VAL:O	1:B:354:GLN:HB2	2.19	0.42
2:N:439:PHE:C	2:N:440:ARG:HD2	2.39	0.42
1:A:374:THR:HA	1:A:386:ILE:O	2.20	0.42
1:B:287:LEU:O	1:B:291:ILE:HG12	2.20	0.42
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.49	0.42
1:D:298:MET:HE2	1:D:298:MET:HB3	1.57	0.42
2:M:259:ASP:OD1	2:M:262:LYS:HD2	2.19	0.42
2:M:269:ALA:HA	2:M:272:THR:HG22	2.02	0.42
2:O:406:ARG:HG3	2:O:456:PHE:CZ	2.54	0.42
1:B:324:MET:HE3	1:B:430:GLY:HA2	2.01	0.42
1:C:317:CYS:O	1:C:321:GLU:HG2	2.19	0.42
2:N:714:TYR:CZ	2:N:718:LYS:HE3	2.55	0.42
1:C:150:VAL:HG13	1:C:184:THR:CG2	2.50	0.42
2:M:240:GLN:O	2:M:244:GLN:HG2	2.20	0.42
2:M:445:GLY:HA2	2:M:465:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:655:LYS:HG2	2:N:685:ARG:NH1	2.35	0.42
2:O:428:LEU:HD12	2:O:428:LEU:N	2.34	0.42
1:B:359:SER:O	1:B:363:VAL:HG23	2.20	0.42
1:A:584:MET:HG3	1:B:73:ALA:HB2	2.01	0.42
1:B:98:VAL:O	1:B:102:VAL:HG12	2.20	0.42
1:C:364:ALA:HB1	1:C:369:THR:HB	2.01	0.42
1:C:428:VAL:HG13	1:C:539:ILE:CD1	2.50	0.42
1:D:482:LEU:HD13	1:D:510:LEU:HD11	2.01	0.42
1:A:662:VAL:HG21	2:M:194:LEU:HD13	2.00	0.42
2:N:524:ARG:NH2	2:N:645:MET:SD	2.85	0.42
2:O:259:ASP:OD1	2:O:262:LYS:HD2	2.20	0.42
2:O:622:THR:OG1	2:O:626:MET:O	2.25	0.42
2:P:219:ALA:O	2:P:223:LEU:HG	2.20	0.42
2:P:236:ALA:O	2:P:240:GLN:HG2	2.20	0.42
2:P:602:MET:HE3	2:P:645:MET:CE	2.49	0.42
1:A:591:ILE:HG23	1:A:594:TRP:CZ2	2.55	0.42
1:B:256:PHE:CD2	1:B:289:GLU:HG3	2.55	0.42
1:C:321:GLU:OE1	1:C:325:ARG:NH1	2.40	0.42
1:D:330:LEU:HD11	1:D:503:GLN:CD	2.40	0.42
2:M:226:GLY:HA2	2:M:243:TYR:CE1	2.54	0.42
2:N:602:MET:O	2:N:644:PHE:HA	2.20	0.42
1:A:112:ALA:HA	1:B:217:ASN:OD1	2.20	0.42
1:C:655:LYS:HG3	2:O:191:GLU:HG2	2.02	0.42
2:M:141:VAL:HG22	2:M:221:TYR:CZ	2.54	0.42
2:N:406:ARG:HB3	2:N:410:PHE:CE2	2.55	0.42
2:N:383:PRO:O	2:N:469:THR:HA	2.20	0.42
2:N:470:ASP:O	2:N:474:VAL:HG23	2.19	0.42
2:O:129:PRO:O	2:O:132:TRP:HB2	2.20	0.42
2:O:668:VAL:HG12	2:O:720:HIS:CE1	2.55	0.42
2:P:470:ASP:HB3	2:P:473:LYS:HG2	2.01	0.42
1:A:326:GLN:HB2	1:A:328:ILE:HG12	2.01	0.41
1:C:299:GLU:HG2	1:C:303:LYS:HE2	2.02	0.41
1:C:591:ILE:HG23	1:C:594:TRP:CZ2	2.55	0.41
2:M:360:GLU:O	2:M:360:GLU:HG2	2.20	0.41
2:M:622:THR:HB	2:M:623:PRO:HD2	2.02	0.41
2:O:376:ILE:HD12	2:O:376:ILE:C	2.40	0.41
1:B:574:VAL:O	1:B:576:PHE:N	2.53	0.41
2:M:18:PRO:HG3	2:M:288:ILE:HG12	2.02	0.41
2:O:622:THR:HB	2:O:623:PRO:HD2	2.01	0.41
2:O:585:TYR:CE1	2:O:656:LYS:HD2	2.55	0.41
1:A:374:THR:HB	1:A:388:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:VAL:O	1:C:354:GLN:HB2	2.20	0.41
2:M:223:LEU:HA	2:M:244:GLN:NE2	2.35	0.41
1:A:256:PHE:CD2	1:A:289:GLU:HG3	2.56	0.41
1:D:316:CYS:HB3	1:D:317:CYS:H	1.64	0.41
2:M:129:PRO:O	2:M:132:TRP:HB2	2.20	0.41
2:N:185:ILE:HG22	2:N:190:VAL:CG2	2.51	0.41
2:N:403:LEU:HD21	2:N:460:VAL:CG2	2.49	0.41
2:P:503:PHE:O	2:P:551:ILE:N	2.46	0.41
2:P:670:MET:HE3	2:P:674:LEU:HG	2.02	0.41
1:A:266:ALA:O	1:A:267:ASN:CB	2.68	0.41
1:C:559:LEU:O	1:C:563:MET:HG3	2.20	0.41
1:C:641:ALA:O	1:C:645:ILE:HG13	2.21	0.41
1:D:484:VAL:O	1:D:488:LEU:HG	2.21	0.41
2:M:277:ILE:HD12	2:M:277:ILE:N	2.34	0.41
2:M:373:ILE:HG22	2:M:440:ARG:HG3	2.03	0.41
2:O:109:ALA:O	2:O:113:ILE:HG13	2.21	0.41
2:P:373:ILE:HG22	2:P:440:ARG:HG3	2.03	0.41
2:P:527:LEU:HD12	2:P:528:CYS:N	2.35	0.41
2:P:583:CYS:HB3	2:P:586:THR:HG22	2.02	0.41
2:P:598:PHE:CE1	2:P:601:ILE:HD11	2.56	0.41
1:A:158:SER:OG	1:A:161:GLU:HG3	2.20	0.41
1:A:227:PRO:O	1:A:231:VAL:HG23	2.21	0.41
2:N:132:TRP:HA	2:N:208:PRO:HB2	2.03	0.41
2:N:142:ARG:CZ	2:N:632:ALA:HB1	2.51	0.41
2:O:403:LEU:HD21	2:O:460:VAL:CG2	2.50	0.41
2:P:142:ARG:CZ	2:P:632:ALA:HB1	2.50	0.41
2:P:602:MET:O	2:P:644:PHE:HA	2.19	0.41
1:B:572:PRO:HG2	1:B:674:TYR:CZ	2.55	0.41
2:M:374:ASP:HB3	2:M:440:ARG:HH21	1.85	0.41
2:N:586:THR:HG23	2:N:661:ASP:OD1	2.20	0.41
2:O:169:LEU:HG	2:O:193:LEU:HD21	2.01	0.41
2:O:282:LEU:CB	2:O:287:GLN:HG3	2.50	0.41
2:O:457:PRO:O	2:O:458:ALA:HB3	2.21	0.41
2:O:63:PRO:HB3	2:O:224:ARG:HG3	2.03	0.41
2:O:80:PRO:HB2	2:O:81:PRO:CD	2.50	0.41
1:A:168:GLU:O	1:A:172:GLU:HG3	2.21	0.41
1:D:607:MET:HE3	1:D:608:PRO:HD2	2.03	0.41
2:O:104:GLU:OE1	2:O:237:ARG:HD2	2.20	0.41
2:O:442:LYS:O	2:O:446:GLU:HG3	2.21	0.41
1:A:537:ILE:N	1:A:537:ILE:HD12	2.36	0.41
1:B:316:CYS:O	1:B:503:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:583:CYS:HB2	2:M:586:THR:CG2	2.50	0.41
2:N:456:PHE:HA	2:N:542:ILE:CD1	2.51	0.41
2:O:678:LEU:O	2:O:682:PHE:HB2	2.21	0.41
2:P:237:ARG:O	2:P:241:ARG:HG3	2.21	0.41
2:P:408:HIS:O	2:P:412:ASN:ND2	2.54	0.41
2:P:457:PRO:O	2:P:458:ALA:HB3	2.21	0.41
2:P:65:ILE:HG12	2:P:108:TYR:CD1	2.56	0.41
1:A:24:ASN:O	1:A:27:ARG:HG2	2.20	0.41
1:B:138:LYS:HD2	1:B:256:PHE:HA	2.02	0.41
1:B:426:ARG:HH22	1:B:539:ILE:CG1	2.33	0.41
1:B:456:ILE:HD13	1:B:463:GLY:HA2	2.03	0.41
1:D:238:ALA:O	1:D:241:ASP:HB3	2.21	0.41
1:D:574:VAL:O	1:D:576:PHE:N	2.53	0.41
1:D:65:GLY:CA	1:D:609:PRO:HB2	2.51	0.41
2:N:157:ALA:HB3	2:N:183:LEU:HD23	2.02	0.41
2:N:160:LEU:HD13	2:N:215:ILE:HD13	2.02	0.41
2:N:169:LEU:HG	2:N:193:LEU:HD21	2.03	0.41
2:P:399:PHE:CZ	2:P:541:GLU:HG3	2.56	0.41
2:P:572:TYR:HA	2:P:579:LEU:O	2.21	0.41
1:A:26:ASP:HA	1:A:37:LEU:HD13	2.02	0.41
1:A:320:ASN:O	1:A:324:MET:HG2	2.21	0.41
1:A:342:CYS:HA	1:A:367:TYR:CZ	2.55	0.41
1:A:574:VAL:O	1:A:576:PHE:N	2.51	0.41
1:A:70:PHE:CZ	1:A:100:ARG:HB3	2.56	0.41
1:B:280:LEU:HD21	1:B:291:ILE:HG21	2.03	0.41
1:B:570:ASP:HB3	1:B:572:PRO:HD2	2.03	0.41
1:D:660:LYS:O	1:D:664:GLU:HG3	2.21	0.41
2:M:80:PRO:HB2	2:M:81:PRO:HD3	2.03	0.41
2:O:497:ASP:OD2	2:O:585:TYR:OH	2.26	0.41
2:O:551:ILE:HG21	2:O:567:VAL:HG22	2.03	0.41
2:P:318:LEU:N	2:P:318:LEU:HD12	2.36	0.41
1:A:66:ILE:CG2	1:A:612:GLY:HA3	2.47	0.40
1:B:351:VAL:HB	1:B:356:ILE:CD1	2.51	0.40
1:C:218:GLN:HG2	1:D:377:ASN:HB2	2.03	0.40
1:D:278:PHE:HB3	1:D:312:LEU:HD23	2.03	0.40
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.56	0.40
1:D:3:ARG:O	2:P:162:ARG:NH1	2.54	0.40
2:M:456:PHE:HD2	2:M:542:ILE:HD11	1.86	0.40
2:O:342:MET:HE2	2:O:384:LEU:HD22	2.04	0.40
2:P:209:LEU:HD11	2:P:218:ALA:HB2	2.03	0.40
2:P:278:THR:HG21	2:P:282:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:393:ARG:H	2:P:393:ARG:HG2	1.65	0.40
1:A:186:LEU:CD2	1:A:205:PRO:HD2	2.50	0.40
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.22	0.40
1:A:256:PHE:CG	1:A:289:GLU:HG3	2.56	0.40
1:B:330:LEU:HD13	1:B:503:GLN:HG2	2.02	0.40
1:B:261:PRO:HA	1:B:429:ALA:O	2.20	0.40
1:C:615:LEU:HD23	1:C:615:LEU:C	2.42	0.40
2:N:528:CYS:HB3	3:N:801:SF4:S3	2.61	0.40
1:A:241:ASP:O	1:A:245:GLU:HG3	2.20	0.40
1:B:28:THR:HG21	1:B:33:VAL:CG1	2.51	0.40
1:B:317:CYS:O	1:B:321:GLU:HG2	2.22	0.40
1:D:279:VAL:HA	1:D:313:VAL:HG23	2.03	0.40
1:D:482:LEU:HD12	1:D:486:LYS:HE3	2.03	0.40
1:D:428:VAL:HG13	1:D:539:ILE:HD11	2.02	0.40
1:A:619:ILE:HG13	2:M:260:MET:HE1	2.04	0.40
2:M:538:ALA:O	2:M:542:ILE:HG13	2.21	0.40
2:P:80:PRO:HB2	2:P:81:PRO:HD3	2.02	0.40
1:A:594:TRP:O	1:A:598:LEU:HG	2.20	0.40
1:A:655:LYS:HG3	2:M:191:GLU:HG2	2.03	0.40
1:B:472:ASN:ND2	1:B:606:THR:HG21	2.37	0.40
1:C:61:ILE:HD13	1:C:77:ARG:CZ	2.49	0.40
1:D:61:ILE:HD13	1:D:77:ARG:NE	2.26	0.40
2:N:149:VAL:CG1	2:N:509:CYS:HA	2.47	0.40
2:O:602:MET:HE3	2:O:645:MET:CE	2.51	0.40
2:O:603:ALA:HB3	2:O:612:MET:CG	2.52	0.40
1:A:607:MET:HE3	1:A:634:PHE:CG	2.57	0.40
1:B:264:SER:OG	1:B:265:GLU:N	2.54	0.40
1:D:173:ASP:O	1:D:208:ILE:HG13	2.21	0.40
1:D:316:CYS:O	1:D:503:GLN:NE2	2.55	0.40
1:D:39:LYS:NZ	1:D:43:ASP:OD2	2.49	0.40
1:D:65:GLY:HA3	1:D:609:PRO:HB2	2.04	0.40
1:D:658:VAL:O	1:D:662:VAL:HG23	2.22	0.40
2:O:209:LEU:HD11	2:O:218:ALA:HB2	2.02	0.40
2:P:376:ILE:HD12	2:P:376:ILE:C	2.42	0.40
2:P:406:ARG:HB3	2:P:410:PHE:CZ	2.56	0.40
2:P:470:ASP:OD2	2:P:472:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	673/674 (100%)	647 (96%)	25 (4%)	1 (0%)	51	71
1	B	673/674 (100%)	648 (96%)	24 (4%)	1 (0%)	51	71
1	C	673/674 (100%)	650 (97%)	22 (3%)	1 (0%)	51	71
1	D	672/674 (100%)	648 (96%)	23 (3%)	1 (0%)	51	71
2	M	726/729 (100%)	702 (97%)	23 (3%)	1 (0%)	51	71
2	N	726/729 (100%)	699 (96%)	25 (3%)	2 (0%)	41	59
2	O	724/729 (99%)	696 (96%)	24 (3%)	4 (1%)	25	40
2	P	726/729 (100%)	700 (96%)	24 (3%)	2 (0%)	41	59
All	All	5593/5612 (100%)	5390 (96%)	190 (3%)	13 (0%)	47	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	187	ASP
2	O	187	ASP
1	A	267	ASN
2	M	596	GLY
2	N	596	GLY
2	O	596	GLY
2	P	187	ASP
2	P	596	GLY
2	O	427	TRP
1	B	354	GLN
1	C	354	GLN
1	D	354	GLN
2	O	205	ILE

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	544/543 (100%)	540 (99%)	4 (1%)	84	93
1	B	544/543 (100%)	541 (99%)	3 (1%)	86	94
1	C	544/543 (100%)	540 (99%)	4 (1%)	84	93
1	D	543/543 (100%)	538 (99%)	5 (1%)	78	91
2	M	610/611 (100%)	607 (100%)	3 (0%)	88	95
2	N	610/611 (100%)	606 (99%)	4 (1%)	84	93
2	O	608/611 (100%)	605 (100%)	3 (0%)	88	95
2	P	610/611 (100%)	607 (100%)	3 (0%)	88	95
All	All	4613/4616 (100%)	4584 (99%)	29 (1%)	86	94

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	118	ASN
1	A	206	PHE
1	A	546	HIS
1	B	9	HIS
1	B	118	ASN
1	B	546	HIS
1	C	9	HIS
1	C	118	ASN
1	C	318	THR
1	C	546	HIS
1	D	9	HIS
1	D	118	ASN
1	D	298	MET
1	D	318	THR
1	D	546	HIS
2	M	149	VAL
2	M	254	TYR
2	M	598	PHE

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Mol	Chain	Res	Type
2	N	96	PHE
2	N	149	VAL
2	N	254	TYR
2	N	598	PHE
2	O	96	PHE
2	O	254	TYR
2	O	317	LYS
2	P	96	PHE
2	P	149	VAL
2	P	254	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	503	GLN
1	C	503	GLN
2	P	426	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	$\# Z > 2$
4	XCC	C	703	1,10	0,11,11	0.00	-	-		
8	CMO	M	804	-	0,1,1	0.00	-	-		
8	CMO	N	804	7	0,1,1	0.00	-	-		
5	PGE	A	704	-	9,9,9	0.35	0	8,8,8	0.20	0
3	SF4	D	701	1	0,12,12	0.00	-	-		
3	SF4	O	900	2	0,12,12	0.00	-	-		
3	SF4	P	801	2	0,12,12	0.00	-	-		
3	SF4	B	701	1	0,12,12	0.00	-	-		
3	SF4	N	801	2	0,12,12	0.00	-	-		
3	SF4	C	701	1	0,12,12	0.00	-	-		
3	SF4	M	801	2	0,12,12	0.00	-	-		
3	SF4	A	702	1	0,12,12	0.00	-	-		
8	CMO	P	804	7	0,1,1	0.00	-	-		
6	PG5	C	704	-	11,11,11	0.20	0	10,10,10	0.28	0
4	XCC	D	702	1	0,11,11	0.00	-	-		
3	SF4	A	701	1	0,12,12	0.00	-	-		
3	SF4	C	702	1	0,12,12	0.00	-	-		
4	XCC	A	703	1,10	0,11,11	0.00	-	-		
4	XCC	B	702	1,10	0,11,11	0.00	-	-		

