Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2020 – 08:16 AM GMT

PDB ID	:	6YTT
Title	:	CO-dehydrogenase/Acetyl-CoA synthase (CODH/ACS) from Clostridium autoethanogenum at 3.0-A resolution
Authors	:	Wagner, T.; Lemaire, O.N.
Deposited on	:	2020-04-24
Resolution	:	3.01 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:

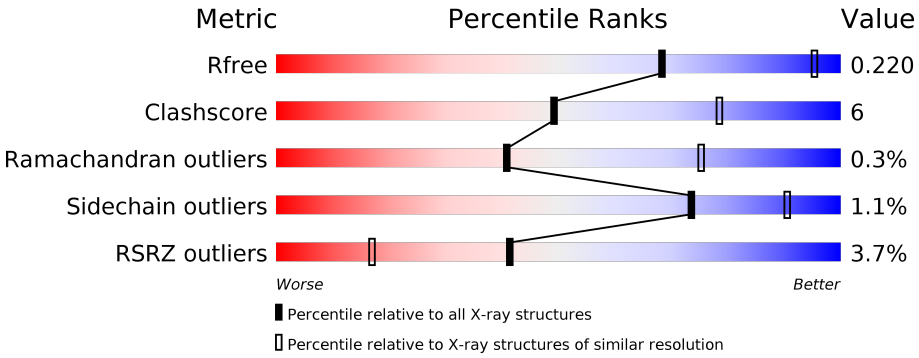
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	708	5% 77% 23%
1	D	708	8% 80% 19%
2	B	631	91% 9%
2	C	631	92% 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	705	-	-	-	X
3	GOL	B	706	-	-	-	X
3	GOL	C	1001	-	-	-	X
3	GOL	C	1003	-	-	-	X
6	F	A	806	-	-	-	X
6	F	C	1007	-	-	-	X
9	NA	B	711	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20389 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

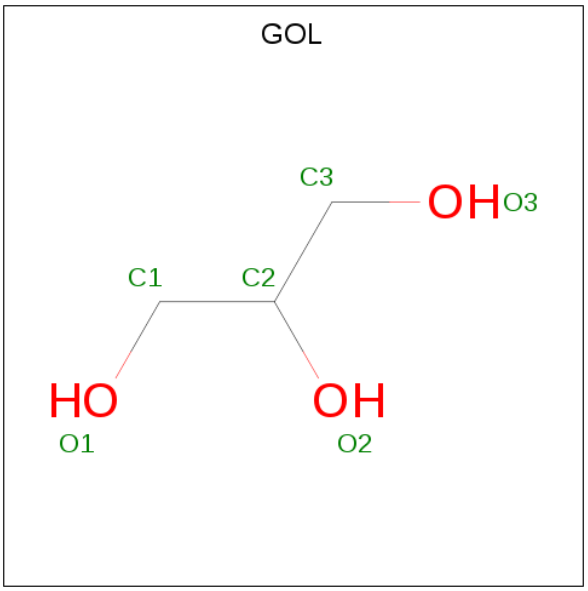
- Molecule 1 is a protein called CO dehydrogenase/acetyl-CoA synthase complex, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5392	3449	884	1023	36			
1	D	705	Total	C	N	O	S	0	0	0
			5368	3433	880	1019	36			

- Molecule 2 is a protein called Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor).

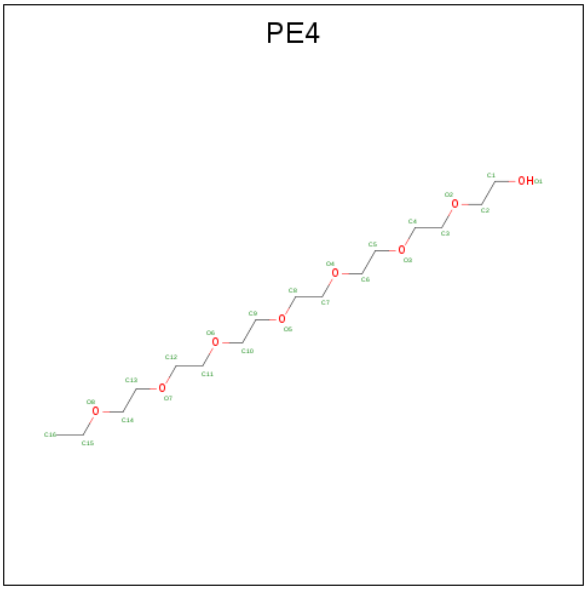
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	629	Total	C	N	O	S	0	0	0
			4723	2967	814	902	40			
2	C	630	Total	C	N	O	S	0	0	0
			4732	2972	815	905	40			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



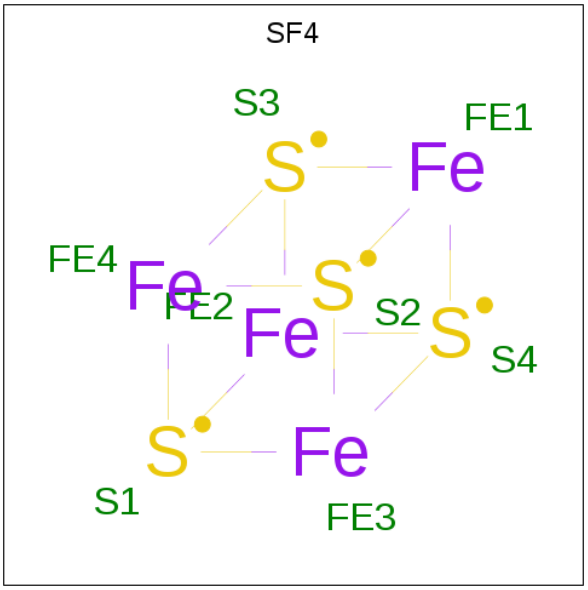
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 13 7	0	0
4	B	1	Total C O 11 8 3	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0
5	C	1	Total Fe S 8 4 4	0	0
5	D	1	Total Fe S 8 4 4	0	0

- Molecule 6 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total F 1 1	0	0
6	A	2	Total F 2 2	0	0

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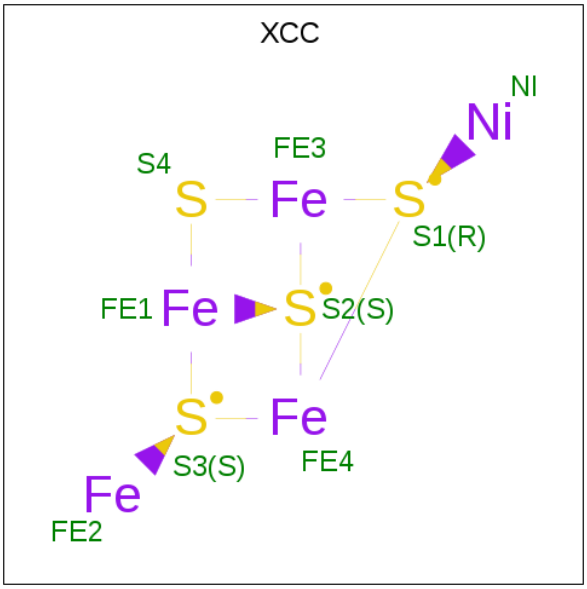
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	6	Total F 6 6	0	0

- 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	A	2	Total Ni 2 2	0	0
7	D	2	Total Ni 2 2	0	0

- Molecule 8 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by author).



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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total Na 3 3	0	0

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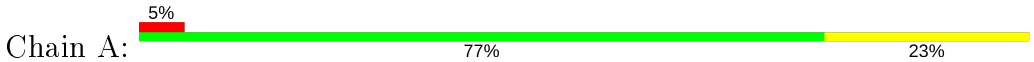
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total Na 3 3	0	0

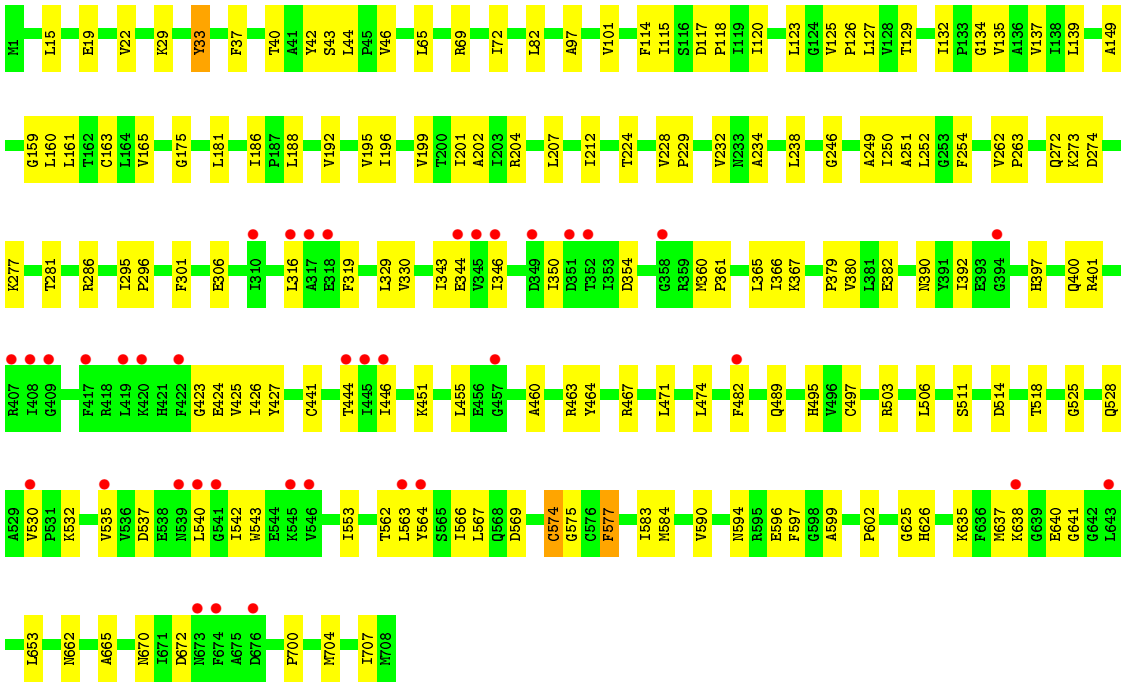
3 Residue-property plots (i)

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

- Molecule 1: CO dehydrogenase/acetyl-CoA synthase complex, beta subunit

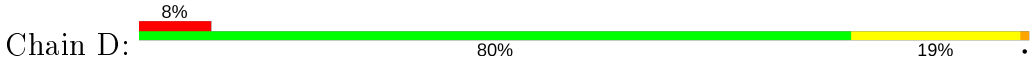
Chain A:

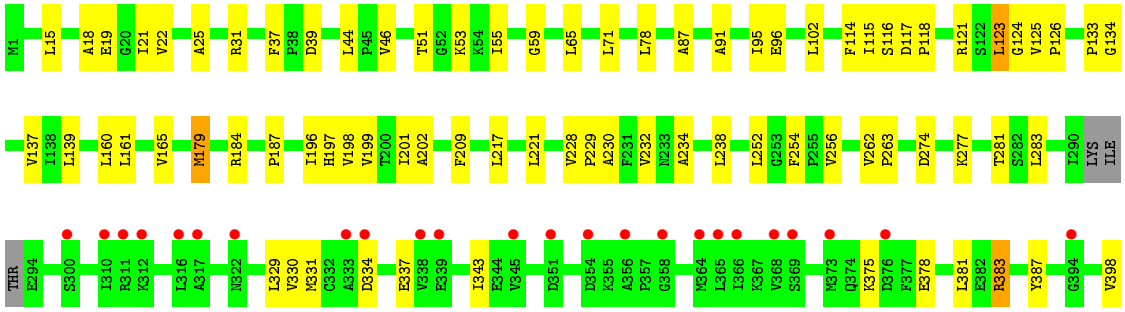


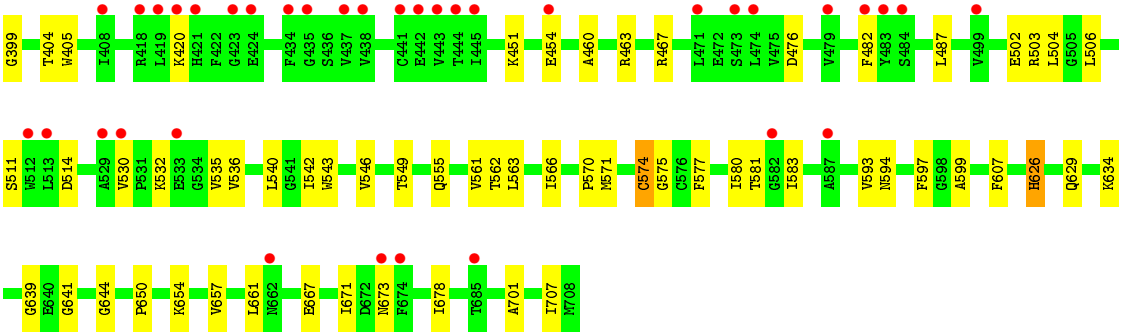


- Molecule 1: CO dehydrogenase/acetyl-CoA synthase complex, beta subunit

Chain D:

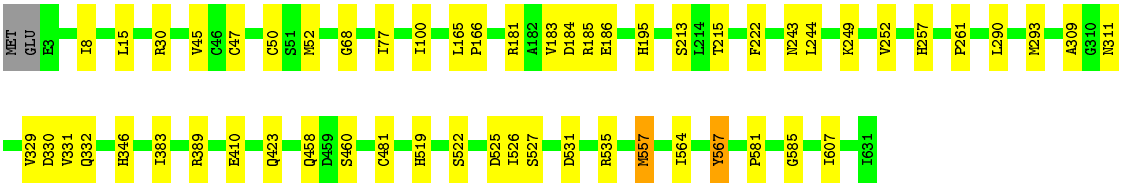






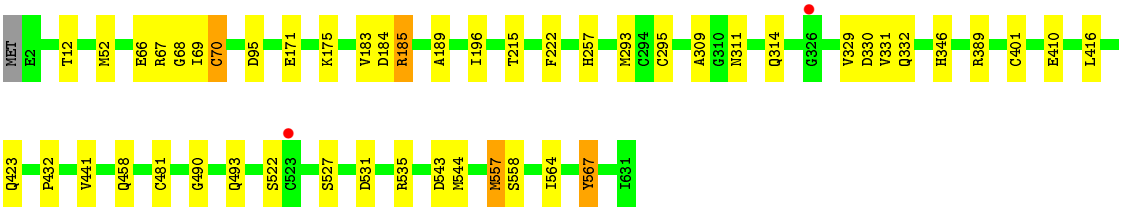
• Molecule 2: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain B:



• Molecule 2: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	298.94Å 298.94Å 128.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.01 49.15 – 3.01	Depositor EDS
% Data completeness (in resolution range)	70.4 (49.15-3.01) 70.4 (49.15-3.01)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.192 , 0.220 0.191 , 0.220	Depositor DCC
R_{free} test set	4156 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	87.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20389	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, F, PE4, NA, SF4, XCC, NI

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	0.26	0/5488	0.44	0/7428
1	D	0.25	0/5463	0.43	0/7393
2	B	0.25	0/4797	0.44	0/6488
2	C	0.25	0/4806	0.43	0/6500
All	All	0.25	0/20554	0.43	0/27809

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

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	5392	0	5492	104	0
1	D	5368	0	5460	84	0
2	B	4723	0	4813	34	0
2	C	4732	0	4818	31	0
3	A	12	0	16	1	0
3	B	30	0	40	0	0
3	C	18	0	24	0	0
3	D	6	0	8	0	0
4	A	20	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	15	1	0
5	A	8	0	0	0	0
5	B	16	0	0	1	0
5	C	8	0	0	1	0
5	D	8	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	6	0	0	0	0
7	A	2	0	0	0	0
7	D	2	0	0	0	0
8	B	9	0	0	0	0
8	C	9	0	0	0	0
9	B	3	0	0	0	0
9	C	3	0	0	0	0
All	All	20389	0	20711	242	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 6.