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
4	XCC	C	703	1,10	-	-	0/3/3/3
3	SF4	C	701	1	-	-	0/6/5/5
3	SF4	D	701	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
3	SF4	P	801	2	-	-	0/6/5/5
3	SF4	B	701	1	-	-	0/6/5/5
3	SF4	N	801	2	-	-	0/6/5/5
5	PGE	A	704	-	-	3/7/7/7	-
3	SF4	A	701	1	-	-	0/6/5/5
3	SF4	M	801	2	-	-	0/6/5/5
3	SF4	A	702	1	-	-	0/6/5/5
4	XCC	B	702	1,10	-	-	0/3/3/3
4	XCC	D	702	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG5	C	704	-	-	4/9/9/9	-
3	SF4	C	702	1	-	-	0/6/5/5
4	XCC	A	703	1,10	-	-	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	704	PGE	O3-C5-C6-O4
5	A	704	PGE	O1-C1-C2-O2
6	C	704	PG5	C3-C2-O1-C1
6	C	704	PG5	O1-C2-C3-O2
6	C	704	PG5	O2-C4-C5-O3
6	C	704	PG5	O3-C6-C7-O4
5	A	704	PGE	O2-C3-C4-O3

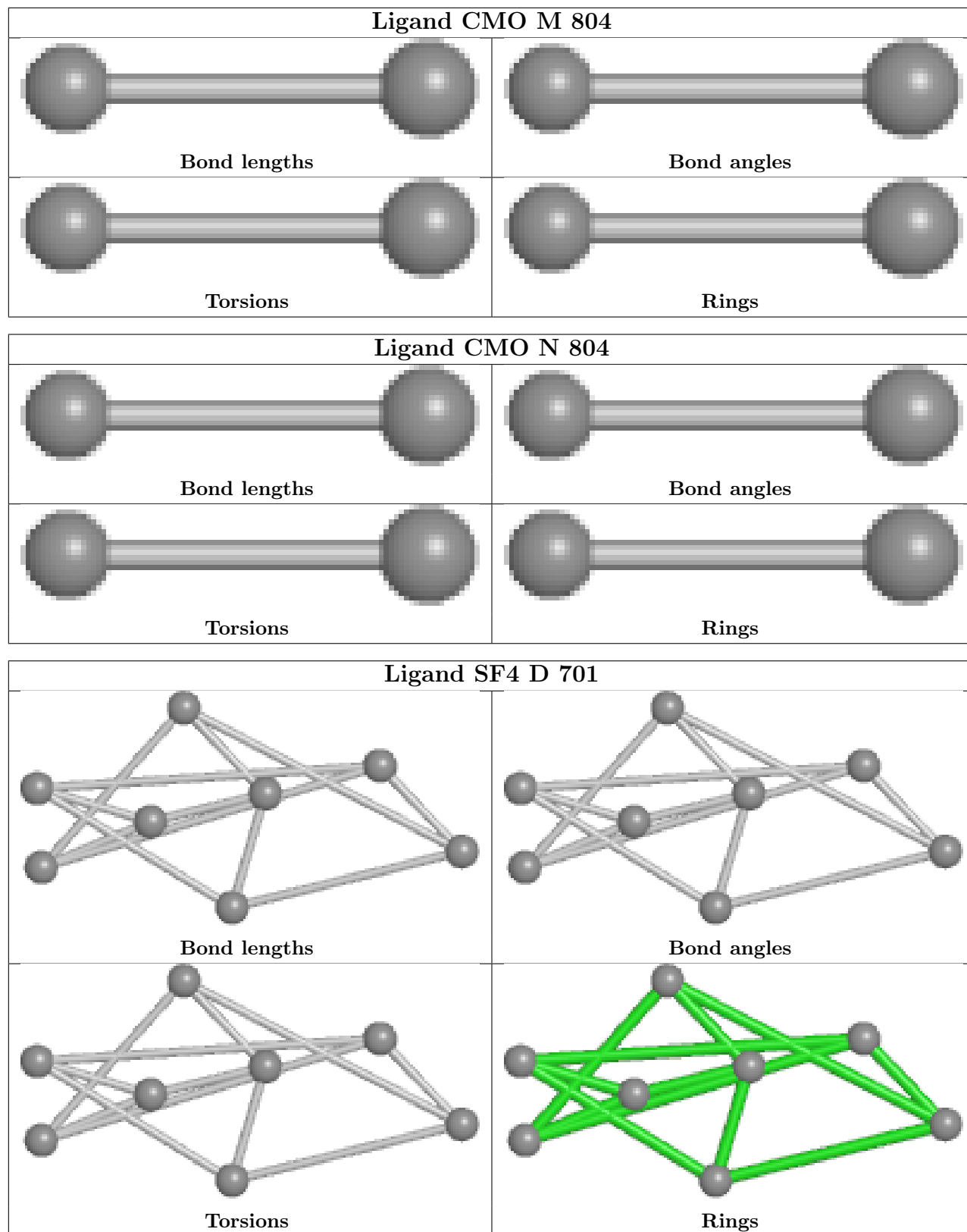
There are no ring outliers.

7 monomers are involved in 12 short contacts:

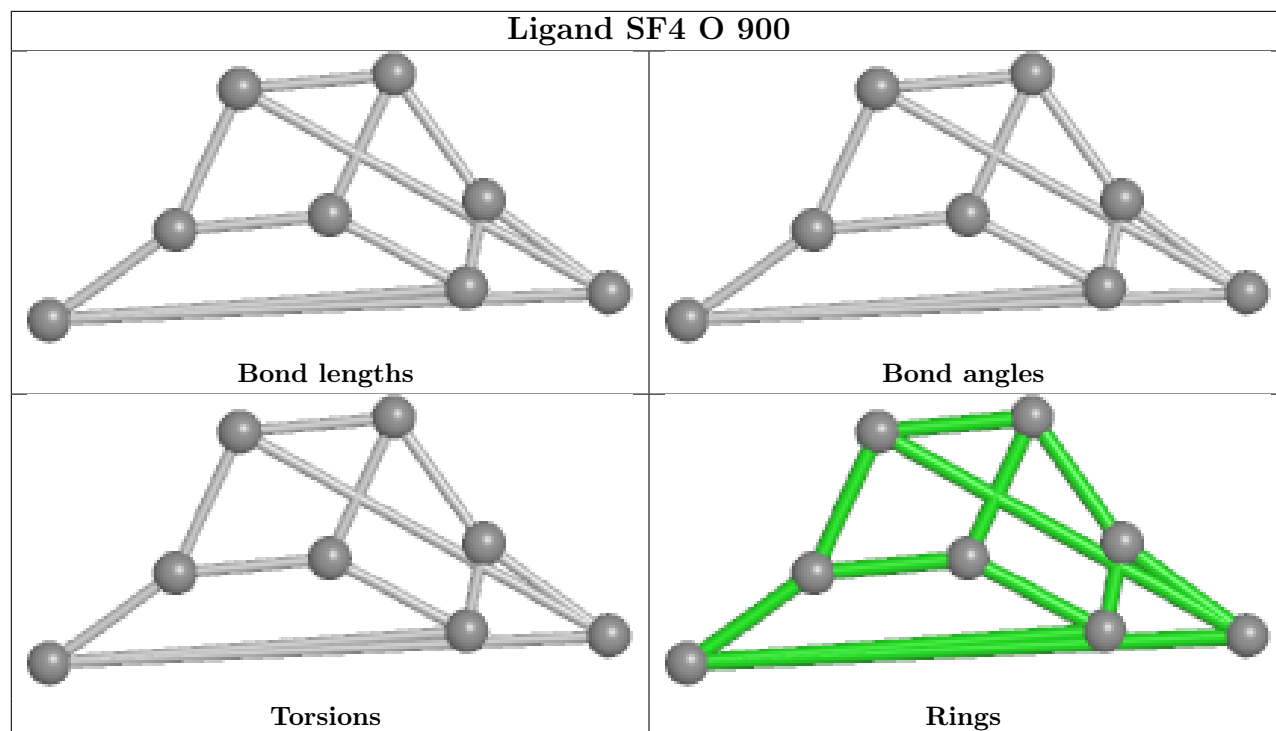
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	703	XCC	2	0
3	P	801	SF4	1	0
3	N	801	SF4	1	0
6	C	704	PG5	1	0
4	D	702	XCC	3	0
4	A	703	XCC	2	0
4	B	702	XCC	2	0

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

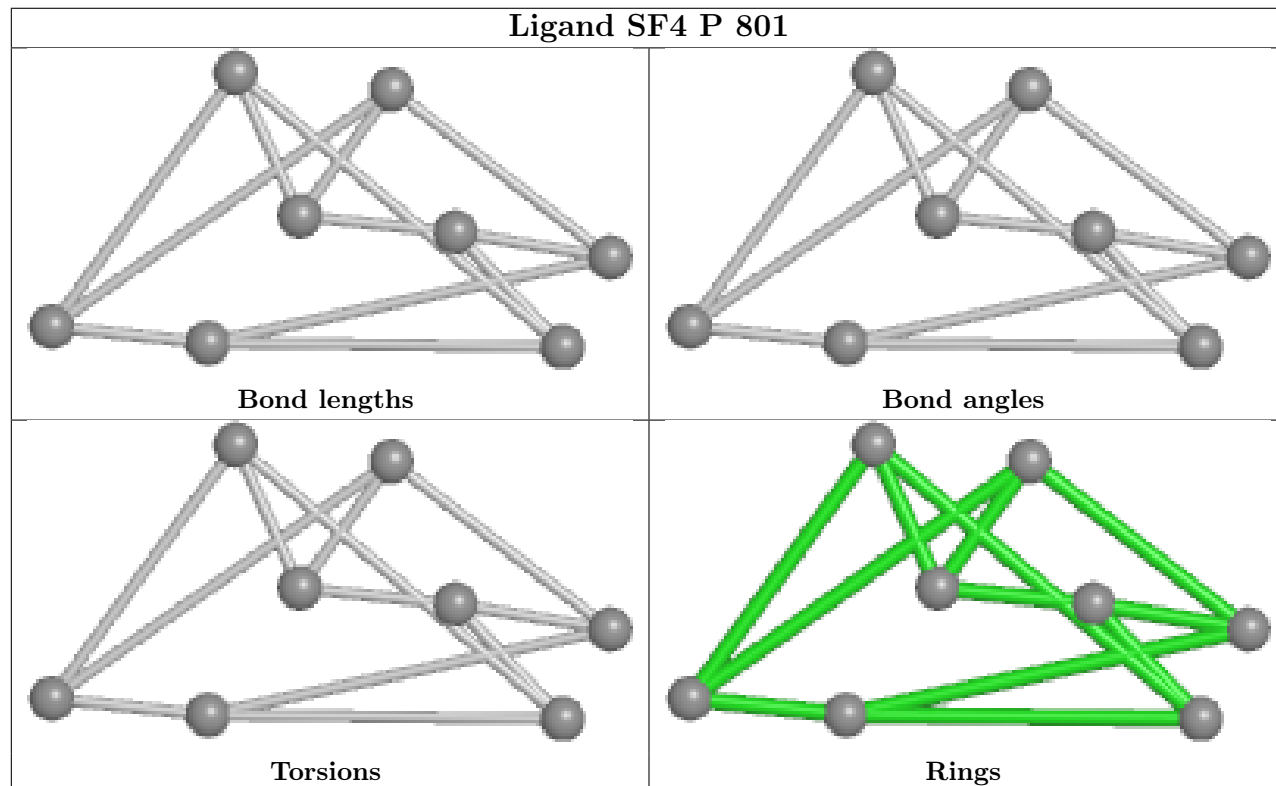
equivalents in the CSD to analyse the geometry.