All (242) 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:A:281:THR:HG22	2:B:423:GLN:HB2	1.60	0.80
1:D:121:ARG:HD3	1:D:555:GLN:HB3	1.68	0.75
1:D:581:THR:HG1	1:D:626:HIS:HE2	1.36	0.72
2:B:257:HIS:HB3	2:B:329:VAL:HG12	1.73	0.69
2:B:557:MET:HG3	2:C:52:MET:HG3	1.74	0.69
2:C:423:GLN:HB2	1:D:281:THR:HG22	1.74	0.69
1:A:379:PRO:HG3	1:A:467:ARG:HD3	1.75	0.68
1:A:234:ALA:HB1	1:A:238:LEU:HD21	1.76	0.67
1:D:199:VAL:HG13	1:D:252:LEU:HD11	1.76	0.67
1:D:22:VAL:HG11	1:D:65:LEU:HD11	1.76	0.66
1:A:46:VAL:HG21	1:A:196:ILE:HD11	1.78	0.65
2:B:183:VAL:HG22	2:B:215:THR:HB	1.78	0.65
1:A:272:GLN:HE21	1:A:281:THR:HG21	1.60	0.64
1:D:44:LEU:HD12	1:D:55:ILE:HD12	1.80	0.64
1:A:365:LEU:HD21	1:A:367:LYS:HE3	1.80	0.64
1:D:657:VAL:HG12	1:D:661:LEU:HB2	1.80	0.63
2:B:330:ASP:OD1	2:B:331:VAL:N	2.30	0.63
2:C:66:GLU:HG3	2:C:67:ARG:HG3	1.83	0.60
1:A:134:GLY:O	1:A:160:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:SER:H	1:A:514:ASP:HB2	1.67	0.60
2:B:290:LEU:H	4:B:703:PE4:H132	1.67	0.60
1:D:234:ALA:HB1	1:D:238:LEU:HD21	1.83	0.59
1:A:662:ASN:ND2	1:A:672:ASP:O	2.36	0.58
2:B:52:MET:HG3	2:C:557:MET:HG3	1.85	0.58
2:C:401:CYS:SG	2:C:490:GLY:HA2	2.42	0.58
1:A:583:ILE:HA	1:A:590:VAL:HG12	1.85	0.57
1:A:495:HIS:HE2	1:A:497:CYS:HG	1.50	0.57
1:A:506:LEU:HD11	1:A:574:CYS:SG	2.44	0.57
1:D:378:GLU:OE1	1:D:467:ARG:NH2	2.38	0.57
1:D:398:VAL:HG23	1:D:405:TRP:HB3	1.86	0.57
1:A:274:ASP:HB3	1:A:277:LYS:HG2	1.87	0.57
2:B:213:SER:HB2	2:B:567:TYR:HB3	1.88	0.56
1:A:22:VAL:HG11	1:A:65:LEU:HD11	1.88	0.56
1:D:262:VAL:HG22	1:D:263:PRO:HD2	1.87	0.56
1:D:123:LEU:HD11	1:D:161:LEU:HD22	1.88	0.56
1:D:21:ILE:HG21	1:D:95:ILE:HG23	1.87	0.56
1:D:329:LEU:HD22	1:D:460:ALA:HA	1.88	0.55
1:D:561:VAL:HG11	1:D:571:MET:HG3	1.87	0.55
1:A:535:VAL:HB	1:A:543:TRP:CZ3	2.42	0.55
1:A:346:ILE:HG21	1:A:451:LYS:HD3	1.90	0.54
1:D:31:ARG:O	1:D:59:GLY:N	2.39	0.54
1:D:274:ASP:HB3	1:D:277:LYS:HG2	1.90	0.54
2:C:311:ASN:HB2	2:C:481:CYS:SG	2.47	0.54
2:C:401:CYS:SG	2:C:493:GLN:NE2	2.81	0.54
1:D:46:VAL:HG21	1:D:196:ILE:HD11	1.90	0.54
1:D:134:GLY:HA2	1:D:229:PRO:HG2	1.91	0.53
2:B:249:LYS:O	2:B:389:ARG:NH1	2.42	0.53
1:D:124:GLY:HA3	1:D:209:PHE:CZ	2.43	0.53
1:A:181:LEU:HD12	1:A:186:ILE:HD11	1.91	0.53
1:A:380:VAL:HG13	1:A:518:THR:HG22	1.90	0.53
1:A:471:LEU:HD11	1:A:511:SER:HB2	1.90	0.53
1:D:330:VAL:HG11	1:D:381:LEU:HB2	1.91	0.53
1:D:37:PHE:HD2	1:D:114:PHE:CG	2.27	0.52
1:A:161:LEU:HD11	1:A:186:ILE:HD12	1.91	0.52
2:B:311:ASN:HB2	2:B:481:CYS:SG	2.49	0.52
1:D:334:ASP:HB2	1:D:337:GLU:HG2	1.90	0.52
1:A:316:LEU:HD12	1:A:350:ILE:HD11	1.91	0.52
2:C:257:HIS:HB3	2:C:329:VAL:HG12	1.92	0.52
1:A:542:ILE:HG12	1:A:562:THR:HG22	1.91	0.52
2:B:257:HIS:O	2:B:329:VAL:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:LYS:NZ	1:D:667:GLU:OE1	2.34	0.52
1:A:594:ASN:HD22	1:A:653:LEU:HG	1.75	0.52
1:D:96:GLU:HG2	1:D:197:HIS:NE2	2.24	0.51
1:A:330:VAL:HB	1:A:382:GLU:HG3	1.93	0.51
1:D:91:ALA:O	1:D:95:ILE:HG13	2.11	0.51
2:B:581:PRO:HD2	2:B:607:ILE:HD13	1.93	0.51
2:B:30:ARG:HD2	2:C:68:GLY:O	2.11	0.51
1:D:343:ILE:HD13	1:D:420:LYS:HG3	1.92	0.51
1:D:503:ARG:NH1	1:D:563:LEU:O	2.43	0.51
2:C:410:GLU:OE2	2:C:410:GLU:N	2.38	0.51
1:D:134:GLY:O	1:D:160:LEU:HB2	2.10	0.51
1:A:43:SER:OG	1:A:44:LEU:N	2.43	0.51
2:B:252:VAL:HG11	2:B:383:ILE:HA	1.93	0.51
1:D:671:ILE:HG22	1:D:673:ASN:H	1.75	0.51
2:C:295:CYS:SG	2:C:522:SER:HB2	2.50	0.50
1:D:644:GLY:O	1:D:701:ALA:HB2	2.10	0.50
2:B:410:GLU:OE2	2:B:410:GLU:N	2.37	0.50
1:D:543:TRP:HB2	1:D:546:VAL:HB	1.92	0.50
1:A:495:HIS:CE1	1:A:497:CYS:HG	2.29	0.50
1:D:25:ALA:HA	1:D:102:LEU:HD21	1.93	0.50
1:D:121:ARG:HB3	1:D:555:GLN:HG3	1.93	0.50
1:D:506:LEU:HD11	1:D:574:CYS:SG	2.52	0.50
1:D:15:LEU:O	1:D:19:GLU:HG3	2.11	0.50
1:A:344:GLU:HB3	1:A:444:THR:HG23	1.93	0.50
1:A:125:VAL:HG13	1:A:126:PRO:HD3	1.92	0.50
1:A:163:CYS:HB3	1:A:188:LEU:HD21	1.93	0.50
1:A:15:LEU:O	1:A:19:GLU:HG3	2.12	0.49
1:A:199:VAL:HG13	1:A:252:LEU:HD11	1.95	0.49
1:D:597:PHE:CZ	1:D:599:ALA:HB3	2.47	0.49
1:D:583:ILE:HD11	1:D:707:ILE:HG21	1.94	0.49
1:A:69:ARG:O	1:A:72:ILE:HG22	2.12	0.48
2:B:15:LEU:HD12	2:B:244:LEU:HD13	1.95	0.48
2:C:257:HIS:O	2:C:329:VAL:HA	2.13	0.48
1:D:504:LEU:HD23	1:D:511:SER:HA	1.95	0.48
1:A:366:ILE:HD11	1:A:426:ILE:HD13	1.96	0.48
1:A:277:LYS:O	1:A:281:THR:HG23	2.13	0.48
1:A:503:ARG:NH1	1:A:563:LEU:O	2.46	0.48
1:A:295:ILE:HD13	1:A:301:PHE:HB3	1.95	0.48
1:A:665:ALA:HB1	1:A:670:ASN:HB2	1.95	0.48
1:D:530:VAL:HG22	1:D:549:THR:HG21	1.96	0.48
1:A:97:ALA:O	1:A:101:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:ILE:HA	2:B:567:TYR:CE2	2.49	0.48
1:D:542:ILE:HG12	1:D:562:THR:HG22	1.95	0.48
1:A:427:TYR:CD1	1:A:441:CYS:HB2	2.49	0.47
2:C:293:MET:HG2	2:C:309:ALA:HB3	1.96	0.47
1:D:179:MET:HG2	1:D:187:PRO:HD3	1.96	0.47
1:D:37:PHE:HB3	1:D:114:PHE:CE2	2.49	0.47
1:D:383:ARG:HE	1:D:383:ARG:HA	1.80	0.47
2:C:564:ILE:HA	2:C:567:TYR:CE2	2.49	0.47
1:D:202:ALA:HB1	1:D:228:VAL:HG11	1.96	0.47
1:D:230:ALA:HB3	1:D:254:PHE:CD1	2.49	0.47
1:D:535:VAL:HB	1:D:543:TRP:CZ3	2.50	0.47
1:A:149:ALA:HB2	1:A:175:GLY:HA3	1.95	0.47
1:A:566:ILE:HD13	1:A:637:MET:HE3	1.95	0.47
1:A:192:VAL:O	1:A:195:VAL:HG22	2.14	0.47
1:A:390:ASN:ND2	1:A:397:HIS:O	2.45	0.47
1:A:137:VAL:O	1:A:232:VAL:HA	2.15	0.47
1:D:161:LEU:HA	1:D:184:ARG:HB3	1.96	0.47
1:D:18:ALA:HA	1:D:95:ILE:HG12	1.95	0.47
1:A:132:ILE:HG22	1:A:159:GLY:O	2.14	0.47
1:D:671:ILE:H	1:D:671:ILE:HD12	1.79	0.47
1:A:139:LEU:HB2	1:A:165:VAL:HG13	1.97	0.47
1:A:273:LYS:HG3	3:A:802:GOL:H12	1.95	0.46
1:D:125:VAL:HG13	1:D:126:PRO:HD3	1.97	0.46
1:A:115:ILE:O	1:A:204:ARG:NH1	2.39	0.46
1:D:277:LYS:O	1:D:281:THR:HG23	2.16	0.46
2:C:531:ASP:O	2:C:535:ARG:HG3	2.16	0.46
2:C:346:HIS:CE1	2:C:389:ARG:HD3	2.51	0.46
1:A:354:ASP:N	1:A:354:ASP:OD1	2.49	0.46