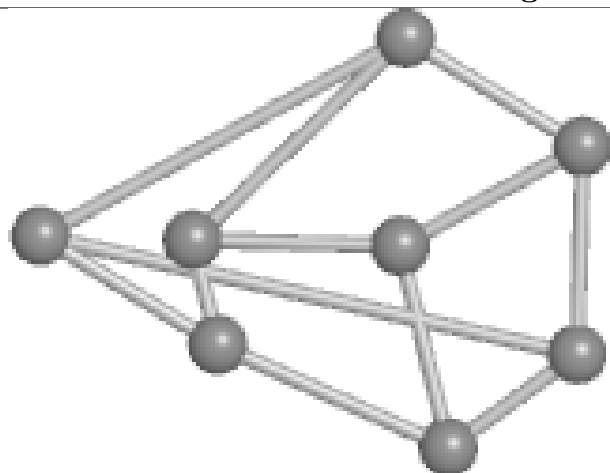
Ligand SF4 O 900



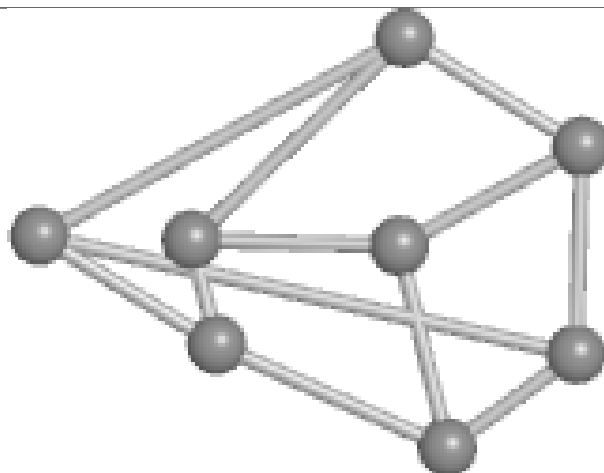
Ligand SF4 P 801



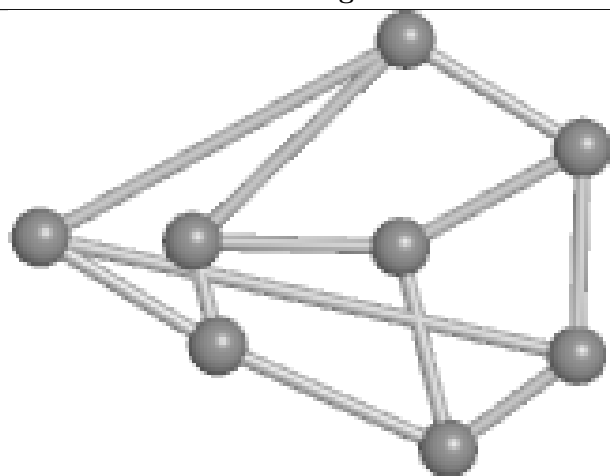
Ligand SF4 B 701



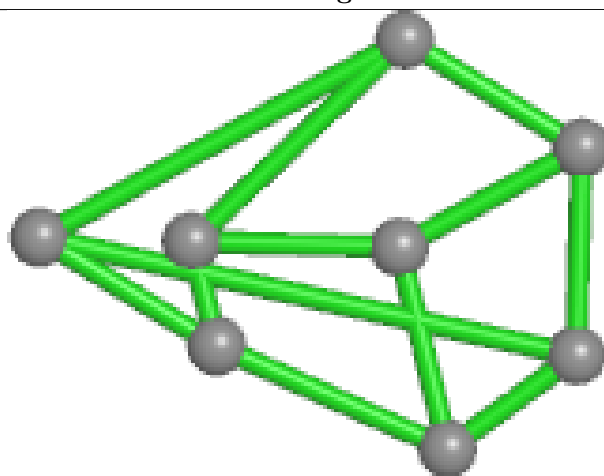
Bond lengths



Bond angles

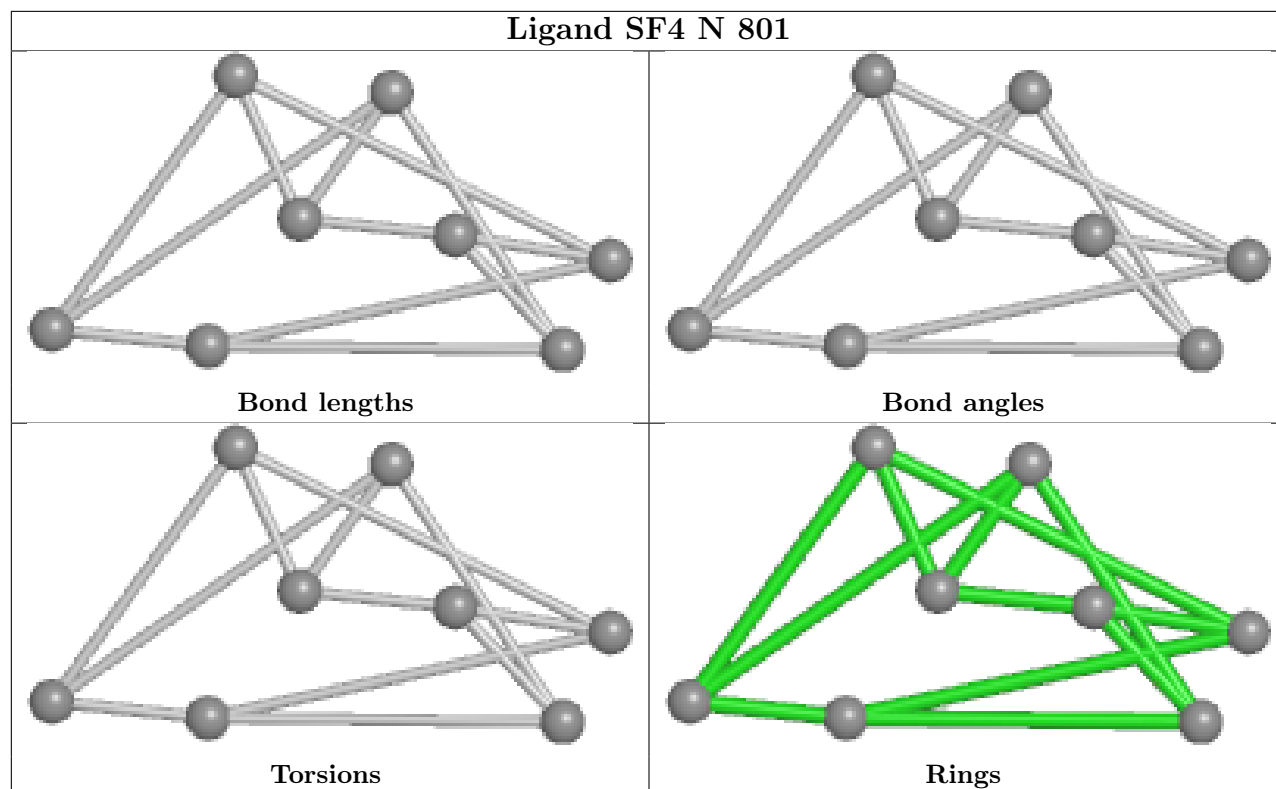


Torsions

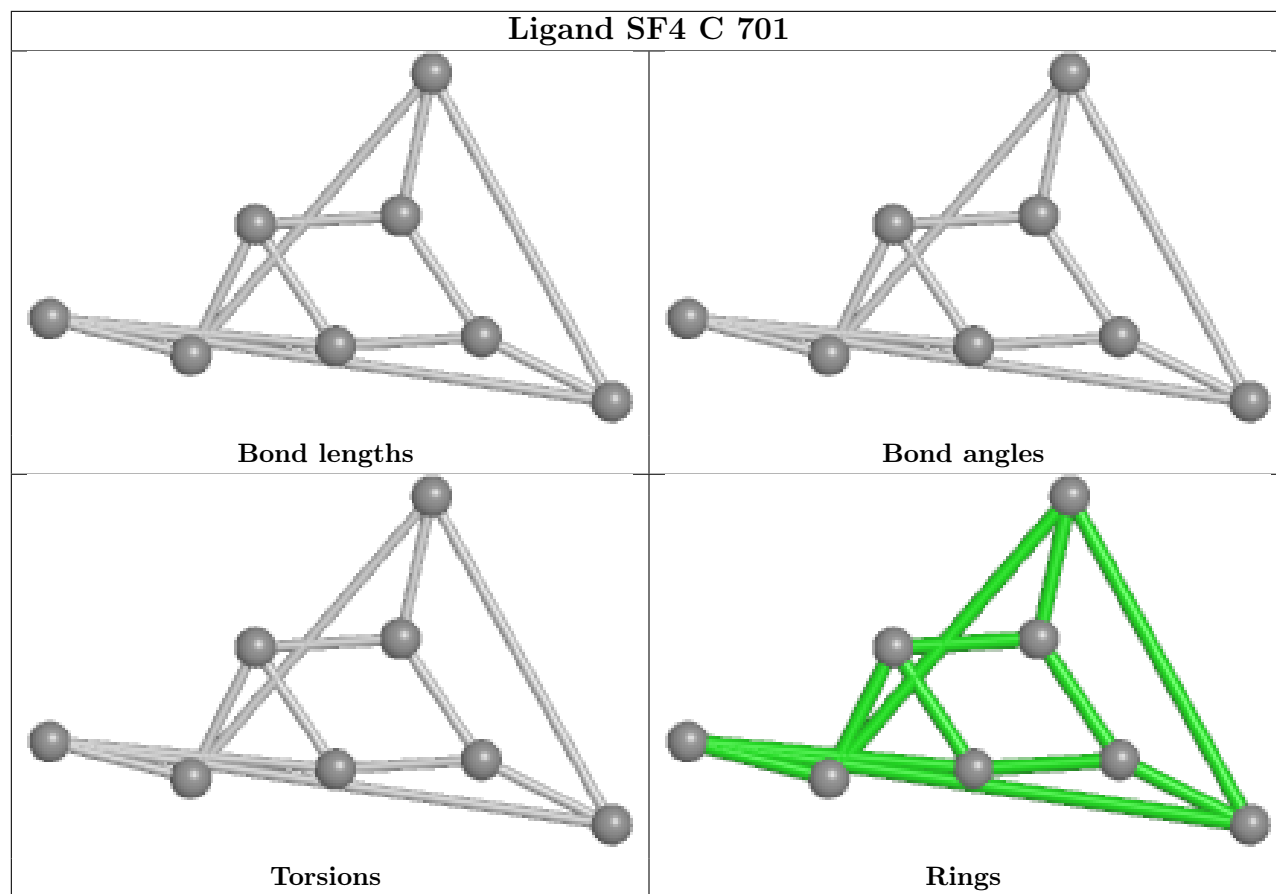


Rings

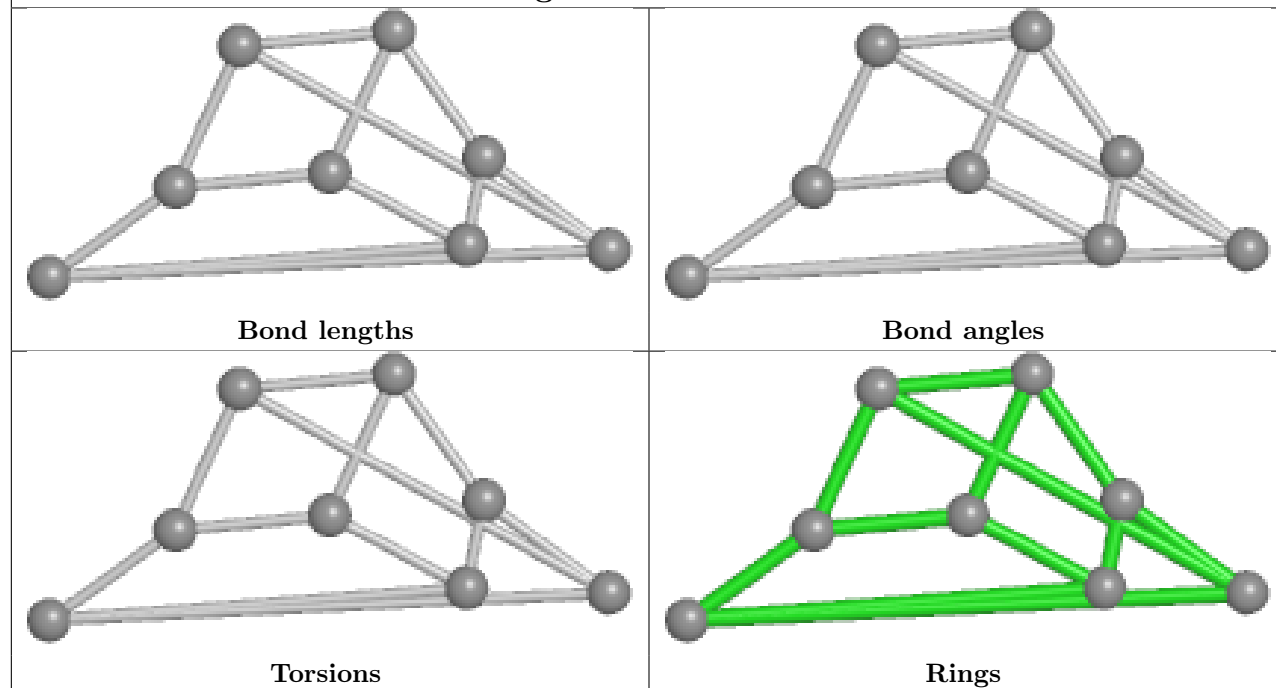
Ligand SF4 N 801



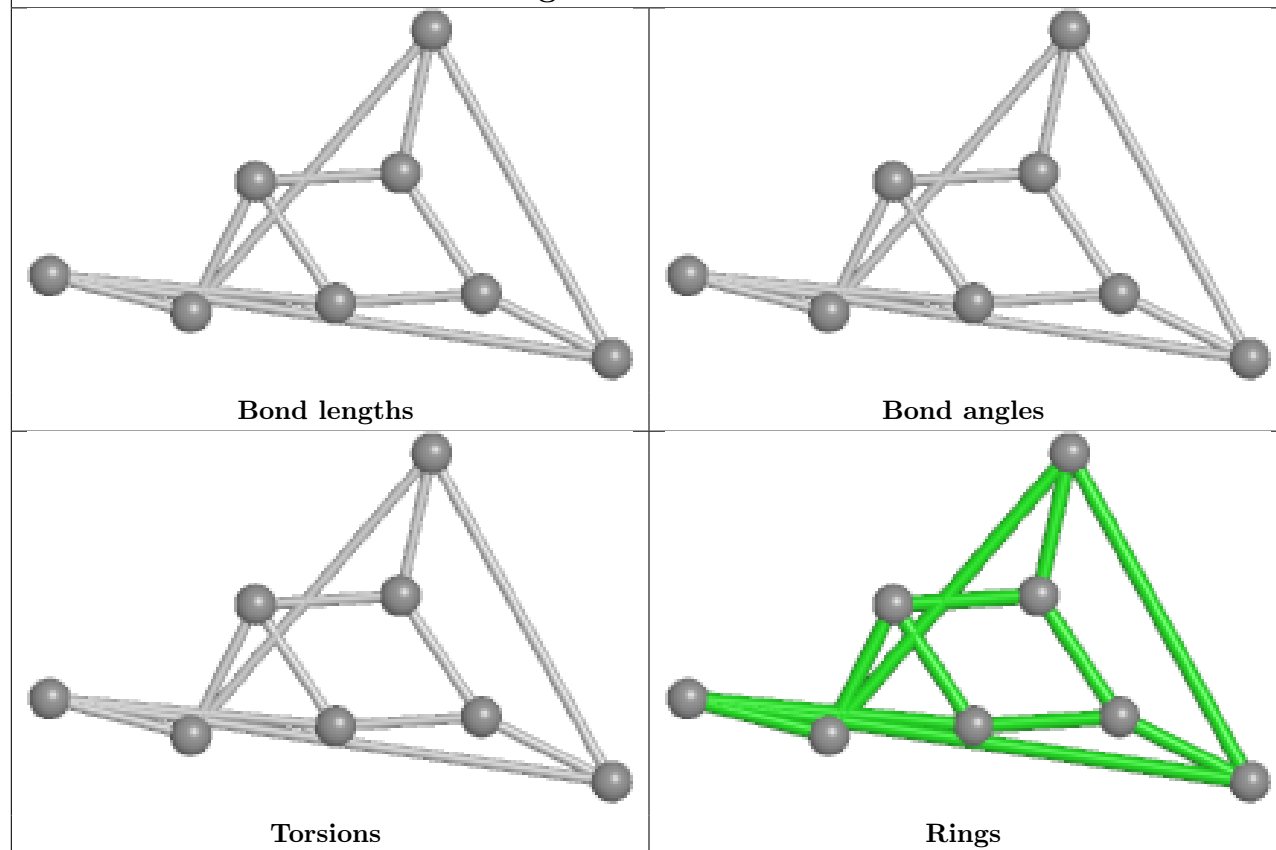
Ligand SF4 C 701

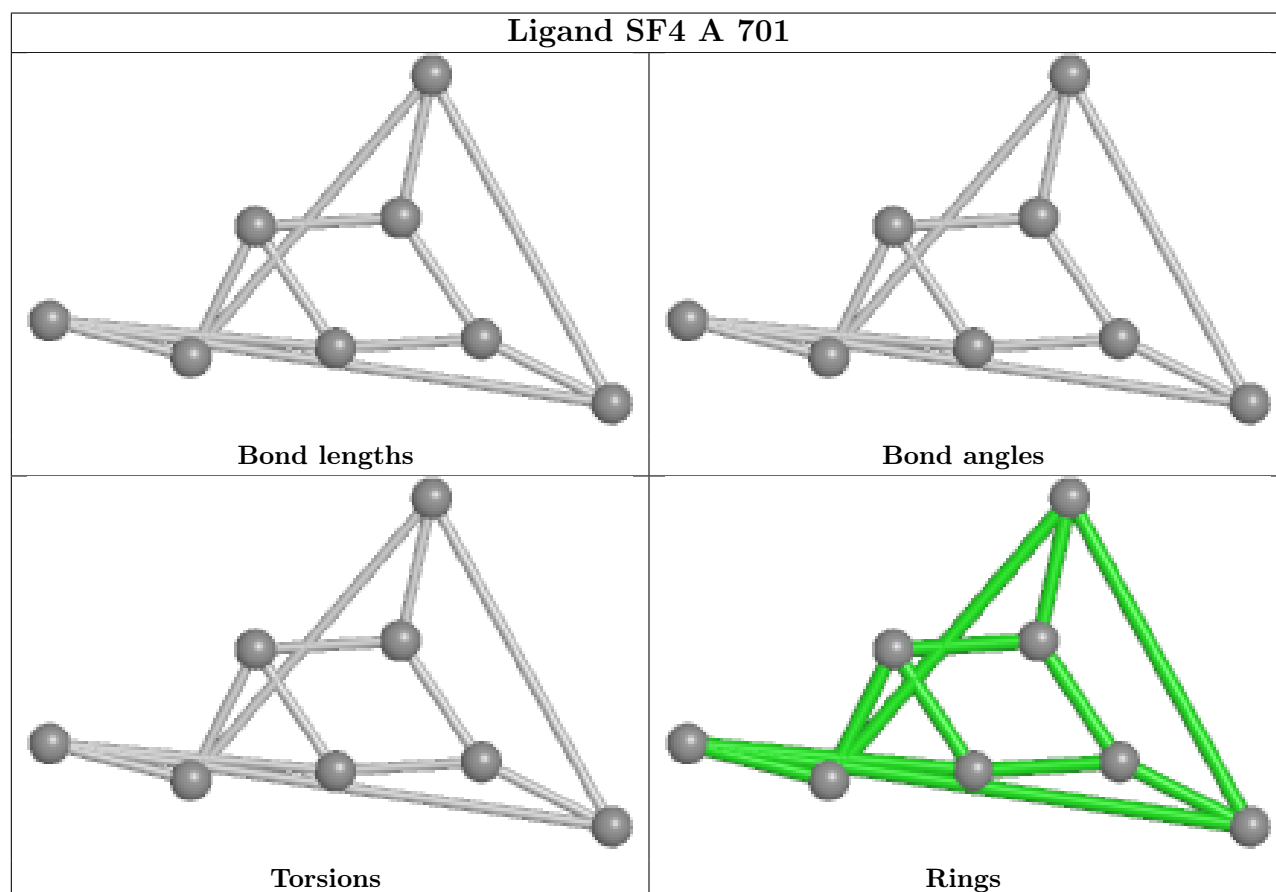
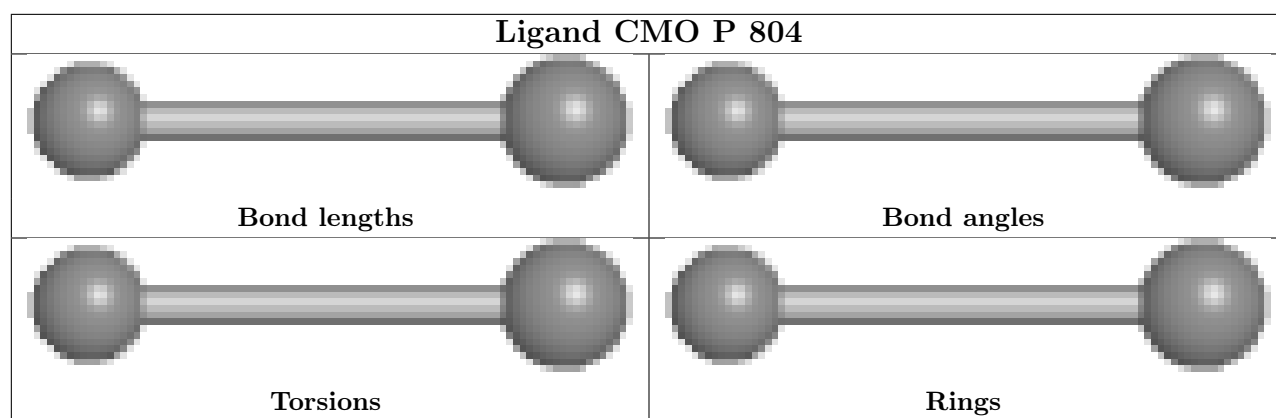


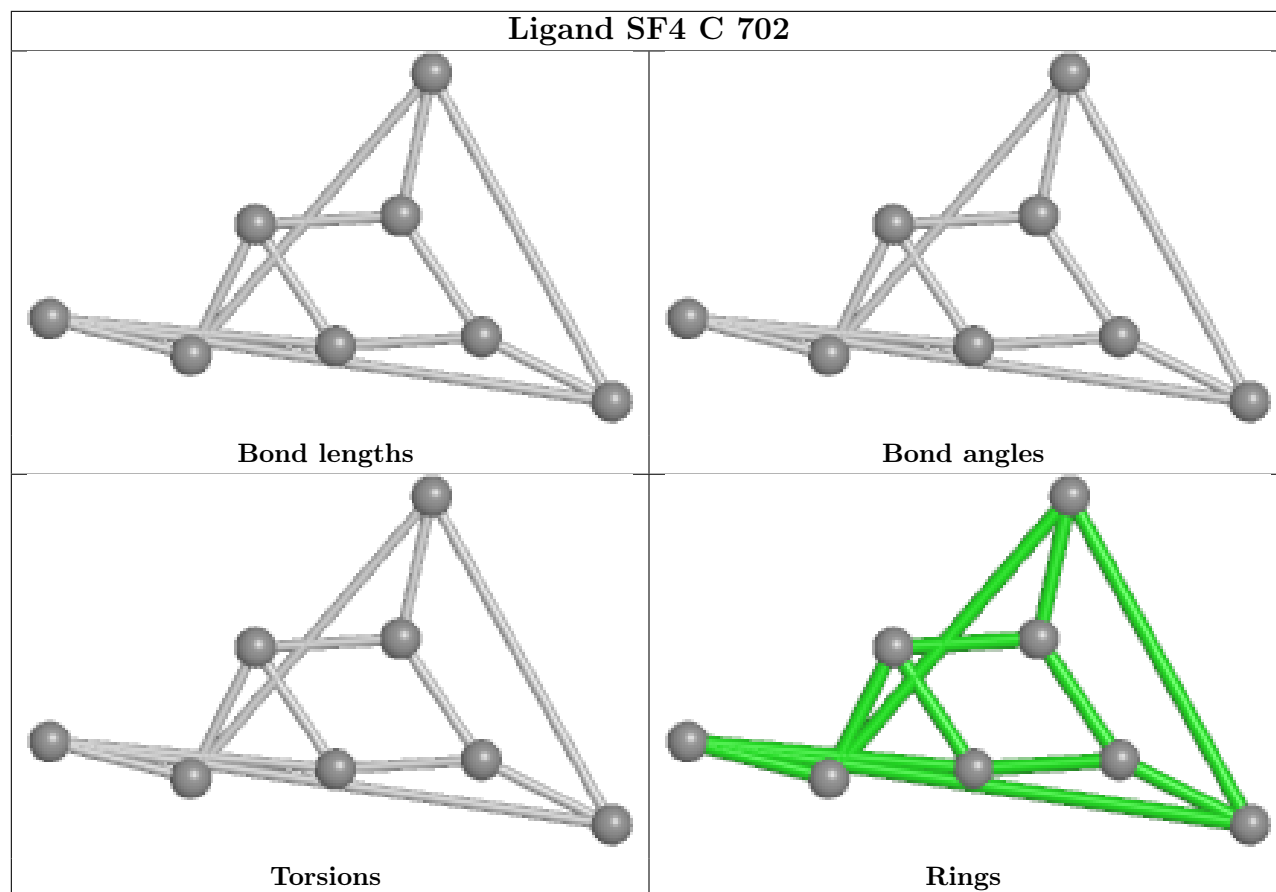
Ligand SF4 M 801



Ligand SF4 A 702







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	672/674 (99%)	-0.08	12 (1%) 68 70	21, 36, 55, 127	0
1	B	672/674 (99%)	-0.15	3 (0%) 92 93	21, 35, 54, 121	0
1	C	672/674 (99%)	0.00	21 (3%) 49 51	26, 40, 61, 109	0
1	D	672/674 (99%)	0.10	19 (2%) 53 55	26, 44, 67, 116	0
2	M	728/729 (99%)	-0.08	11 (1%) 73 75	23, 43, 71, 124	0
2	N	728/729 (99%)	-0.02	17 (2%) 60 62	20, 41, 72, 107	0
2	O	726/729 (99%)	1.59	258 (35%) 0 0	37, 87, 163, 238	0
2	P	728/729 (99%)	0.57	103 (14%) 2 2	28, 57, 117, 194	0
All	All	5598/5612 (99%)	0.25	444 (7%) 12 12	20, 43, 112, 238	0

All (444) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	474	VAL	13.1
2	O	485	TYR	11.6
2	O	356	VAL	10.8
2	O	354	ARG	10.5
2	O	460	VAL	9.5
2	O	481	ALA	9.3
2	O	468	PHE	8.5
2	P	492	MET	8.4
2	P	475	LYS	8.3
2	O	367	GLU	8.3
2	O	399	PHE	8.2
2	O	361	ILE	8.0
2	O	366	ILE	8.0
2	O	486	LYS	7.9
2	N	729	MET	7.8
2	P	474	VAL	7.7

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Mol	Chain	Res	Type	RSRZ
2	O	687	VAL	7.6
2	O	355	THR	7.2
2	O	723	LEU	6.9
2	P	698	LYS	6.8
2	P	483	GLU	6.7
2	O	608	CYS	6.7
2	O	504	TYR	6.6
2	O	461	ASP	6.6
2	O	440	ARG	6.5
2	O	391	TYR	6.4
2	O	373	ILE	6.4
2	O	449	VAL	6.3
2	M	729	MET	6.3
2	O	497	ASP	6.0
2	O	368	VAL	6.0
2	P	361	ILE	5.9
2	O	363	ASP	5.9
2	O	400	GLU	5.8
2	O	352	LEU	5.8
2	O	492	MET	5.8
2	O	465	VAL	5.7
2	O	380	SER	5.7
2	O	339	TYR	5.7
2	P	390	ILE	5.7
2	O	365	LYS	5.7
2	O	369	ILE	5.7
2	O	424	ASN	5.6
2	O	451	LYS	5.5
2	O	704	ILE	5.5
2	O	563	ILE	5.5
2	O	494	GLY	5.4
2	O	572	TYR	5.4
2	O	610	GLY	5.2
2	O	389	ASP	5.2
2	O	353	VAL	5.2
2	O	560	ILE	5.2
2	O	394	LYS	5.2
2	O	533	TRP	5.2
2	O	488	ARG	5.1
2	P	468	PHE	5.1
2	O	571	LEU	5.1
2	P	14	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
2	O	463	VAL	5.0
2	O	471	GLU	5.0
2	O	359	SER	5.0
2	O	653	VAL	4.9
2	O	667	ILE	4.9
2	O	718	LYS	4.9
2	P	469	THR	4.8
2	O	711	ILE	4.8
2	O	379	GLY	4.8
2	O	565	LYS	4.8
1	B	538	GLU	4.7
2	O	695	PHE	4.7
2	O	490	ASP	4.7
2	O	407	ILE	4.7
2	O	664	ILE	4.7
2	O	668	VAL	4.6
2	O	698	LYS	4.6
2	O	692	GLY	4.6
2	O	467	ILE	4.6
2	P	542	ILE	4.6
2	O	381	LYS	4.6
2	O	693	GLU	4.6
2	O	348	PRO	4.5
2	O	691	LEU	4.5
2	O	362	THR	4.5
2	O	484	LYS	4.5
2	P	353	VAL	4.5
2	O	317	LYS	4.5
2	O	14	GLU	4.5
2	O	605	LEU	4.5
2	O	716	GLU	4.5
2	P	384	LEU	4.4
2	O	390	ILE	4.4
2	O	462	ARG	4.4
2	O	397	ALA	4.4
2	P	473	LYS	4.4
2	O	357	SER	4.4
2	O	696	ILE	4.4
2	P	467	ILE	4.4
2	O	464	GLN	4.4
2	O	685	ARG	4.4
2	P	727	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	O	612	MET	4.4
2	O	559	PRO	4.3
2	O	554	GLU	4.3
2	P	490	ASP	4.3
2	O	607	GLU	4.3
2	O	360	GLU	4.2
2	P	696	ILE	4.2
2	O	724	THR	4.2
2	P	362	THR	4.2
2	O	715	LEU	4.2
2	O	623	PRO	4.2
2	O	475	LYS	4.2
2	N	373	ILE	4.2
2	O	699	ILE	4.2
2	O	472	ALA	4.2
2	P	369	ILE	4.1
2	O	371	PRO	4.1
2	P	355	THR	4.1
2	O	372	ASP	4.1
2	O	719	GLY	4.1
2	O	703	THR	4.1
2	P	368	VAL	4.1
2	O	712	LEU	4.1
2	O	469	THR	4.0
2	P	354	ARG	4.0
2	O	382	LEU	4.0
2	P	472	ALA	4.0
1	C	416	ARG	4.0
2	P	425	ILE	3.9
2	P	470	ASP	3.9
2	O	387	LEU	3.9
2	M	379	GLY	3.9
2	O	479	GLU	3.9
2	O	690	GLY	3.9
2	O	350	PHE	3.8
2	O	453	LYS	3.8
2	P	486	LYS	3.8
2	O	694	ASP	3.8
2	P	357	SER	3.8
2	P	359	SER	3.8
2	P	471	GLU	3.8
2	O	721	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	P	382	LEU	3.7
2	P	381	LYS	3.7
1	C	77	ARG	3.7
2	P	485	TYR	3.7
2	O	384	LEU	3.7
2	O	577	ARG	3.7
2	O	398	ASP	3.7
2	O	611	ILE	3.6
2	O	580	GLU	3.6
2	O	495	LEU	3.6
2	O	564	TRP	3.6
2	O	573	THR	3.6
2	O	436	ALA	3.6
2	P	724	THR	3.6
2	P	682	PHE	3.5
2	O	437	LYS	3.5
2	O	545	ALA	3.5
2	O	493	ARG	3.5
2	P	391	TYR	3.5
2	N	608	CYS	3.5
2	O	542	ILE	3.5
2	P	383	PRO	3.5
2	O	418	TRP	3.5
2	P	729	MET	3.5
2	O	404	GLU	3.4
2	O	658	ILE	3.4
2	O	319	ASP	3.4
2	P	695	PHE	3.4
2	O	377	PRO	3.4
2	O	435	VAL	3.4
2	O	570	TYR	3.4
2	O	344	GLY	3.4
2	O	477	TYR	3.4
2	O	613	ILE	3.4
1	D	417	PRO	3.4
2	P	693	GLU	3.3
2	O	406	ARG	3.3
2	O	15	GLY	3.3
2	O	566	SER	3.3
1	B	417	PRO	3.3
2	O	459	ILE	3.3
2	O	583	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	O	714	TYR	3.3
2	O	340	VAL	3.3
2	O	525	VAL	3.3
2	P	482	ARG	3.3
2	O	551	ILE	3.3
2	O	722	ALA	3.3
2	P	664	ILE	3.3
2	O	579	LEU	3.2
2	O	680	ASP	3.2
2	O	710	GLU	3.2
2	O	709	ASP	3.2
2	P	367	GLU	3.2
2	O	402	VAL	3.2
2	O	403	LEU	3.2
2	O	603	ALA	3.2
2	P	334	ARG	3.2
2	P	481	ALA	3.2
2	O	3	ASP	3.2
2	O	697	ASP	3.2
2	O	341	GLU	3.2
2	O	466	THR	3.2
2	O	333	ILE	3.2
2	O	411	ILE	3.2
2	P	459	ILE	3.2
2	P	364	GLY	3.2
2	O	553	LYS	3.2
2	P	387	LEU	3.2
2	O	669	TRP	3.1
2	O	507	VAL	3.1
2	P	728	ILE	3.1
1	D	415	ASN	3.1
2	O	689	GLU	3.1
2	P	462	ARG	3.1
1	D	114[A]	CYS	3.1
2	O	567	VAL	3.1
1	C	417	PRO	3.1
2	O	541	GLU	3.1
2	P	393	ARG	3.1
1	A	306	GLY	3.1
1	C	305	ALA	3.0
2	O	2	THR	3.0
2	O	9	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	O	574	ALA	3.0
1	D	418	VAL	3.0
2	O	609	ASN	3.0
2	P	360	GLU	3.0
1	D	104	LEU	3.0
2	O	293	PHE	3.0
2	O	682	PHE	3.0
2	P	373	ILE	3.0
2	O	345	ASN	3.0
2	O	679	HIS	3.0
2	O	10	GLY	3.0
2	P	379	GLY	3.0
2	P	479	GLU	3.0
2	M	715	LEU	3.0
2	O	499	THR	3.0
2	P	460	VAL	2.9
2	O	544	HIS	2.9
2	O	247	ARG	2.9
2	O	393	ARG	2.9
2	P	570	TYR	2.9
1	A	538	GLU	2.9
2	O	683	VAL	2.9
2	P	365	LYS	2.9
2	P	386	ILE	2.9
2	P	703	THR	2.9
1	A	416	ARG	2.9
1	C	415	ASN	2.9
2	O	684	ARG	2.9
2	P	488	ARG	2.9
2	P	399	PHE	2.9
2	O	383	PRO	2.9
2	O	666	ARG	2.9
2	P	669	TRP	2.9
2	P	15	GLY	2.8
2	P	561	LYS	2.8
2	O	457	PRO	2.8
2	O	670	MET	2.8
2	O	503	PHE	2.8
2	P	363	ASP	2.8
2	O	378	GLU	2.8
2	O	337	ASP	2.8
2	O	452	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	O	427	TRP	2.8
2	P	16	LYS	2.8
2	O	480	VAL	2.8
2	O	606	PRO	2.8
2	P	339	TYR	2.8
2	O	678	LEU	2.8
2	P	718	LYS	2.8
2	O	582	VAL	2.7
2	O	346	ARG	2.7
2	O	672	LYS	2.7
2	O	657	PHE	2.7
2	P	572	TYR	2.7
2	O	423	ARG	2.7
1	C	96	THR	2.7
2	M	16	LYS	2.7
2	O	441	PHE	2.7
2	P	477	TYR	2.7
2	O	443	ASN	2.7
2	O	17	GLU	2.7
2	O	621	MET	2.7
2	O	374	ASP	2.7
2	P	494	GLY	2.7
2	O	470	ASP	2.7
2	O	717	GLU	2.6
2	O	520	VAL	2.6
2	P	721	PRO	2.6
2	O	442	LYS	2.6
2	O	707	THR	2.6
2	P	424	ASN	2.6
2	O	444	TYR	2.6
2	P	491	ARG	2.6
2	O	478	MET	2.6
2	P	493	ARG	2.6
2	O	448	LEU	2.6
1	C	221	MET	2.6
2	O	585	TYR	2.6
2	P	714	TYR	2.6
2	O	622	THR	2.5
2	P	352	LEU	2.5
1	A	106	ILE	2.5
1	A	107	LEU	2.5
2	N	376	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	694	ASP	2.5
2	O	13	PRO	2.5
2	M	474	VAL	2.5
2	P	356	VAL	2.5
2	P	704	ILE	2.5
2	P	461	ASP	2.5
2	O	370	GLY	2.5
2	O	648	GLY	2.5
2	O	489	ASP	2.5
1	D	585	SER	2.5
1	A	550[A]	CYS	2.5
2	O	558	ASP	2.5
1	A	415	ASN	2.5
2	N	367	GLU	2.5
2	O	16	LYS	2.5
1	D	416	ARG	2.4
2	O	447	ILE	2.4
1	D	105	MET	2.4
1	C	230	LEU	2.4
2	O	316	ILE	2.4
2	P	6	LYS	2.4
2	P	684	ARG	2.4
1	C	216	VAL	2.4
2	O	483	GLU	2.4
2	P	388	VAL	2.4
2	N	381	LYS	2.4
2	O	315	LYS	2.4
2	N	560	ILE	2.4
2	O	662	GLY	2.4
2	P	607	GLU	2.4
1	D	535	ALA	2.4
2	P	389	ASP	2.4
2	O	396	GLN	2.4
1	C	227	PRO	2.4
1	B	550[A]	CYS	2.4
2	P	711	ILE	2.4
2	O	476	GLU	2.3
2	P	659	SER	2.3
1	D	106	ILE	2.3
2	O	301	ILE	2.3
2	P	345	ASN	2.3
2	M	723	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	388	VAL	2.3
1	D	23	LYS	2.3
2	N	316	ILE	2.3
2	O	524	ARG	2.3
2	O	386	ILE	2.3
1	C	65	GLY	2.3
1	C	469	GLY	2.3
2	O	584	LEU	2.3
2	M	367	GLU	2.3
2	O	706	THR	2.3
1	D	160	LEU	2.3
2	P	377	PRO	2.3
2	O	491	ARG	2.3
2	M	373	ILE	2.3
2	P	549	GLN	2.3
1	A	153	GLU	2.3
1	C	413	GLU	2.3
2	P	554	GLU	2.3
2	N	559	PRO	2.2
2	O	300	LYS	2.2
2	O	569	ASP	2.2
1	D	112	ALA	2.2
2	P	604	ILE	2.2
2	N	469	THR	2.2
2	O	502	THR	2.2
2	O	578	ASN	2.2
2	N	380	SER	2.2
2	O	334	ARG	2.2
2	N	339	TYR	2.2
2	O	552	PRO	2.2
2	N	440	ARG	2.2
2	O	288	ILE	2.2
1	D	108	THR	2.2
2	P	371	PRO	2.2
1	A	216	VAL	2.2
1	C	223	MET	2.2
1	D	216	VAL	2.2
2	O	482	ARG	2.2
2	P	699	ILE	2.2
2	O	487	GLU	2.2
2	O	392	GLY	2.2
2	O	547	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	727	PRO	2.2
2	P	348	PRO	2.2
1	C	639	GLN	2.2
2	O	375	GLN	2.2
2	O	517	VAL	2.2
1	C	540	GLY	2.2
2	O	456	PHE	2.2
2	P	722	ALA	2.1
2	O	601	ILE	2.1
2	P	560	ILE	2.1
2	P	613	ILE	2.1
1	D	412	LYS	2.1
2	O	656	LYS	2.1
2	N	470	ASP	2.1
2	O	395	MET	2.1
1	D	378	ALA	2.1
1	C	215	LEU	2.1
1	D	538	GLU	2.1
2	P	544	HIS	2.1
1	A	234	ALA	2.1
1	D	590	ALA	2.1
1	C	108	THR	2.1
2	N	366	ILE	2.1
2	P	611	ILE	2.1
2	N	370	GLY	2.1
2	M	371	PRO	2.1
2	O	11	ALA	2.1
2	O	450	ALA	2.1
2	O	713	PRO	2.1
2	O	647	ILE	2.1
2	O	446	GLU	2.1
2	O	705	GLY	2.1
2	P	577	ARG	2.1
1	C	539	ILE	2.0
2	O	581	GLN	2.0
1	C	470	CYS	2.0
2	O	151	TRP	2.0
2	M	124	ASP	2.0
2	O	665	ALA	2.0
2	O	313	LEU	2.0
2	O	587	LEU	2.0
2	N	362	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	2.0
2	M	690	GLY	2.0
2	O	659	SER	2.0
1	C	235	ILE	2.0
2	O	410	PHE	2.0
2	O	688	GLU	2.0
1	A	308	LYS	2.0
2	O	655	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGE	A	704	10/10	0.77	0.21	19,42,52,54	0
6	PG5	C	704	12/12	0.83	0.17	44,58,71,73	0
4	XCC	B	702	9/9	0.97	0.16	41,53,70,82	0
3	SF4	O	900	8/8	0.97	0.11	58,74,80,88	0
7	NI	M	802	1/1	0.97	0.14	48,48,48,48	0
9	MG	N	805	1/1	0.97	0.07	43,43,43,43	0
4	XCC	C	703	9/9	0.97	0.16	45,58,73,104	0
7	NI	O	902	1/1	0.97	0.15	90,90,90,90	0
4	XCC	A	703	9/9	0.97	0.14	43,52,63,69	0
8	CMO	N	804	2/2	0.98	0.21	40,40,40,42	0
7	NI	O	901	1/1	0.98	0.18	75,75,75,75	0
4	XCC	D	702	9/9	0.98	0.16	50,58,74,84	0
3	SF4	D	701	8/8	0.98	0.20	36,38,44,45	0
8	CMO	M	804	2/2	0.98	0.25	43,43,43,44	0
3	SF4	M	801	8/8	0.99	0.15	28,30,34,36	0