1:D:594:ASN:ND2	1:D:650:PRO:HG2	2.31	0.46
2:C:423:GLN:HB3	1:D:277:LYS:HE2	1.97	0.45
2:B:30:ARG:HB3	2:C:69:ILE:HA	1.99	0.45
1:D:482:PHE:O	1:D:530:VAL:N	2.46	0.45
1:A:597:PHE:CZ	1:A:599:ALA:HB3	2.52	0.45
1:D:566:ILE:HA	1:D:570:PRO:HB3	1.98	0.45
2:B:526:ILE:HD12	2:B:564:ILE:HD13	1.99	0.45
1:D:536:VAL:HG23	1:D:542:ILE:HB	1.99	0.45
2:B:222:PHE:CD2	2:B:527:SER:HB2	2.52	0.45
1:D:375:LYS:HD3	1:D:463:ARG:HH22	1.81	0.45
1:A:125:VAL:O	1:A:129:THR:HG23	2.16	0.45
1:A:29:LYS:HB3	1:A:33:TYR:CD2	2.51	0.45
2:C:12:THR:OG1	2:C:314:GLN:NE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLY:O	1:A:528:GLN:NE2	2.47	0.45
1:A:562:THR:HG23	1:A:569:ASP:HB2	1.99	0.45
1:A:82:LEU:HD12	1:A:251:ALA:HA	1.99	0.44
1:A:224:THR:HA	1:A:228:VAL:HG12	1.99	0.44
1:A:319:PHE:CE2	1:A:360:MET:HB2	2.52	0.44
1:D:593:VAL:HG23	1:D:597:PHE:HD2	1.82	0.44
1:A:495:HIS:NE2	1:A:497:CYS:SG	2.82	0.44
1:A:594:ASN:OD1	1:A:596:GLU:HG2	2.17	0.44
1:D:540:LEU:HD23	1:D:639:GLY:HA3	2.00	0.44
1:A:246:GLY:O	1:A:250:ILE:HG12	2.17	0.44
2:B:346:HIS:CE1	2:B:389:ARG:HG3	2.53	0.44
1:A:584:MET:HE1	1:A:602:PRO:HB2	1.99	0.44
1:D:399:GLY:HA3	1:D:404:THR:HA	2.00	0.44
1:A:329:LEU:HD22	1:A:460:ALA:HA	2.00	0.44
1:A:700:PRO:O	1:A:704:MET:HG3	2.18	0.44
2:B:100:ILE:HD11	2:B:261:PRO:HD2	2.00	0.44
2:B:68:GLY:HA3	5:B:708:SF4:S4	2.58	0.44
2:C:70:CYS:HB3	5:C:1004:SF4:S4	2.58	0.44
1:A:286:ARG:NH1	4:A:803:PE4:O1	2.50	0.44
1:D:115:ILE:HG13	1:D:201:ILE:HD11	2.00	0.44
1:A:567:LEU:HD11	1:A:707:ILE:HG22	2.00	0.43
1:A:37:PHE:HB3	1:A:114:PHE:CE2	2.53	0.43
1:D:511:SER:H	1:D:514:ASP:HB2	1.84	0.43
1:A:635:LYS:HD3	1:A:638:LYS:HD2	1.99	0.43
2:B:181:ARG:NE	2:B:186:GLU:OE2	2.36	0.43
1:A:343:ILE:HD12	1:A:423:GLY:HA3	1.99	0.43
1:A:427:TYR:HD1	1:A:441:CYS:HB2	1.83	0.43
1:A:537:ASP:OD2	1:A:540:LEU:HB2	2.18	0.43
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.84	0.43
1:A:139:LEU:CB	1:A:165:VAL:HG13	2.48	0.43
1:A:295:ILE:HG13	1:A:295:ILE:O	2.18	0.43
1:A:115:ILE:HG13	1:A:201:ILE:HD11	1.99	0.43
2:B:165:LEU:HD12	2:B:166:PRO:HD2	1.99	0.43
2:C:543:ASP:OD1	2:C:544:MET:N	2.44	0.43
1:D:232:VAL:HG13	1:D:256:VAL:HG13	2.01	0.43
1:D:654:LYS:HE3	1:D:678:ILE:HG22	2.01	0.43
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.87	0.43
1:A:489:GLN:HE22	1:A:553:ILE:HG22	1.84	0.43
1:A:564:TYR:CD1	1:A:635:LYS:HB3	2.53	0.43
1:A:135:VAL:HA	1:A:161:LEU:O	2.19	0.42
1:A:401:ARG:HD3	1:A:464:TYR:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLN:HG3	1:A:401:ARG:H	1.84	0.42
2:C:416:LEU:HD22	2:C:432:PRO:HB2	2.01	0.42
1:A:360:MET:HE3	1:A:361:PRO:HD2	2.01	0.42
1:D:580:ILE:HG13	1:D:607:PHE:CE1	2.54	0.42
1:A:228:VAL:HA	1:A:229:PRO:HD3	1.89	0.42
1:A:262:VAL:HG22	1:A:263:PRO:HD2	2.00	0.42
1:A:532:LYS:HE3	1:A:543:TRP:CH2	2.54	0.42
1:A:350:ILE:HD12	1:A:350:ILE:HA	1.88	0.42
1:A:482:PHE:CZ	1:A:532:LYS:HD2	2.55	0.42
1:A:463:ARG:O	1:A:467:ARG:HB2	2.19	0.42
1:A:117:ASP:N	1:A:118:PRO:HD2	2.34	0.42
1:A:202:ALA:HB1	1:A:224:THR:HG22	2.02	0.42
1:A:577:PHE:CD2	1:A:625:GLY:HA3	2.55	0.42
2:C:222:PHE:CD2	2:C:527:SER:HB2	2.55	0.42
1:D:532:LYS:HE3	1:D:543:TRP:CH2	2.55	0.42
1:D:51:THR:HB	1:D:53:LYS:HG2	2.01	0.42
1:D:137:VAL:HG22	1:D:198:VAL:HG11	2.01	0.42
1:D:504:LEU:HD13	1:D:629:GLN:HB2	2.01	0.42
2:B:293:MET:HG2	2:B:309:ALA:HB3	2.01	0.41
1:D:160:LEU:HD21	1:D:283:LEU:HD21	2.02	0.41
1:A:249:ALA:HB1	1:A:254:PHE:HB2	2.01	0.41
2:B:195:HIS:CE1	2:C:558:SER:HB2	2.55	0.41
1:D:476:ASP:OD2	1:D:502:GLU:HB2	2.20	0.41
1:D:657:VAL:O	1:D:657:VAL:HG12	2.20	0.41
2:B:184:ASP:HB3	2:C:184:ASP:HB3	2.02	0.41
1:A:202:ALA:HB1	1:A:228:VAL:HG11	2.02	0.41
2:C:185:ARG:NH2	2:C:189:ALA:HB2	2.35	0.41
2:C:441:VAL:HG22	1:D:78:LEU:HD13	2.03	0.41
1:D:139:LEU:HB2	1:D:165:VAL:HG13	2.02	0.41
1:D:39:ASP:HB2	1:D:116:SER:HB3	2.02	0.41
1:A:123:LEU:HD21	1:A:161:LEU:HD22	2.03	0.41
1:A:296:PRO:HG2	1:A:424:GLU:HB3	2.02	0.41
2:B:8:ILE:HD13	2:B:460:SER:HA	2.02	0.41
1:A:590:VAL:HG11	1:A:637:MET:HE3	2.02	0.41
1:D:506:LEU:HB2	1:D:626:HIS:HA	2.03	0.41
1:D:71:LEU:HB3	1:D:87:ALA:HB2	2.02	0.41
1:A:446:ILE:CD1	1:A:455:LEU:HD12	2.51	0.41
1:D:387:TYR:OH	1:D:487:LEU:HB3	2.20	0.41
1:A:329:LEU:HA	1:A:382:GLU:OE1	2.21	0.41
1:A:482:PHE:O	1:A:530:VAL:N	2.52	0.41
2:B:522:SER:O	2:B:525:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:MET:SD	2:C:196:ILE:HD13	2.61	0.41
1:A:120:ILE:CD1	1:A:201:ILE:HD13	2.51	0.41
1:A:40:THR:HG22	1:A:42:TYR:H	1.86	0.41
2:B:531:ASP:O	2:B:535:ARG:HG3	2.19	0.41
1:D:230:ALA:HB3	1:D:254:PHE:CE1	2.56	0.41
1:A:392:ILE:HD11	1:A:425:VAL:HG21	2.03	0.40
1:A:566:ILE:HD13	1:A:637:MET:CE	2.50	0.40
2:B:45:VAL:HG13	2:B:585:GLY:HA3	2.03	0.40
2:B:47:CYS:HB2	2:B:77:ILE:HG23	2.03	0.40
2:C:183:VAL:HG22	2:C:215:THR:HB	2.01	0.40
1:D:117:ASP:N	1:D:118:PRO:HD2	2.36	0.40
1:D:133:PRO:HD2	1:D:160:LEU:HB3	2.03	0.40
1:D:451:LYS:HA	1:D:454:GLU:HB3	2.03	0.40
1:A:207:LEU:HA	1:A:212:ILE:HD12	2.03	0.40
2:C:330:ASP:OD1	2:C:331:VAL:N	2.47	0.40
1:D:217:LEU:O	1:D:221:LEU:HG	2.22	0.40
1:A:127:LEU:HG	1:A:132:ILE:HD11	2.03	0.40
2:C:171:GLU:OE2	2:C:175:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	706/708 (100%)	680 (96%)	24 (3%)	2 (0%)	41	75
1	D	701/708 (99%)	674 (96%)	25 (4%)	2 (0%)	41	75
2	B	627/631 (99%)	592 (94%)	33 (5%)	2 (0%)	41	75
2	C	628/631 (100%)	593 (94%)	34 (5%)	1 (0%)	47	81
All	All	2662/2678 (99%)	2539 (95%)	116 (4%)	7 (0%)	41	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	ASN
2	B	332	GLN
1	D	575	GLY
2	C	332	GLN
1	A	575	GLY
1	A	641	GLY
1	D	641	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/583 (100%)	577 (99%)	6 (1%)	76	91
1	D	580/583 (100%)	573 (99%)	7 (1%)	71	89
2	B	518/520 (100%)	512 (99%)	6 (1%)	71	89
2	C	519/520 (100%)	513 (99%)	6 (1%)	71	89
All	All	2200/2206 (100%)	2175 (99%)	25 (1%)	73	90