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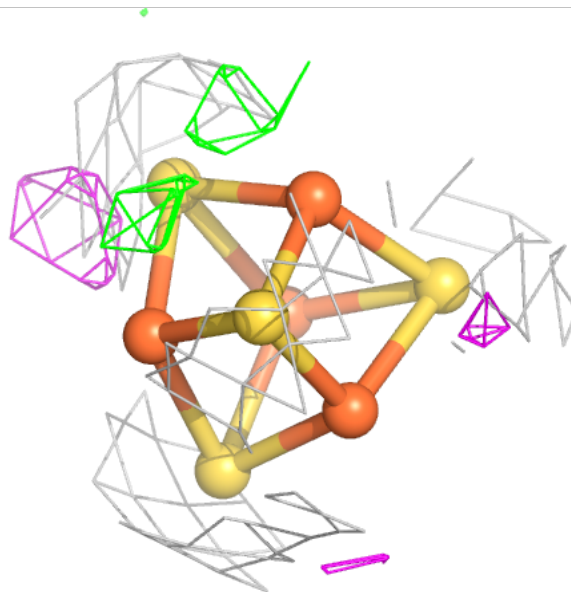
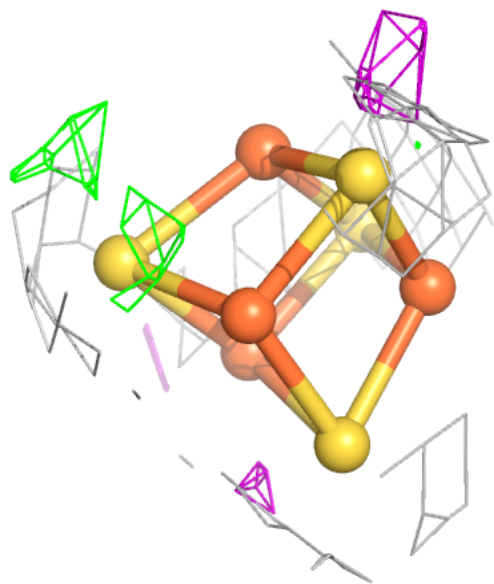
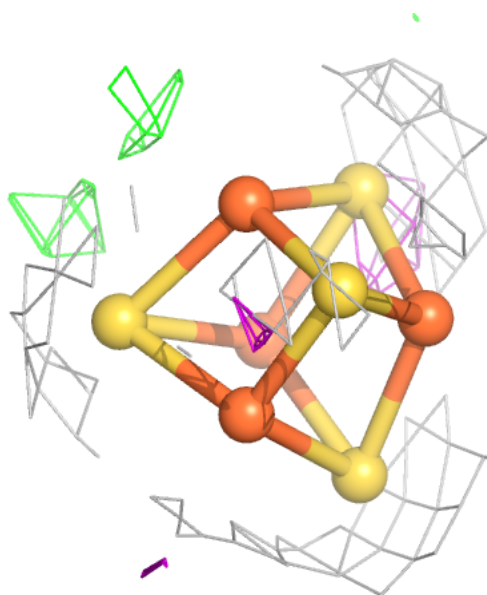
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SF4	B	701	8/8	0.99	0.18	24,27,32,34	0
7	NI	N	802	1/1	0.99	0.12	43,43,43,43	0
7	NI	P	802	1/1	0.99	0.14	61,61,61,61	0
7	NI	M	803	1/1	0.99	0.12	31,31,31,31	0
3	SF4	C	702	8/8	0.99	0.18	35,38,41,43	0
8	CMO	P	804	2/2	0.99	0.19	61,61,61,63	0
3	SF4	P	801	8/8	0.99	0.13	45,49,53,55	0
3	SF4	A	701	8/8	0.99	0.12	21,26,27,29	0
3	SF4	C	701	8/8	0.99	0.14	35,40,42,44	0
3	SF4	A	702	8/8	0.99	0.18	24,26,28,31	0
3	SF4	N	801	8/8	0.99	0.17	27,32,33,35	0
7	NI	P	803	1/1	0.99	0.14	44,44,44,44	0
7	NI	N	803	1/1	1.00	0.18	31,31,31,31	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.

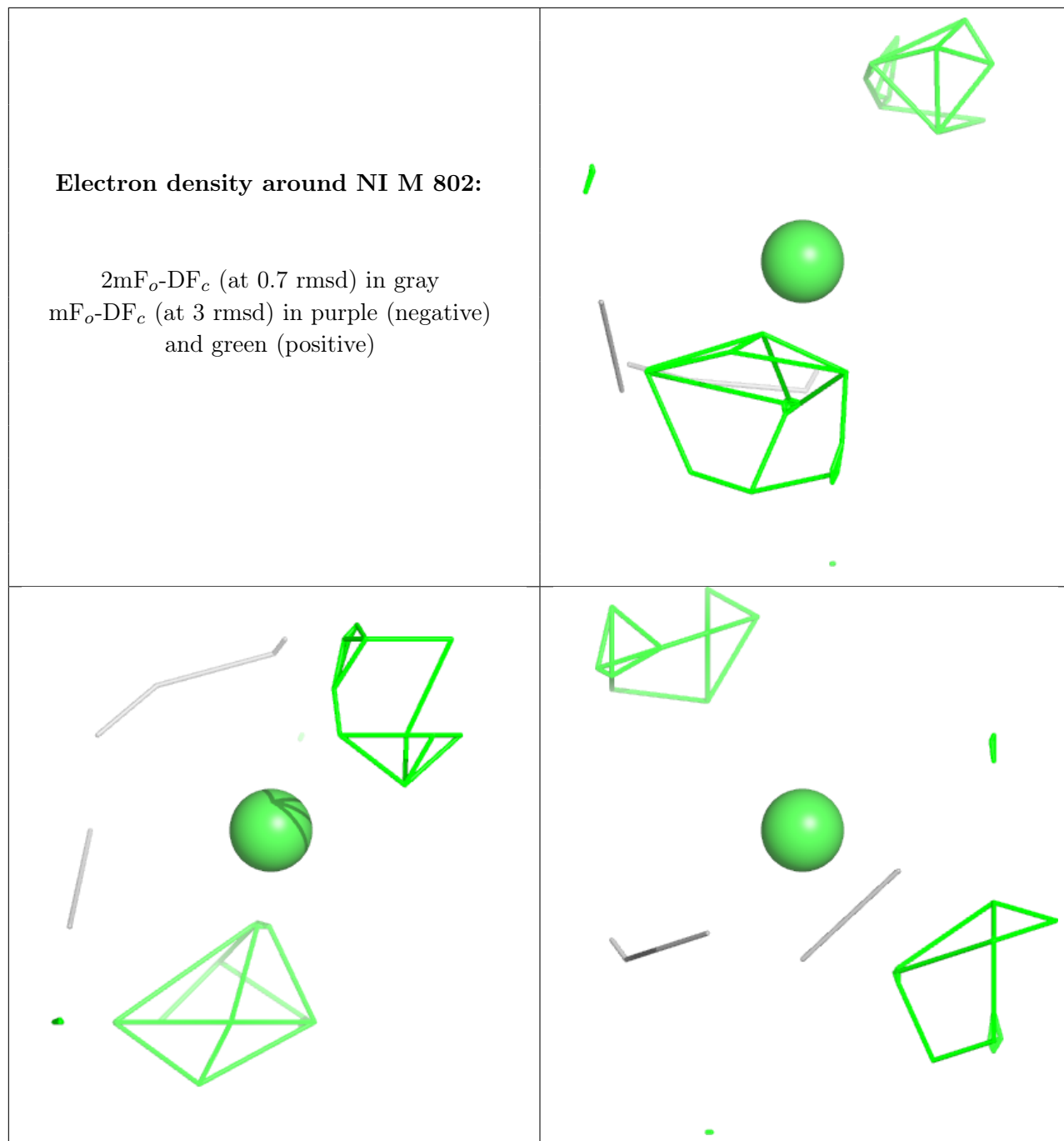
Electron density around SF4 O 900:

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



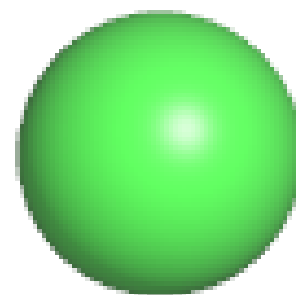
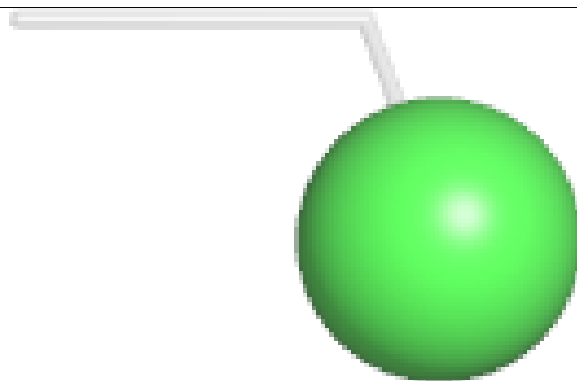
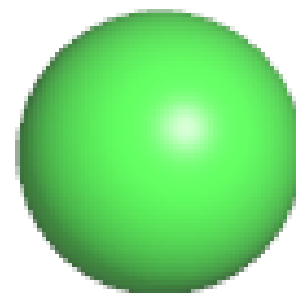
Electron density around NI M 802:

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



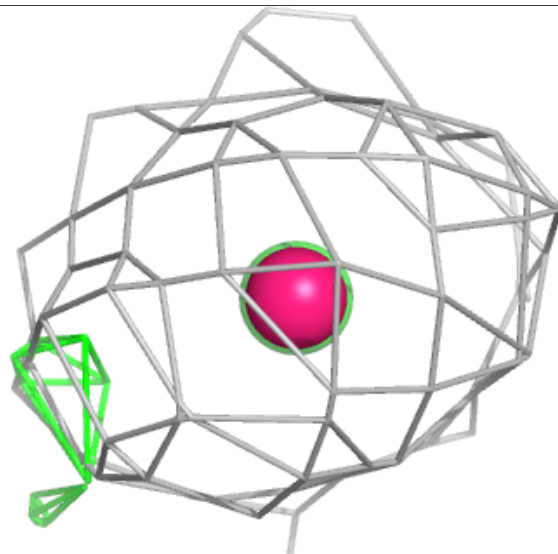
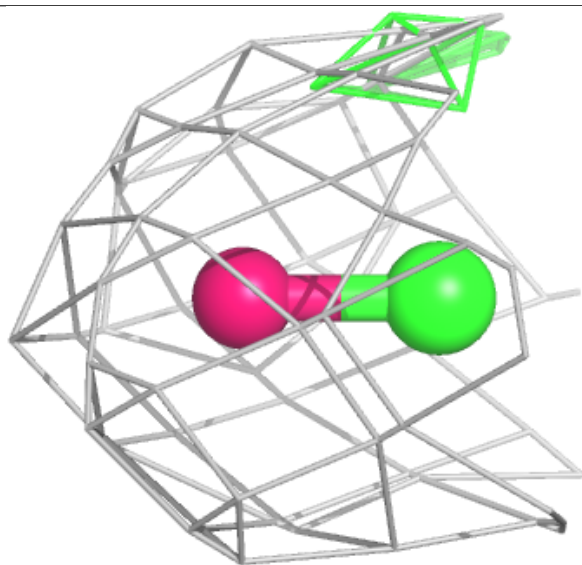
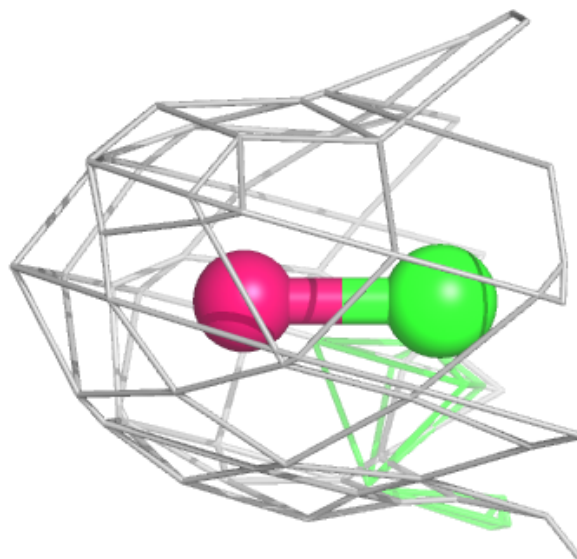
Electron density around NI O 902:

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



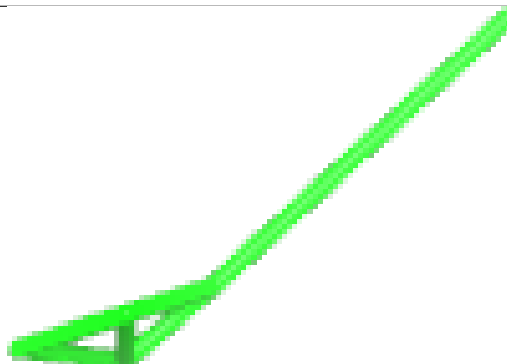
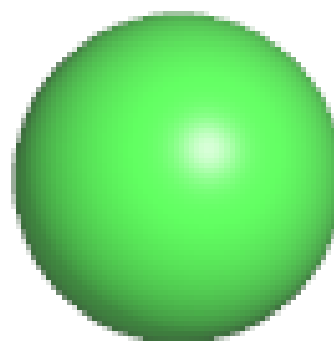
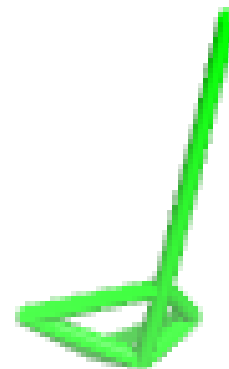
Electron density around CMO N 804:

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



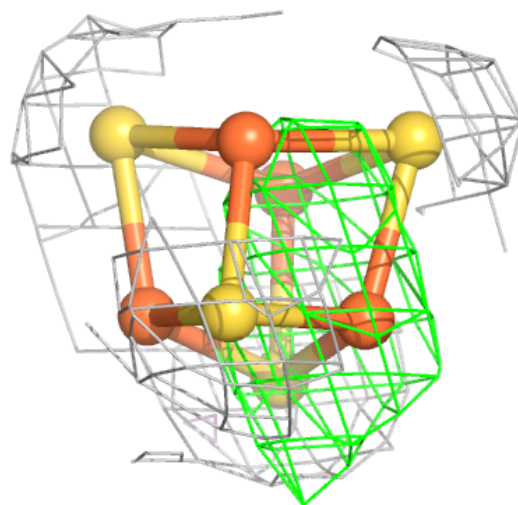
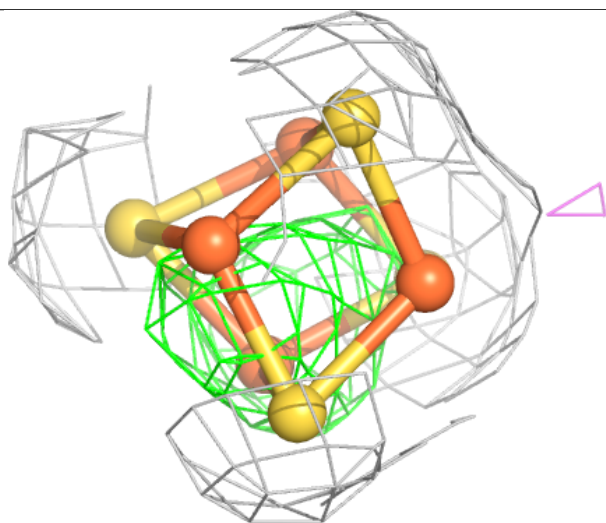
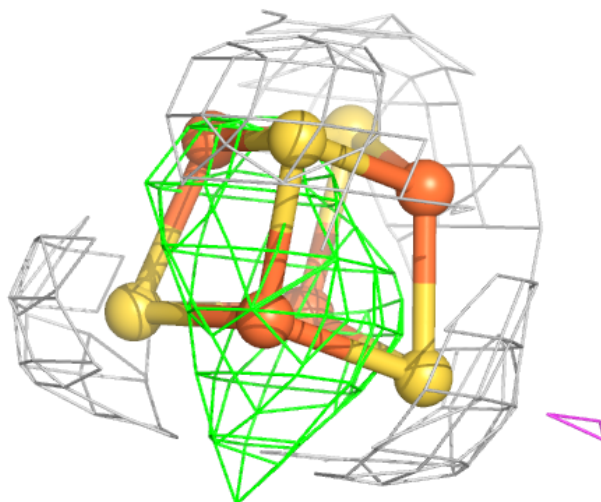
Electron density around NI O 901:

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



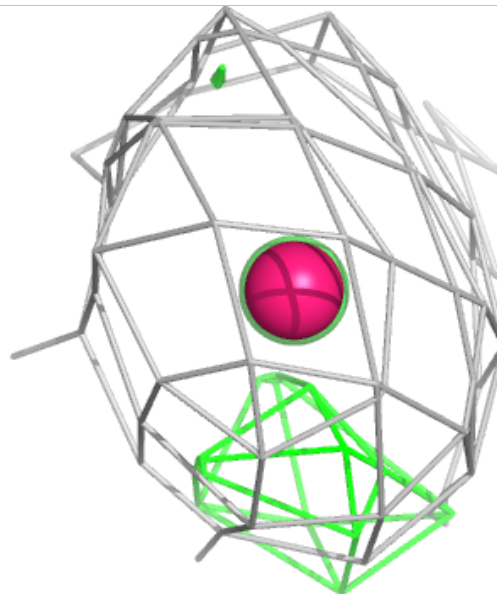
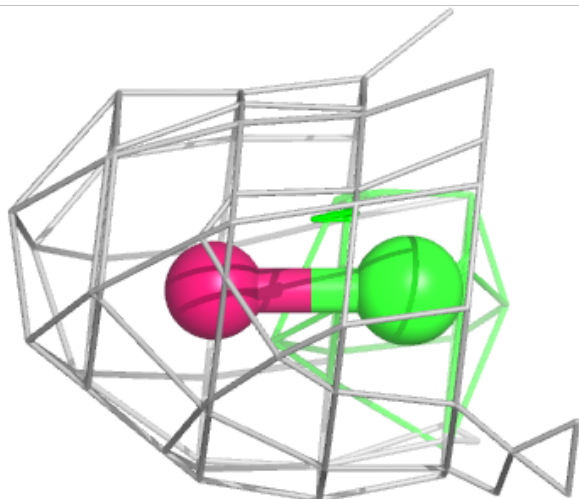
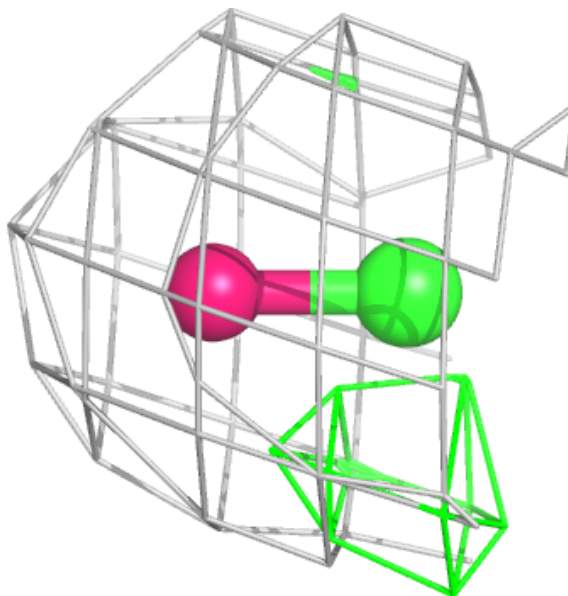
Electron density around SF4 D 701:

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



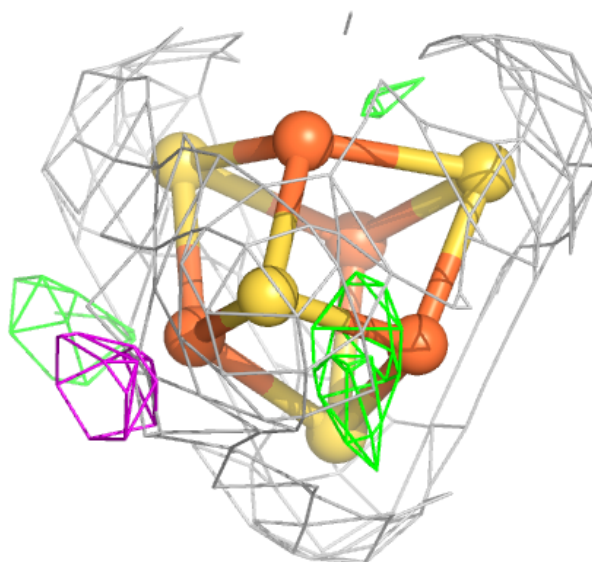
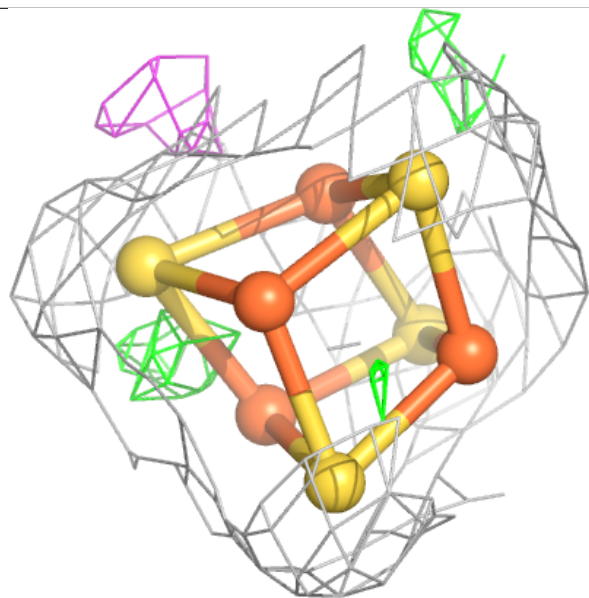
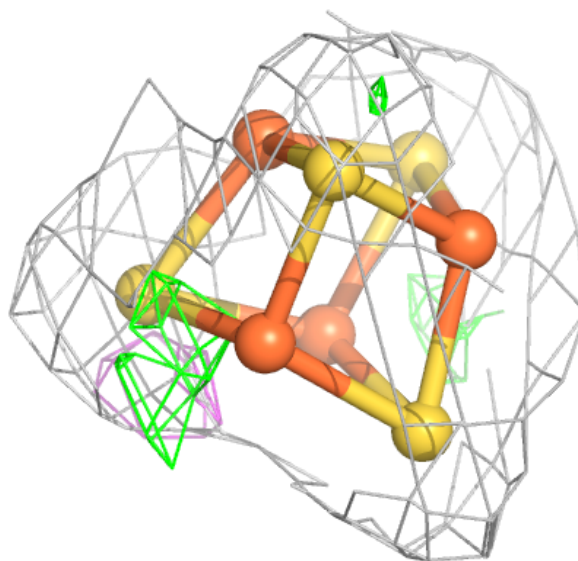
Electron density around CMO M 804:

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



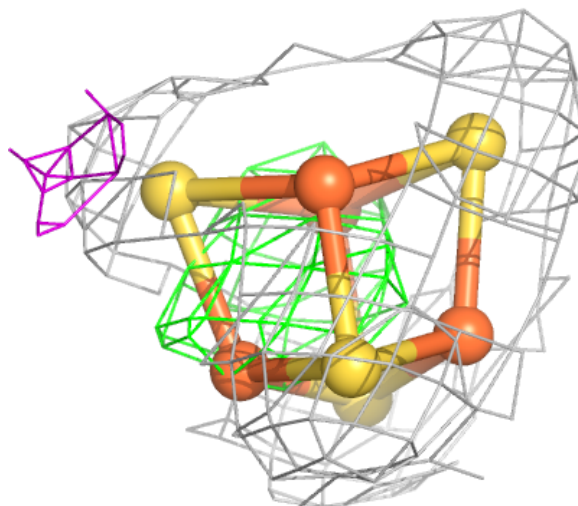
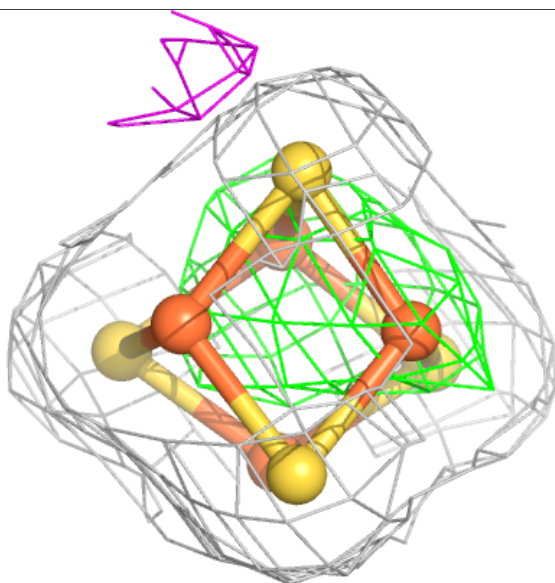
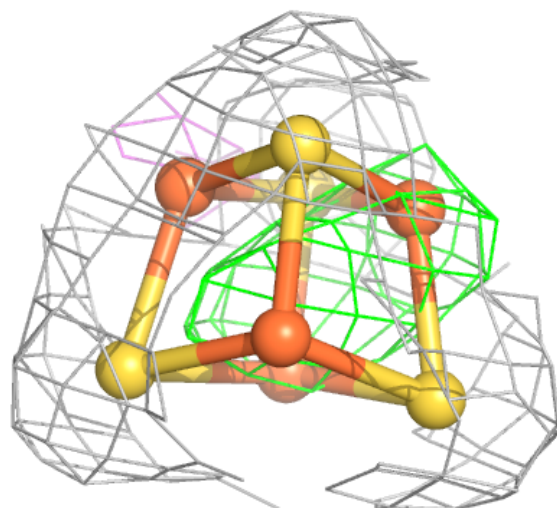
Electron density around SF4 M 801:

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



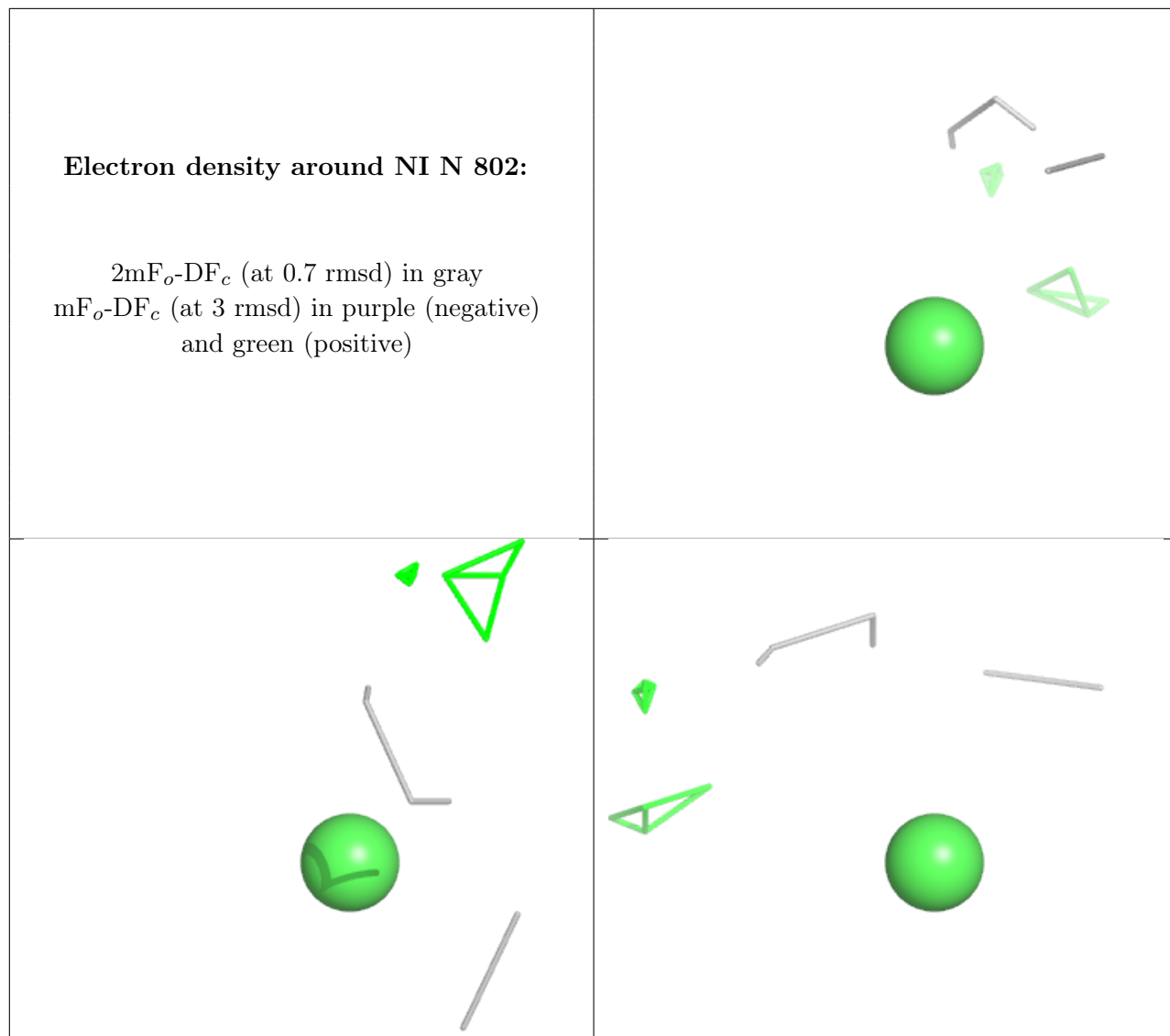
Electron density around SF4 B 701:

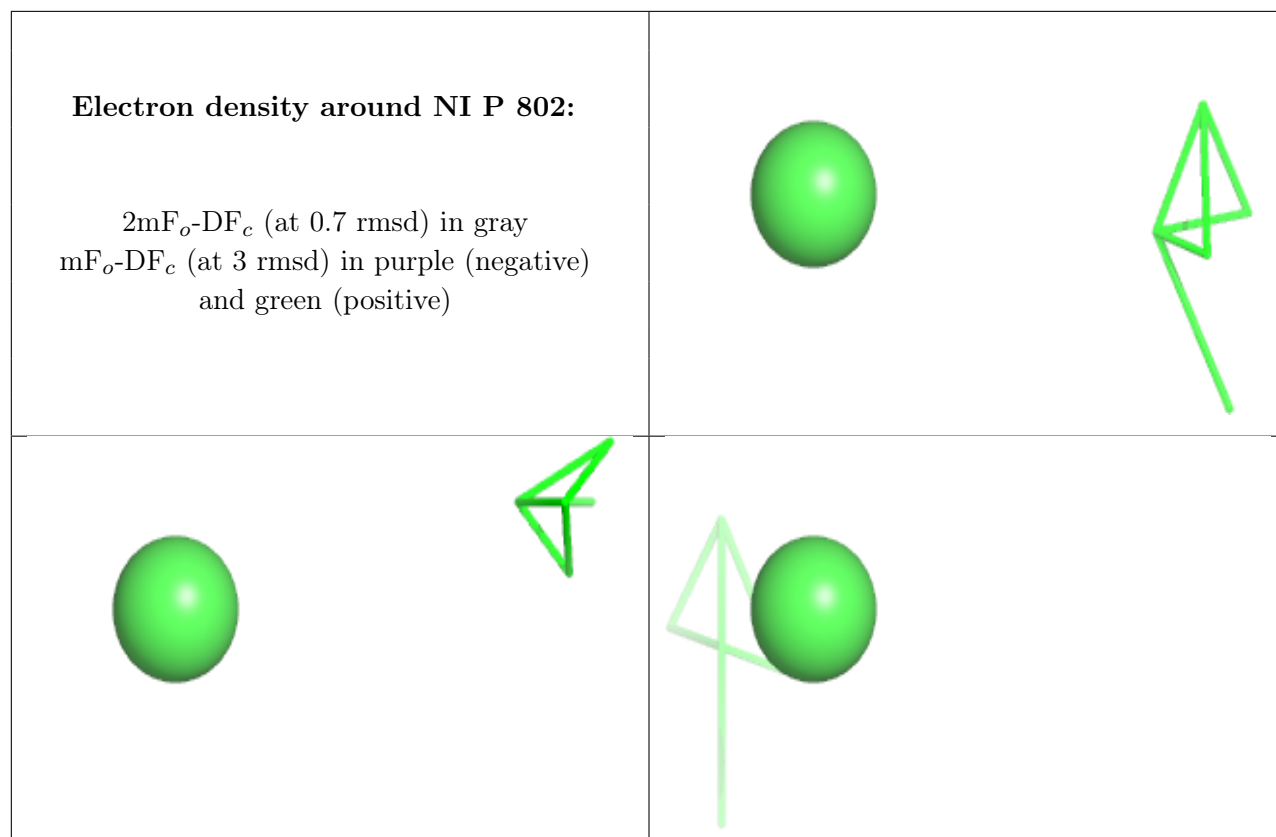
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI N 802:

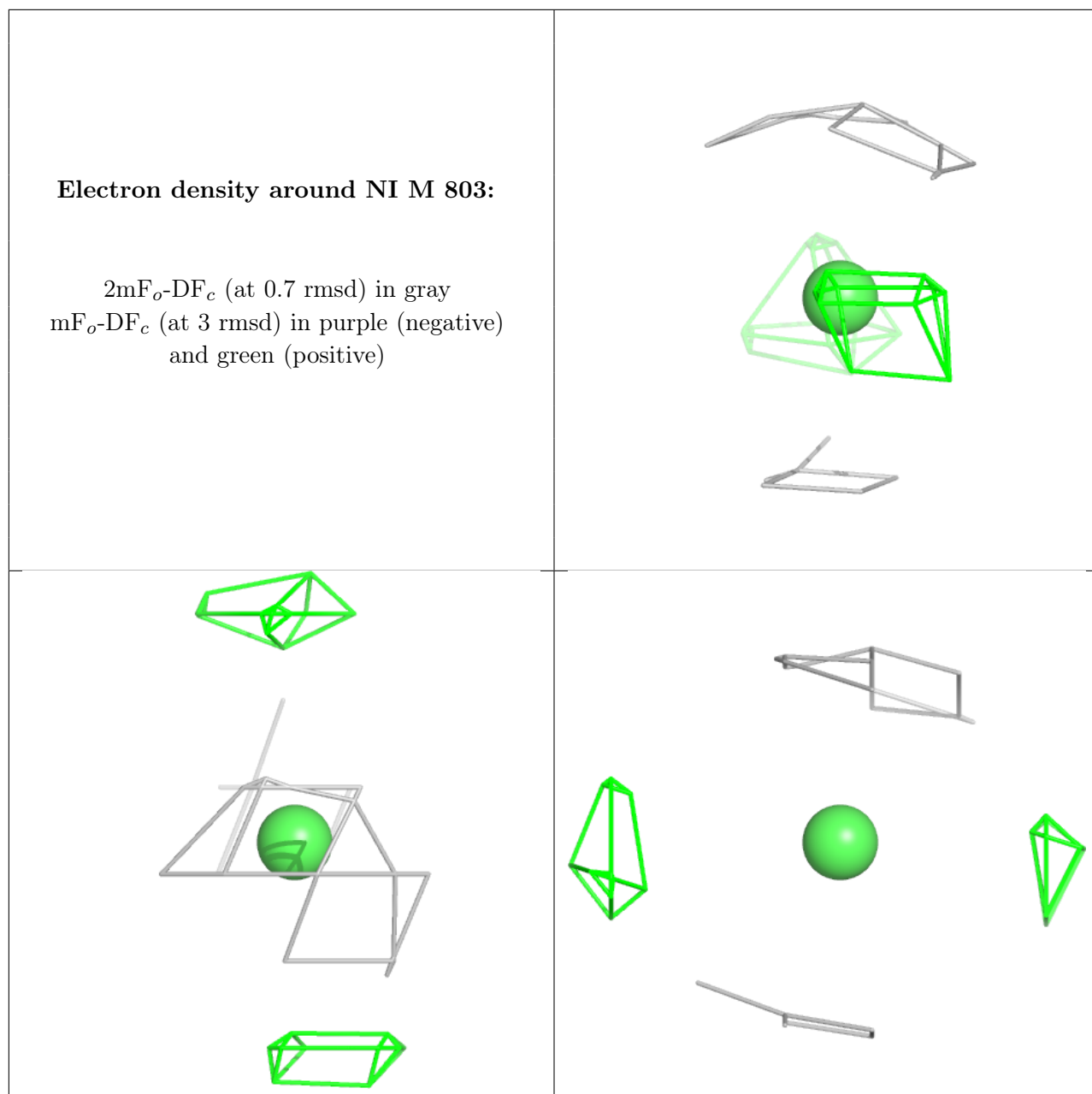
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





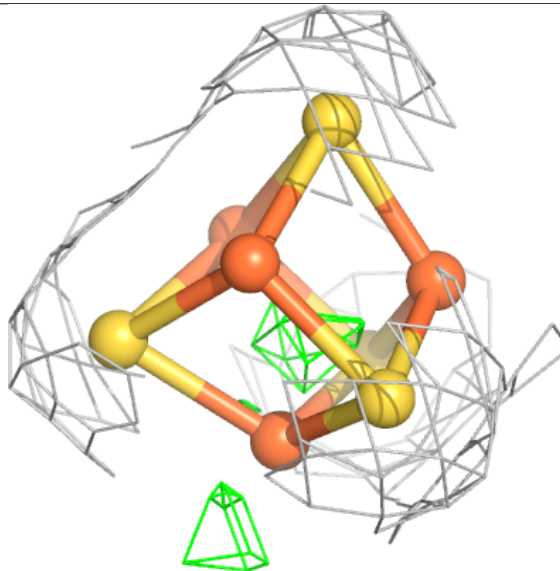
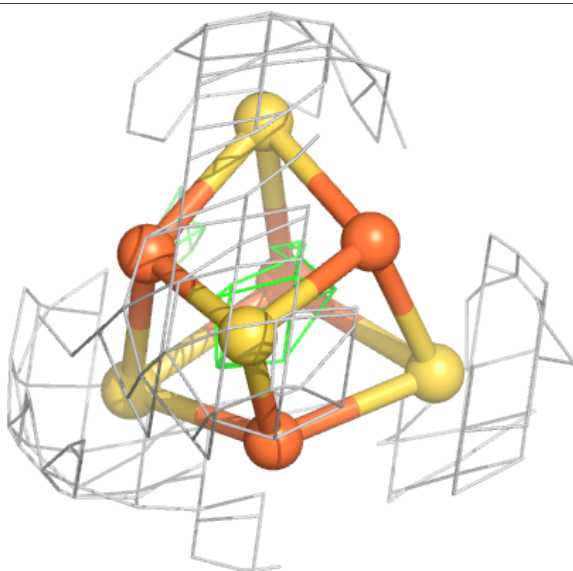
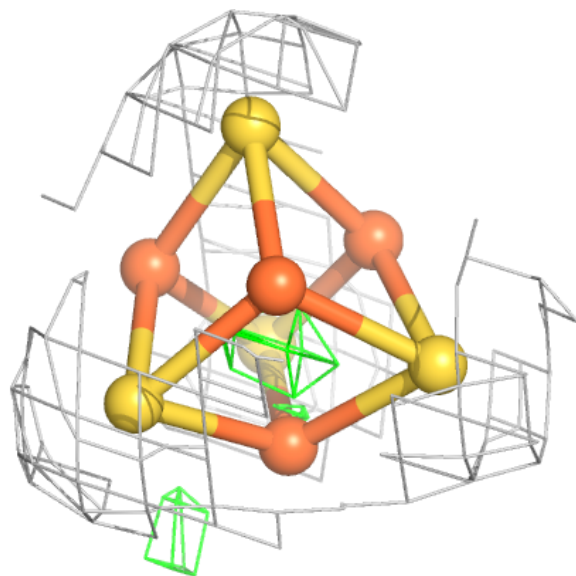
Electron density around NI M 803:

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



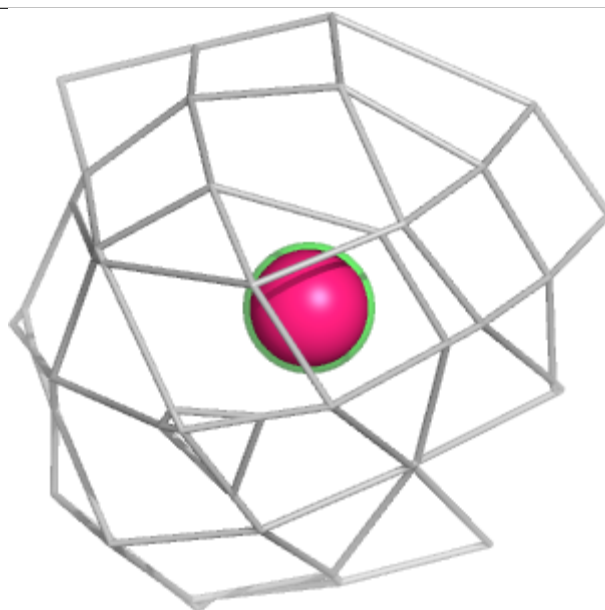
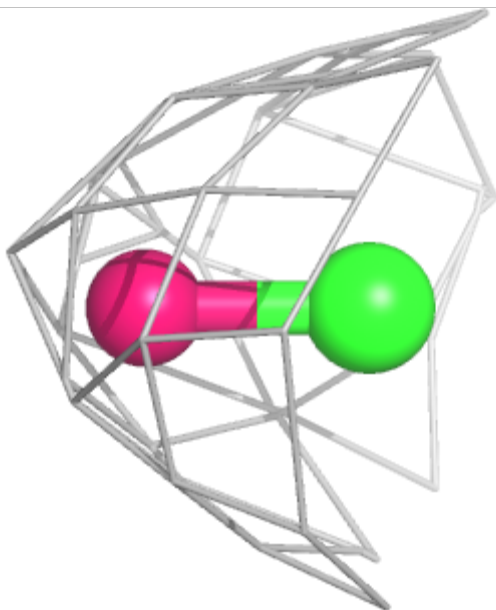
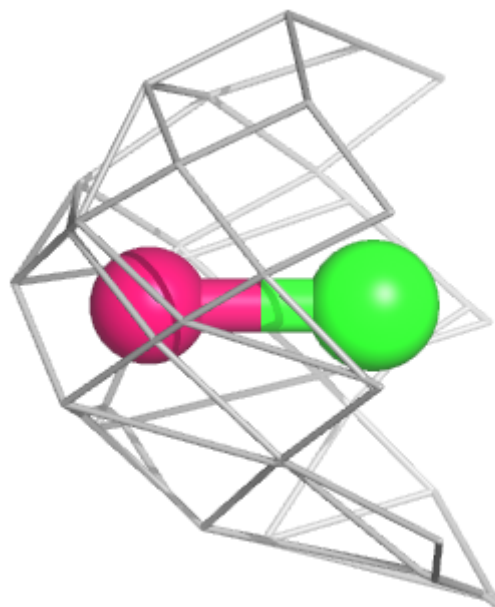
Electron density around SF4 C 702:

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



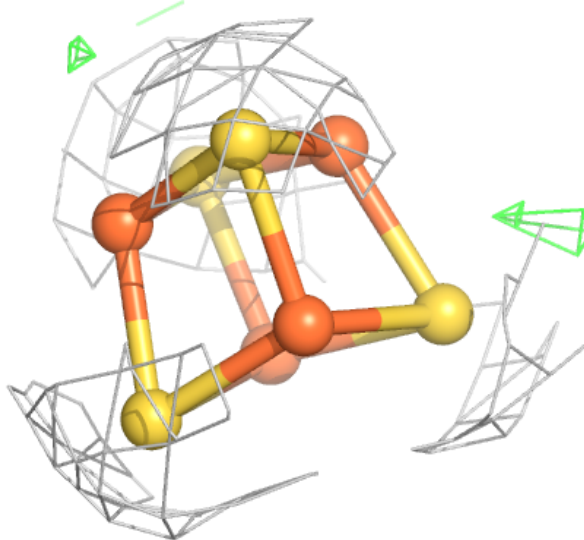
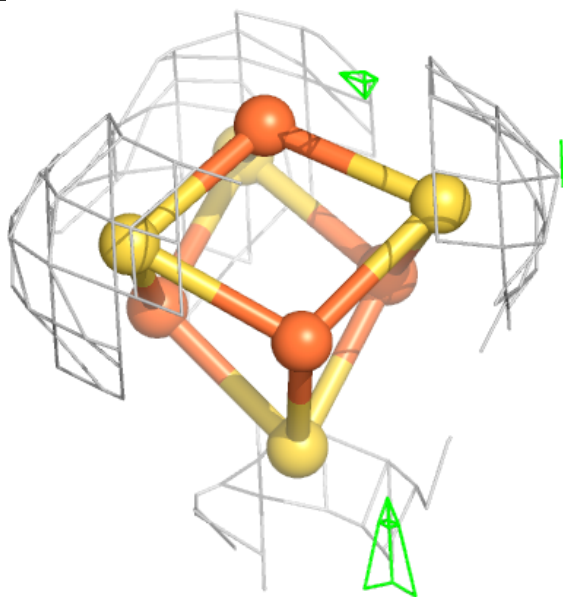
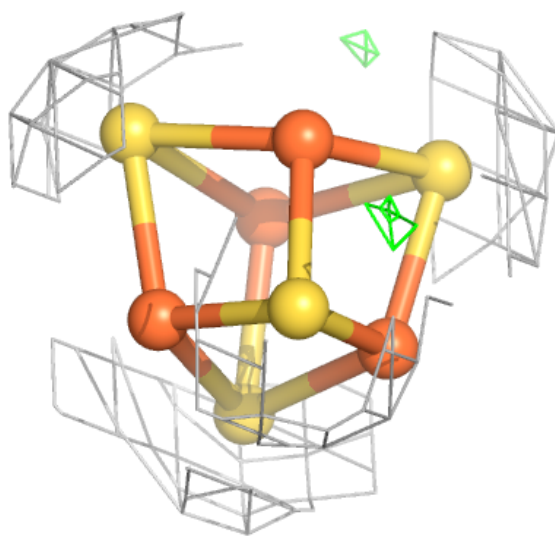
Electron density around CMO P 804:

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



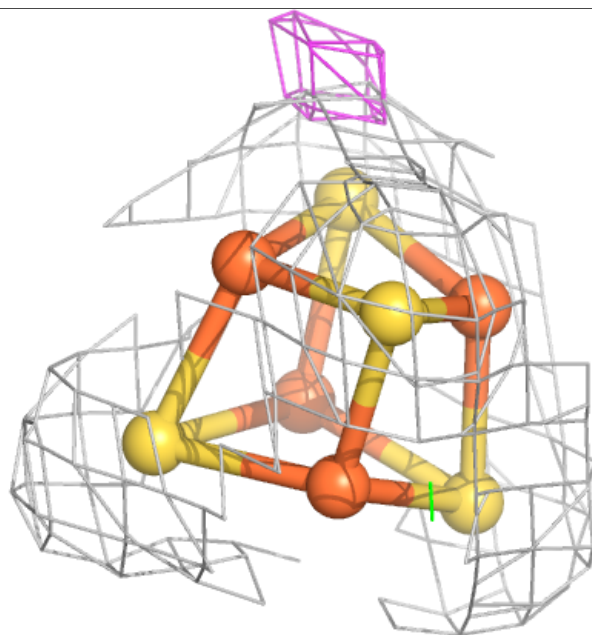
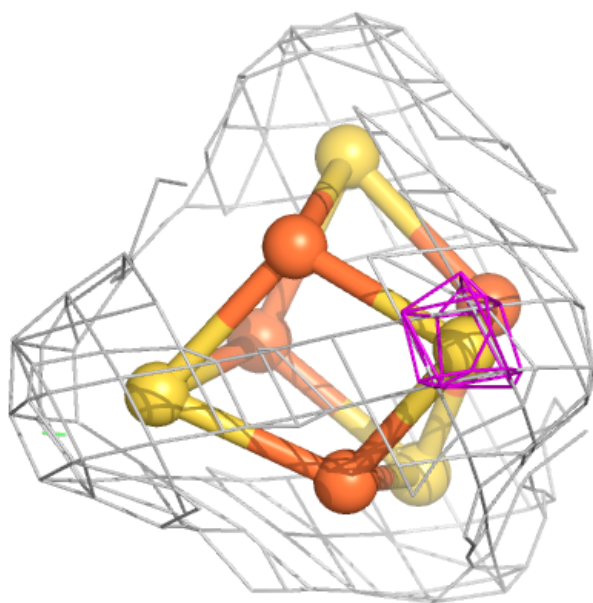
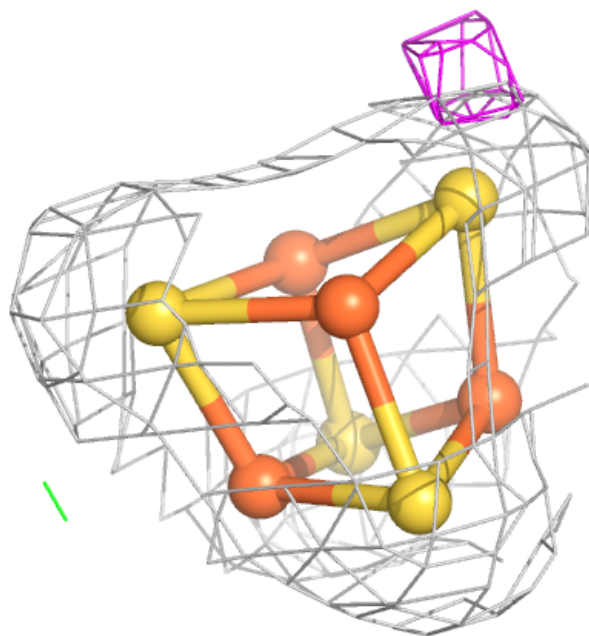
Electron density around SF4 P 801:

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



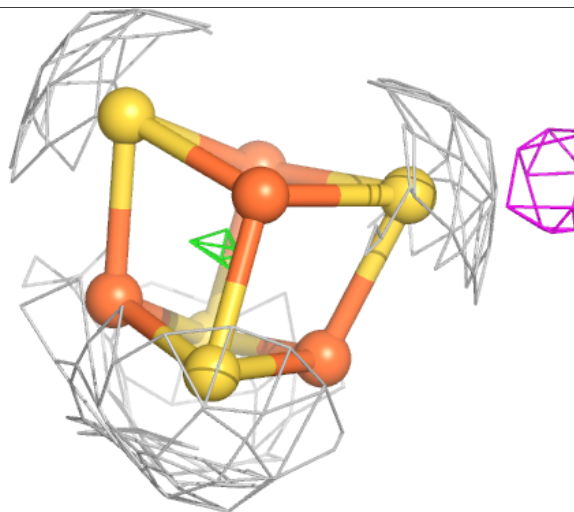
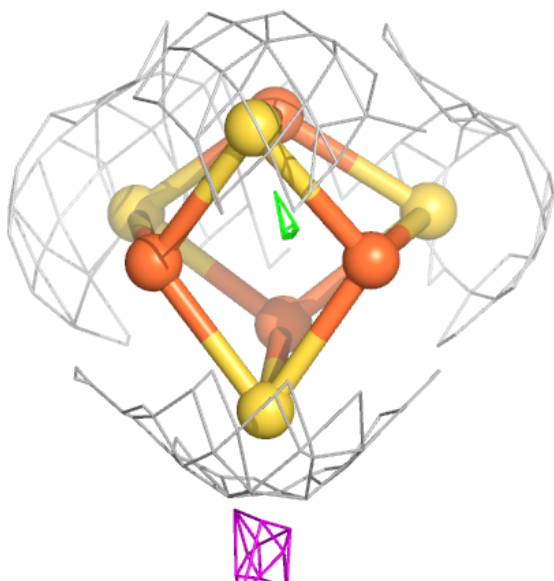
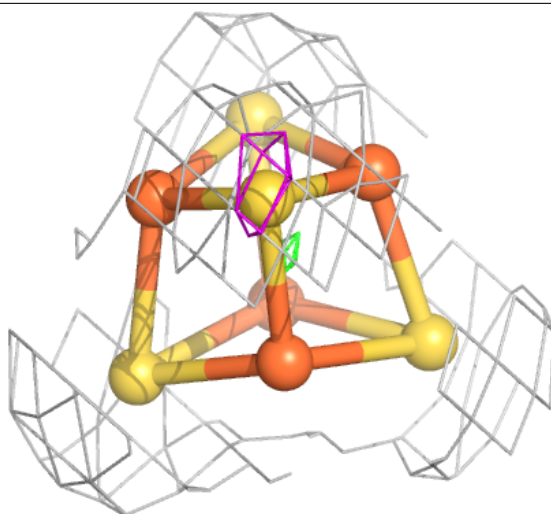
Electron density around SF4 A 701:

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



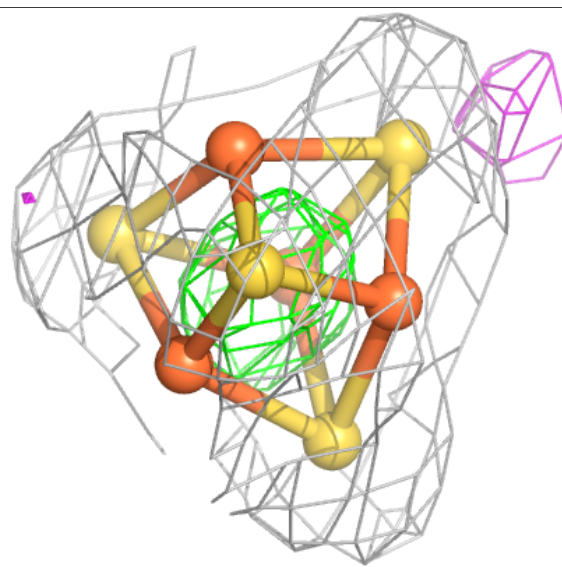
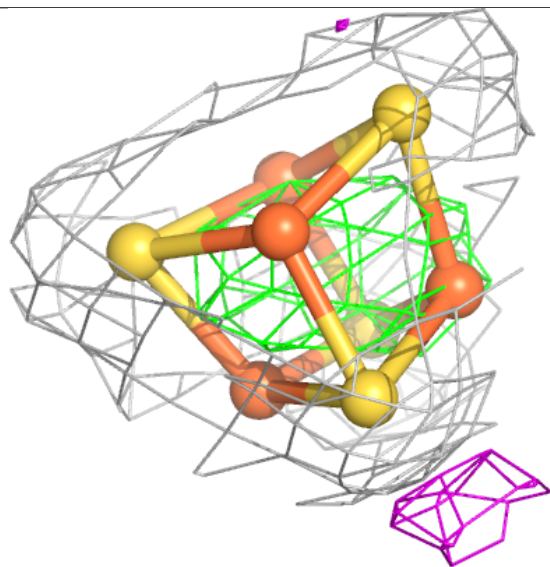
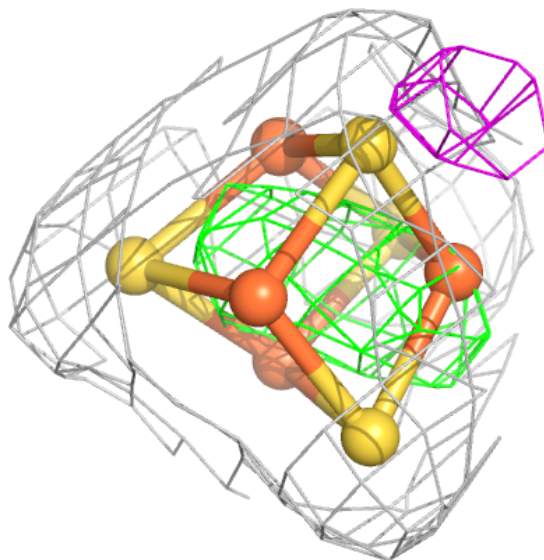
Electron density around SF4 C 701:

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



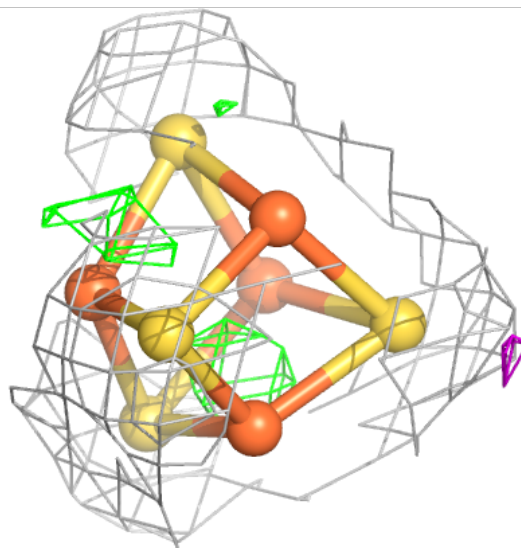
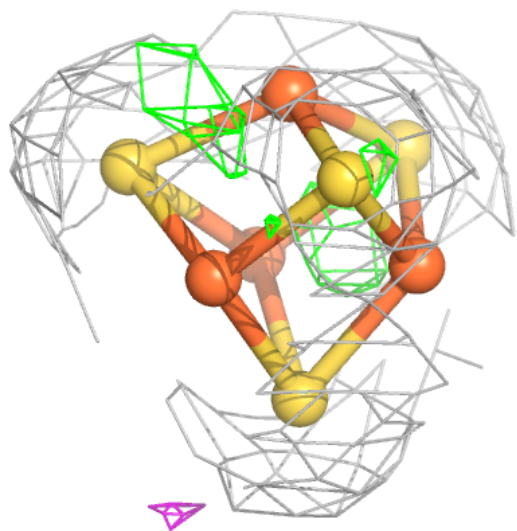
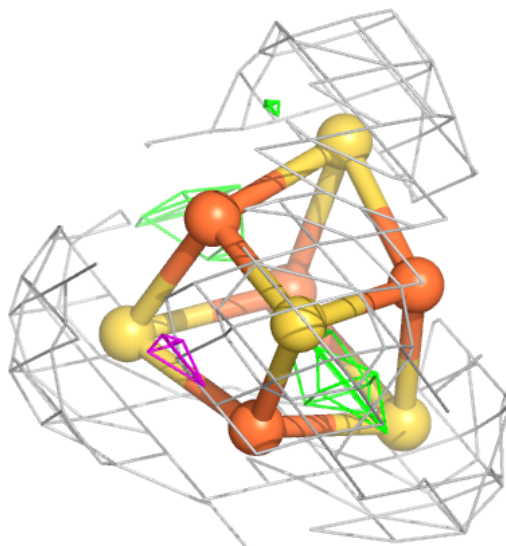
Electron density around SF4 A 702:

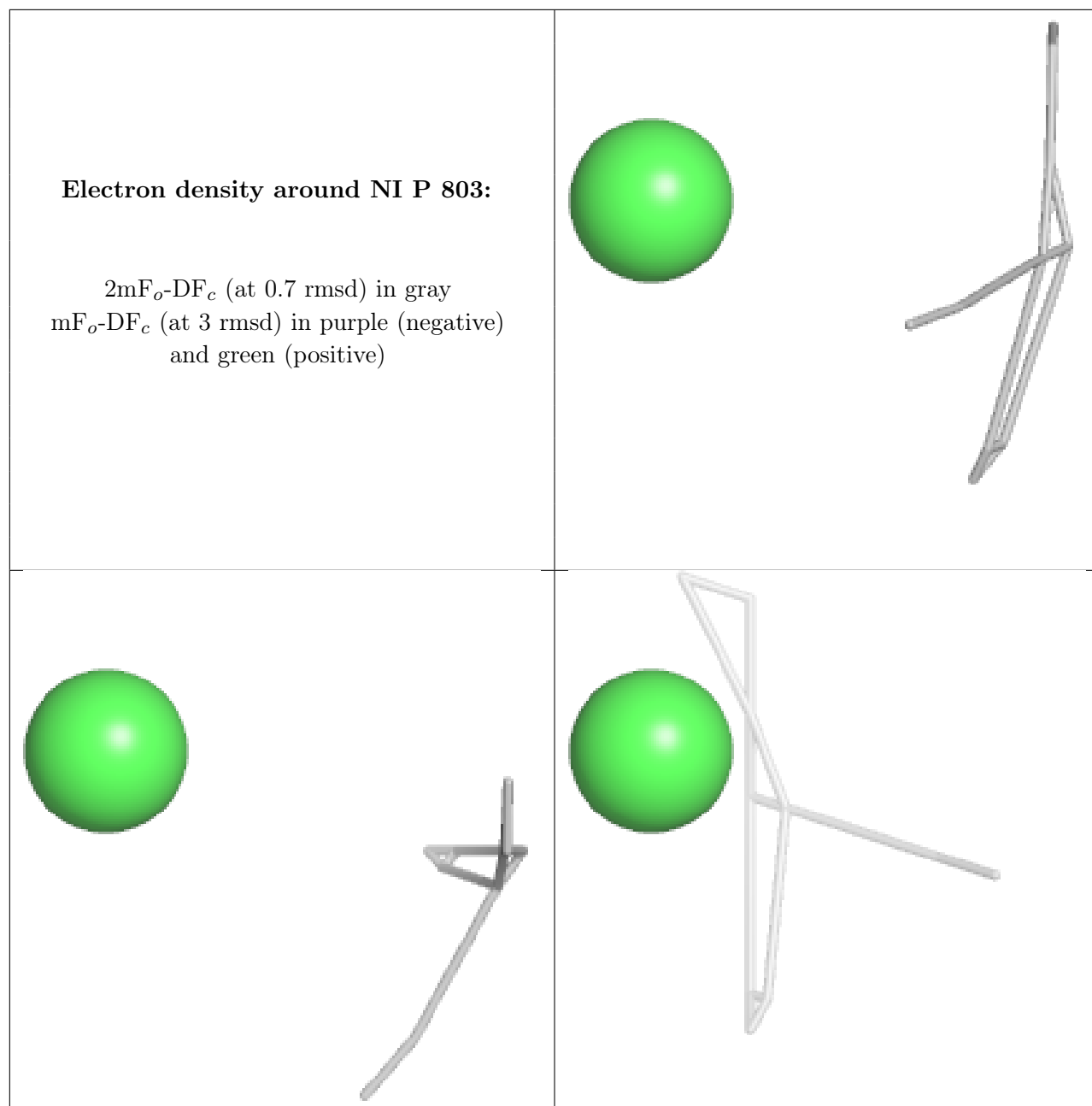
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

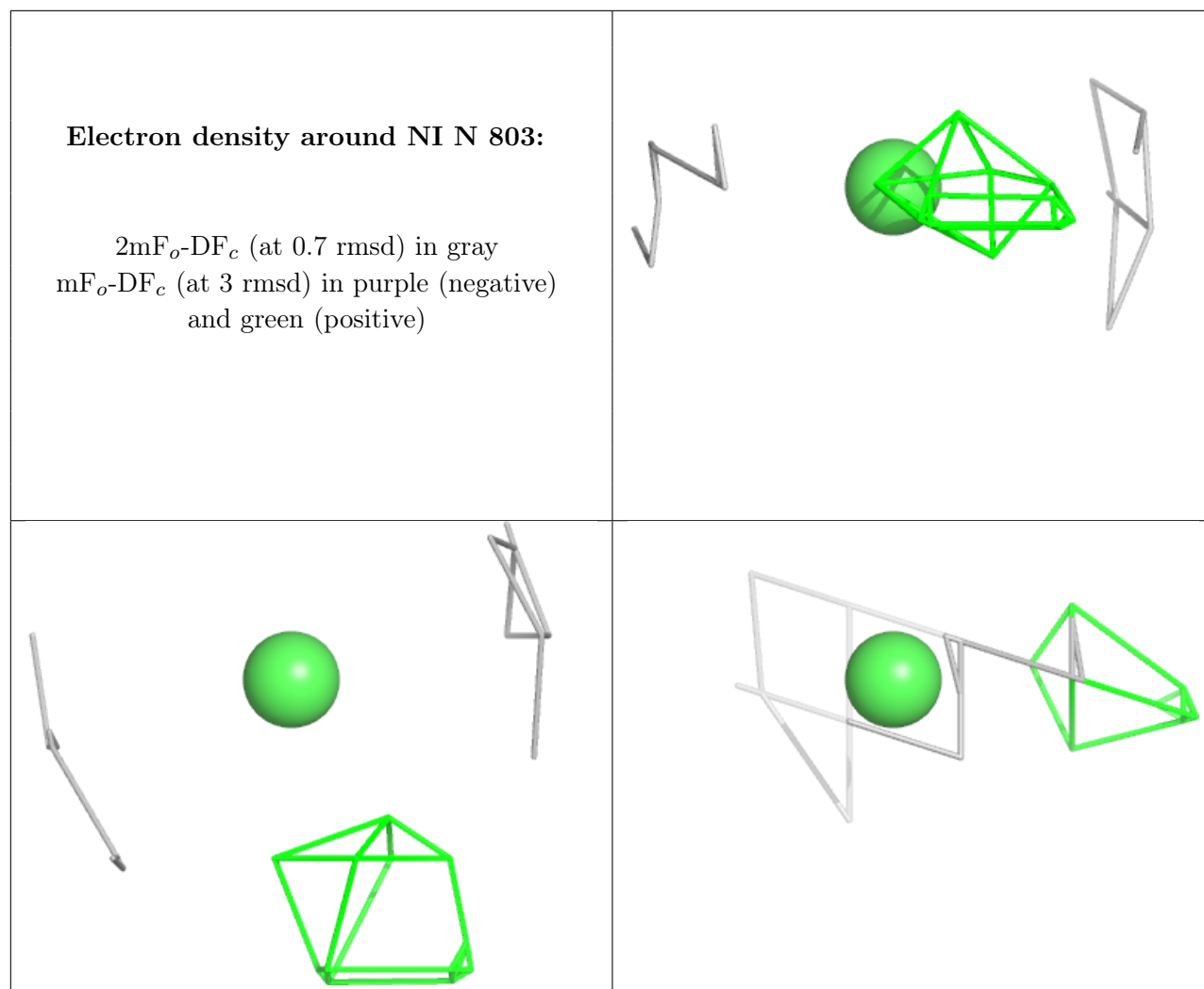


Electron density around SF4 N 801:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.