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	306	GLU
1	A	574	CYS
1	A	577	PHE
1	A	626	HIS
1	A	640	GLU
2	B	50	CYS
2	B	185	ARG
2	B	458	GLN
2	B	519	HIS
2	B	557	MET
2	B	567	TYR
2	C	70	CYS
2	C	95	ASP
2	C	185	ARG

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Mol	Chain	Res	Type
2	C	458	GLN
2	C	557	MET
2	C	567	TYR
1	D	123	LEU
1	D	179	MET
1	D	331	MET
1	D	383	ARG
1	D	574	CYS
1	D	577	PHE
1	D	626	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	493	GLN
2	C	236	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 19 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	1001	-	5,5,5	0.89	0	5,5,5	0.98	0
3	GOL	C	1003	-	5,5,5	0.86	0	5,5,5	1.05	0
5	SF4	D	1002	7	0,12,12	0.00	-	-		
3	GOL	B	704	-	5,5,5	0.84	0	5,5,5	1.03	0
5	SF4	B	708	-	0,12,12	0.00	-	-		
3	GOL	A	802	-	5,5,5	0.85	0	5,5,5	1.01	0
5	SF4	C	1004	2	0,12,12	0.00	-	-		
4	PE4	B	703	-	10,10,23	0.52	0	9,9,22	0.17	0
3	GOL	A	801	-	5,5,5	0.97	0	5,5,5	0.86	0
3	GOL	C	1002	-	5,5,5	0.91	0	5,5,5	0.96	0
8	XCC	C	1005	2	0,11,11	0.00	-	-		
4	PE4	A	803	-	19,19,23	0.50	0	18,18,22	0.22	0
8	XCC	B	709	2	0,11,11	0.00	-	-		
3	GOL	B	706	-	5,5,5	0.85	0	5,5,5	1.05	0
3	GOL	C	1001	-	5,5,5	0.86	0	5,5,5	1.04	0
3	GOL	B	705	-	5,5,5	0.85	0	5,5,5	1.01	0
3	GOL	B	702	-	5,5,5	0.85	0	5,5,5	1.01	0
5	SF4	B	707	-	0,12,12	0.00	-	-		
3	GOL	B	701	-	5,5,5	0.92	0	5,5,5	0.96	0
5	SF4	A	804	7	0,12,12	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
3	GOL	D	1001	-	-	4/4/4/4	-
3	GOL	C	1003	-	-	0/4/4/4	-
5	SF4	D	1002	7	-	-	0/6/5/5
3	GOL	B	704	-	-	0/4/4/4	-
5	SF4	B	708	-	-	-	0/6/5/5
3	GOL	A	802	-	-	0/4/4/4	-
5	SF4	C	1004	2	-	-	0/6/5/5
4	PE4	B	703	-	-	6/8/8/21	-
3	GOL	A	801	-	-	2/4/4/4	-
3	GOL	C	1002	-	-	4/4/4/4	-
8	XCC	C	1005	2	-	-	0/3/3/3
4	PE4	A	803	-	-	12/17/17/21	-
8	XCC	B	709	2	-	-	0/3/3/3
3	GOL	B	706	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	1001	-	-	1/4/4/4	-
3	GOL	B	705	-	-	0/4/4/4	-
3	GOL	B	702	-	-	0/4/4/4	-
5	SF4	B	707	-	-	-	0/6/5/5
3	GOL	B	701	-	-	2/4/4/4	-
5	SF4	A	804	7	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	GOL	O1-C1-C2-O2
3	D	1001	GOL	C1-C2-C3-O3
3	D	1001	GOL	O2-C2-C3-O3
3	A	801	GOL	O1-C1-C2-C3
4	A	803	PE4	C1-C2-O2-C3
4	B	703	PE4	O6-C11-C12-O7
4	A	803	PE4	O2-C3-C4-O3
4	A	803	PE4	O1-C1-C2-O2
4	A	803	PE4	C9-C10-O6-C11
3	B	701	GOL	O1-C1-C2-C3
3	D	1001	GOL	O1-C1-C2-C3
3	C	1002	GOL	O1-C1-C2-C3
3	C	1002	GOL	C1-C2-C3-O3
3	A	801	GOL	O1-C1-C2-O2
3	C	1002	GOL	O2-C2-C3-O3
4	A	803	PE4	O4-C7-C8-O5
4	A	803	PE4	O6-C10-C9-O5
4	A	803	PE4	C5-C6-O4-C7
4	A	803	PE4	C8-C7-O4-C6
4	B	703	PE4	C11-C12-O7-C13
4	A	803	PE4	C4-C3-O2-C2
4	B	703	PE4	C14-C13-O7-C12
4	A	803	PE4	C6-C5-O3-C4
4	B	703	PE4	C9-C10-O6-C11
3	C	1002	GOL	O1-C1-C2-O2
4	B	703	PE4	C16-C15-O8-C14
3	D	1001	GOL	O1-C1-C2-O2
3	B	706	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	803	PE4	C11-C12-O7-C13
3	C	1001	GOL	O2-C2-C3-O3
4	A	803	PE4	O3-C5-C6-O4
4	B	703	PE4	O7-C13-C14-O8

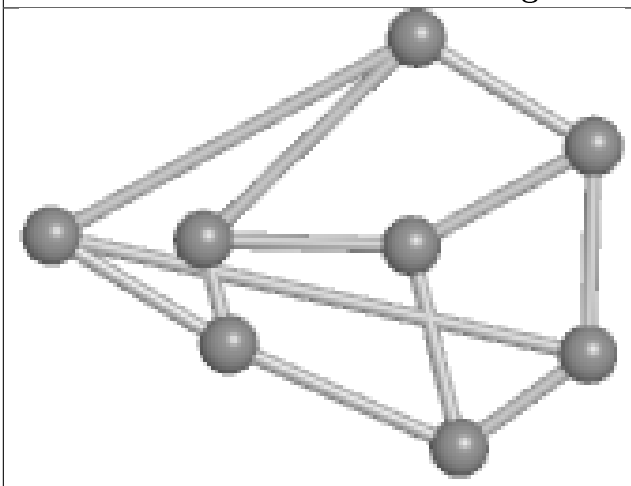
There are no ring outliers.

5 monomers are involved in 5 short contacts:

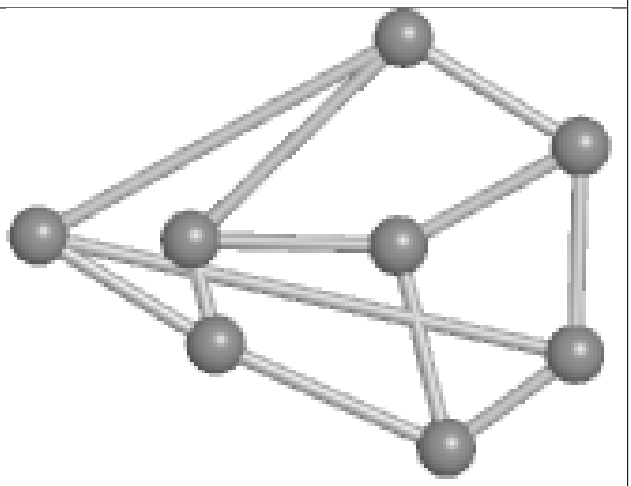
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	708	SF4	1	0
3	A	802	GOL	1	0
5	C	1004	SF4	1	0
4	B	703	PE4	1	0
4	A	803	PE4	1	0

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

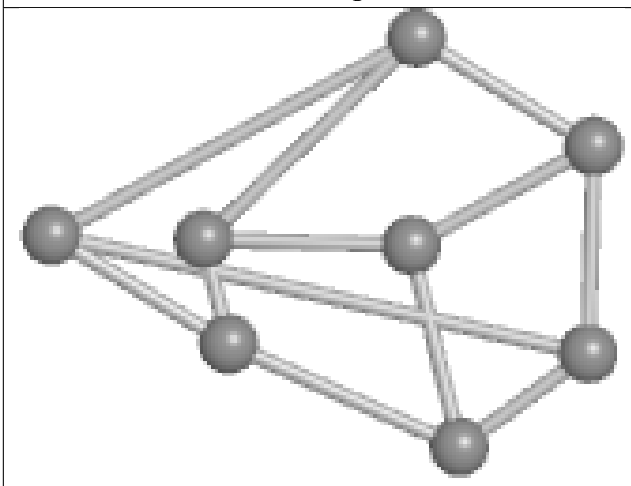
Ligand SF4 D 1002



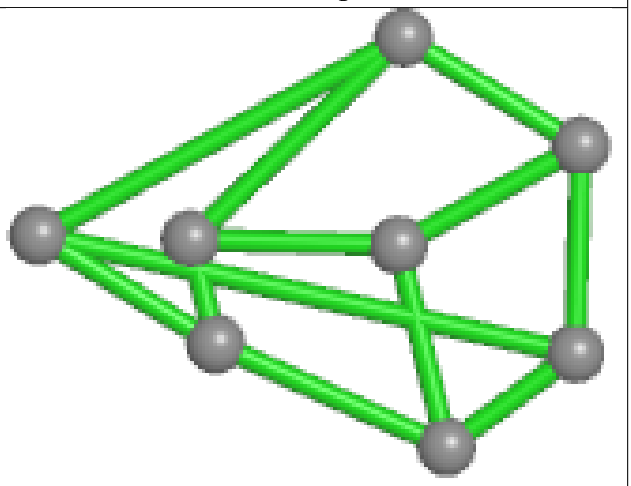
Bond lengths



Bond angles

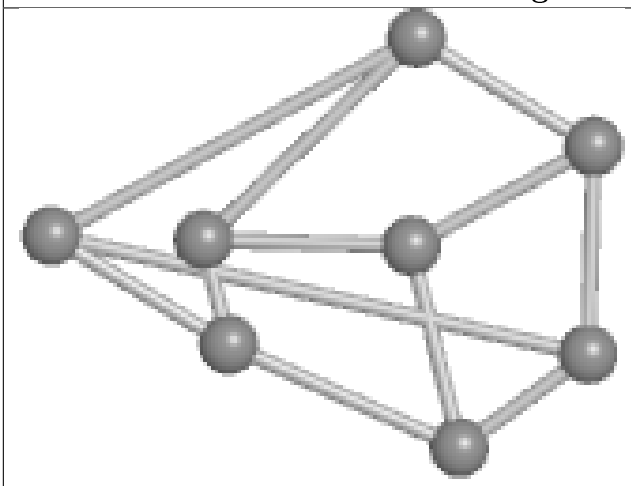


Torsions

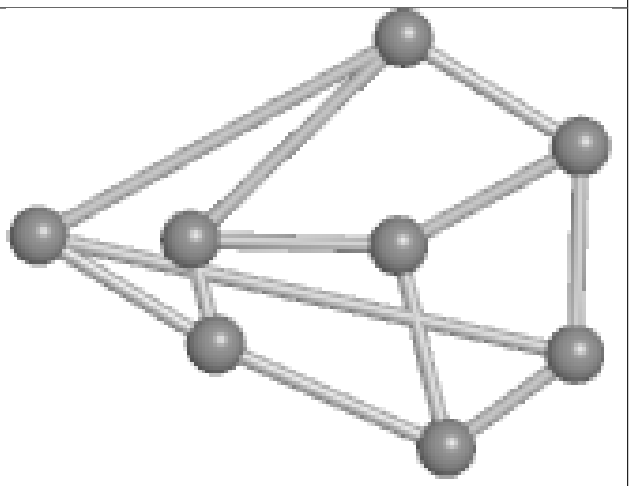


Rings

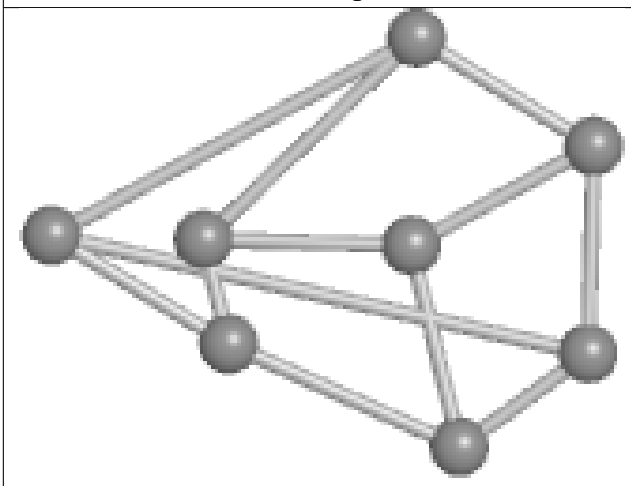
Ligand SF4 B 708



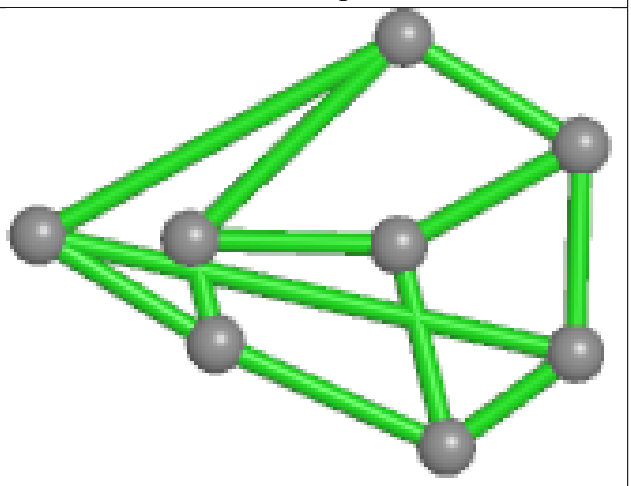
Bond lengths



Bond angles

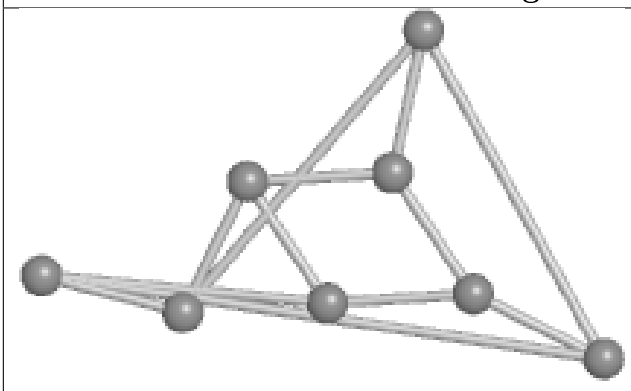


Torsions

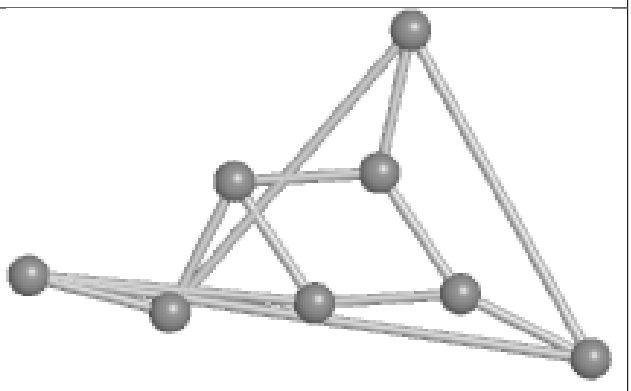


Rings

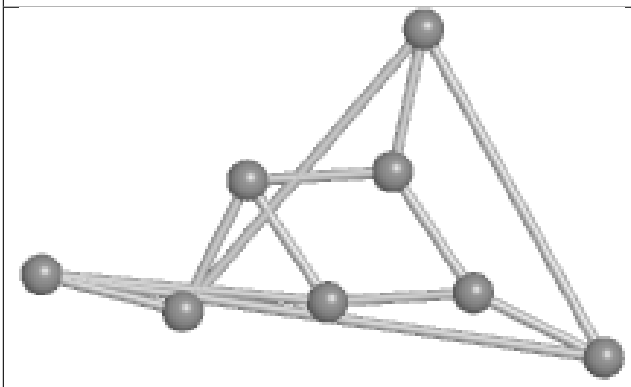
Ligand SF4 C 1004



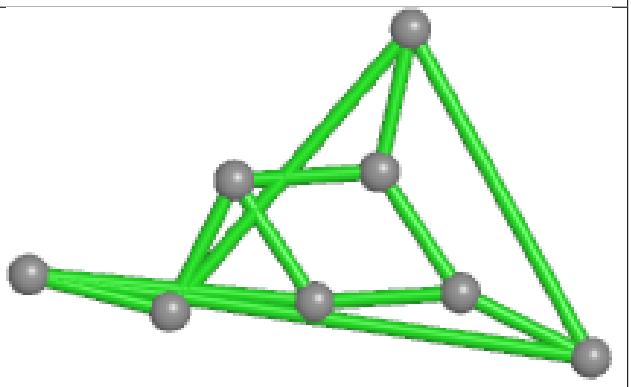
Bond lengths



Bond angles



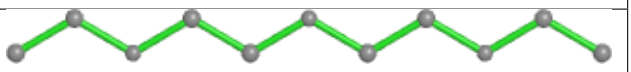
Torsions



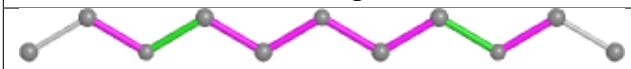
Rings

Ligand PE4 B 703

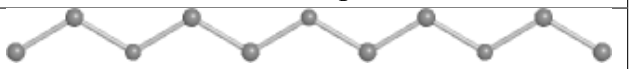
Bond lengths



Bond angles

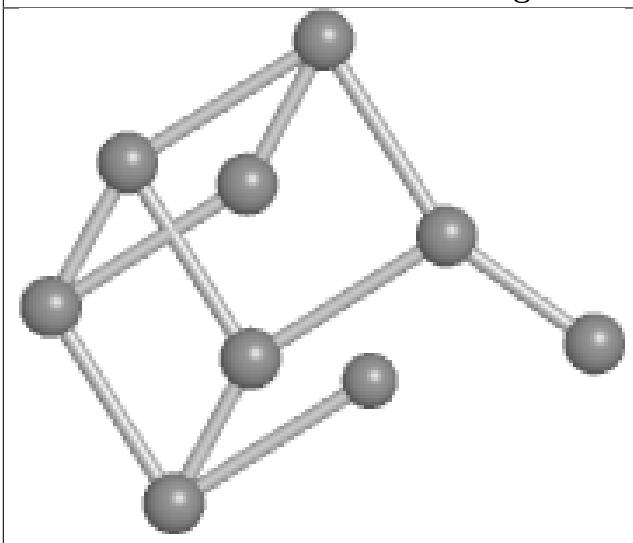


Torsions

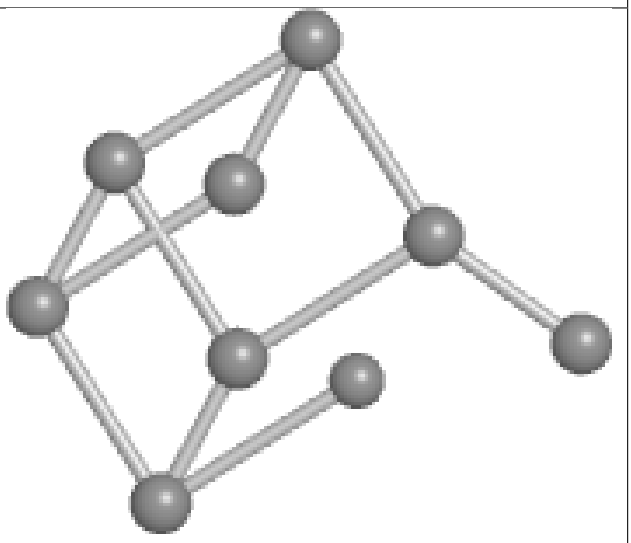


Rings

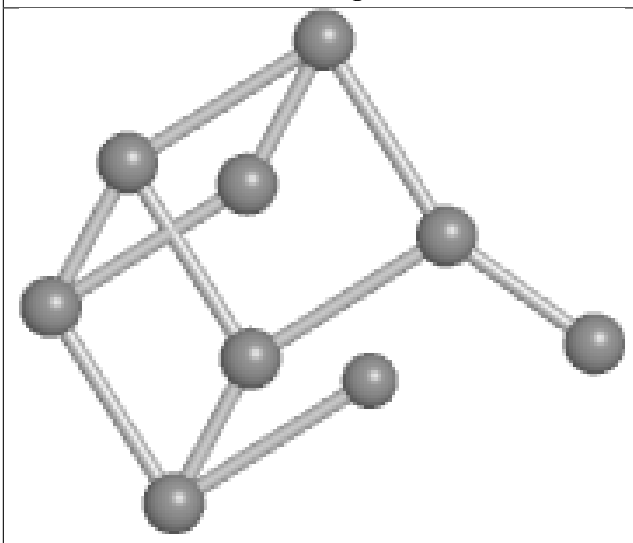
Ligand XCC C 1005



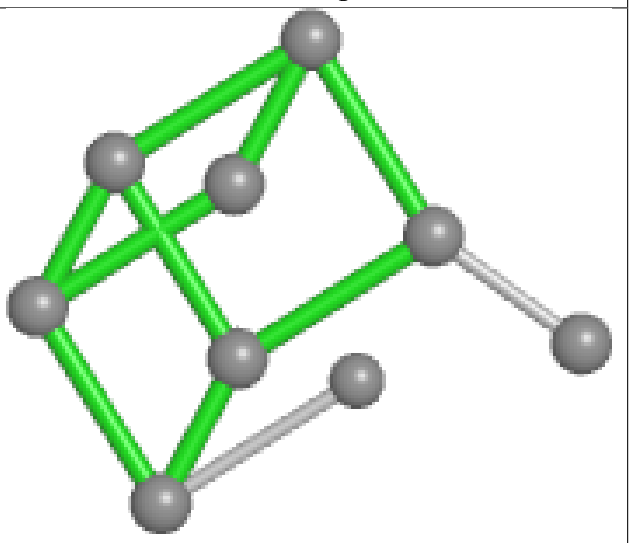
Bond lengths



Bond angles



Torsions

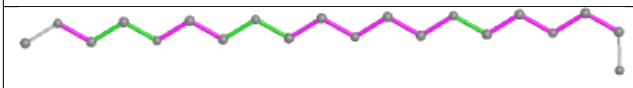


Rings

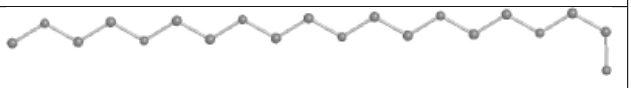
Ligand PE4 A 803

Bond lengths

Bond angles

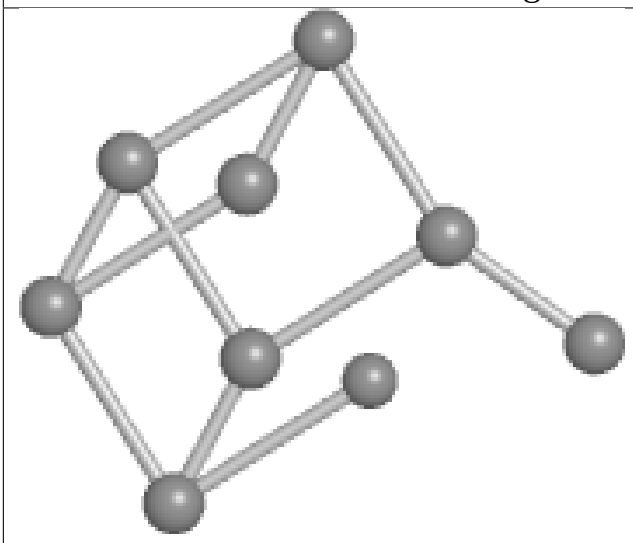


Torsions

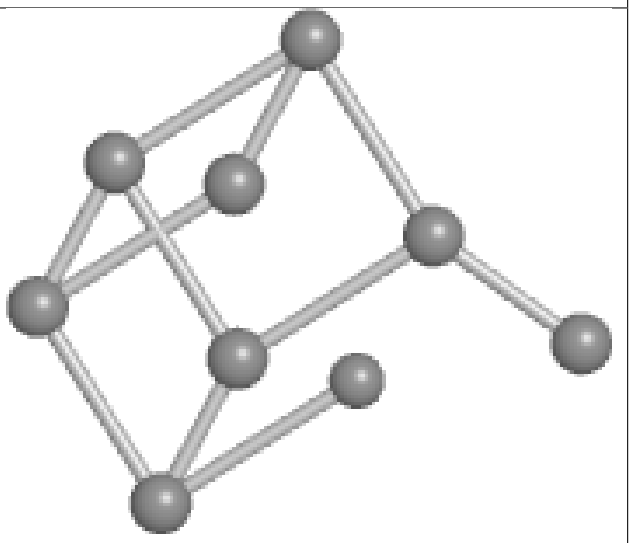


Rings

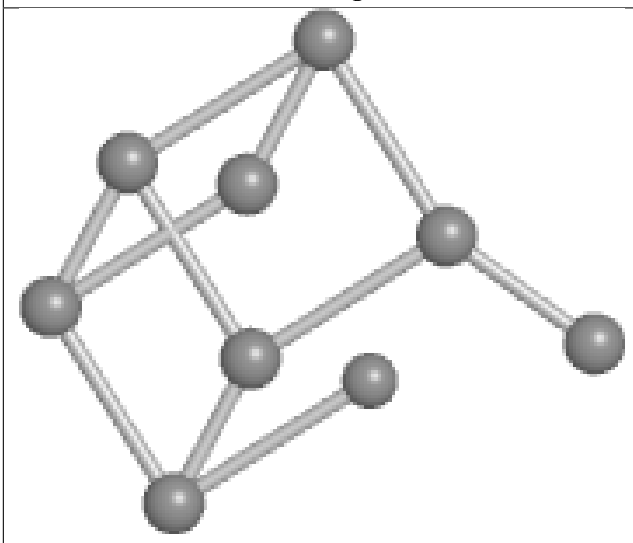
Ligand XCC B 709



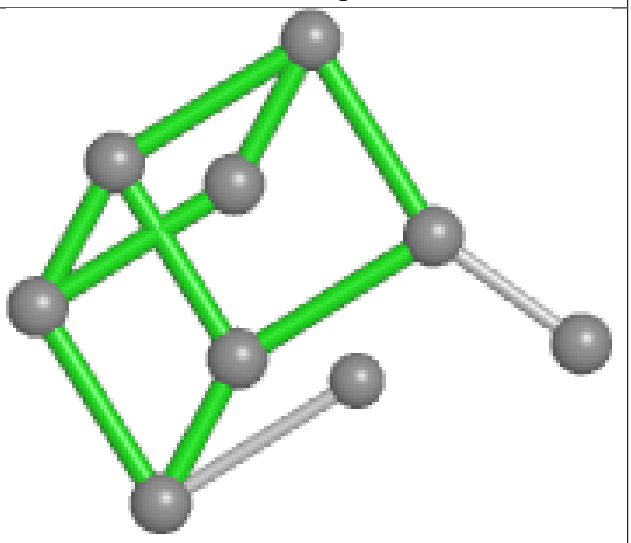
Bond lengths



Bond angles

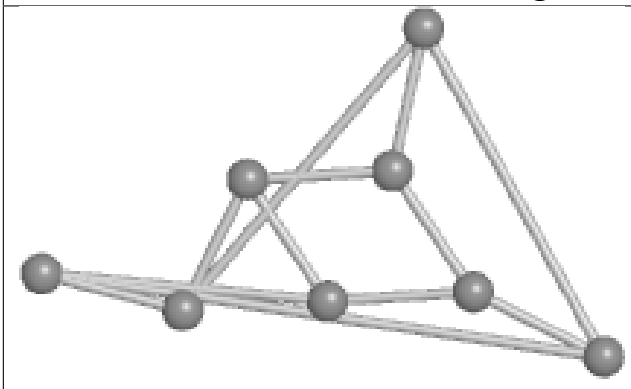


Torsions

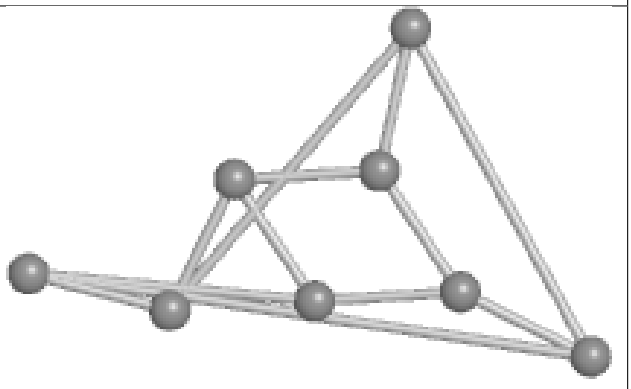


Rings

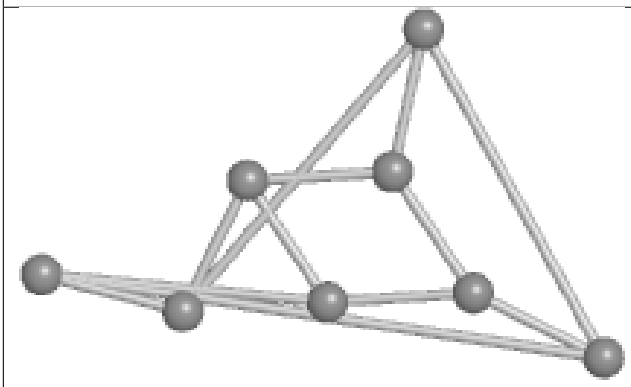
Ligand SF4 B 707



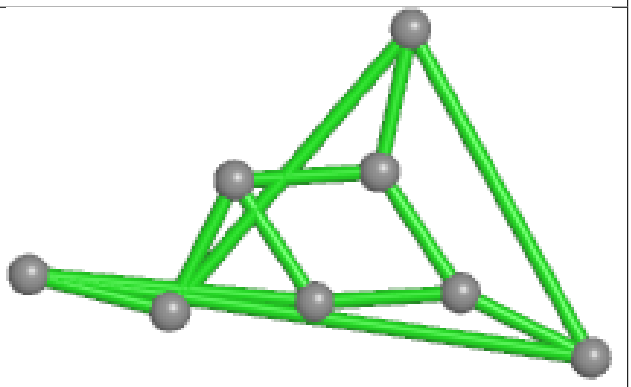
Bond lengths



Bond angles

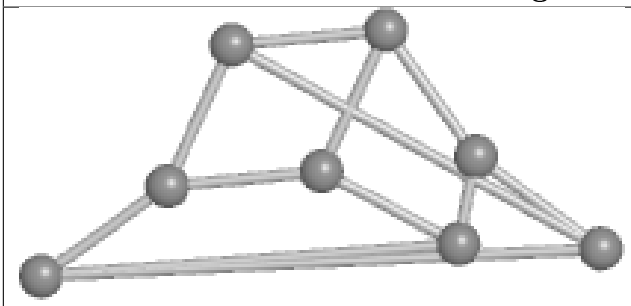


Torsions

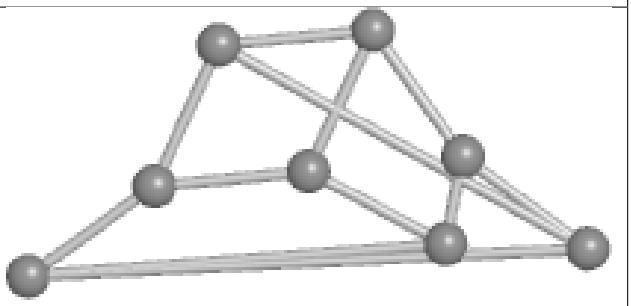


Rings

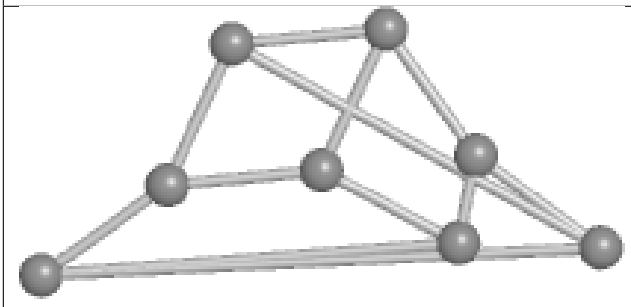
Ligand SF4 A 804



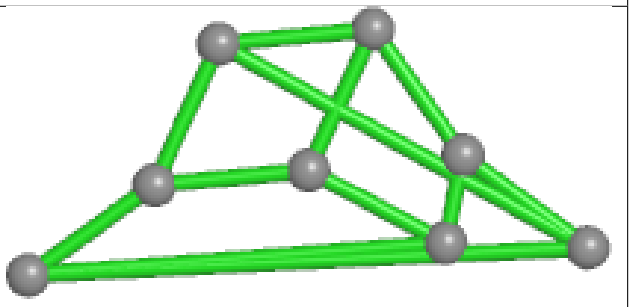
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	708/708 (100%)	0.00	38 (5%) 25 9	39, 110, 179, 218	0
1	D	705/708 (99%)	0.23	60 (8%) 10 3	71, 132, 220, 265	0
2	B	629/631 (99%)	-0.51	0 100 100	30, 53, 82, 115	0
2	C	630/631 (99%)	-0.42	2 (0%) 94 83	40, 73, 110, 147	0
All	All	2672/2678 (99%)	-0.16	100 (3%) 41 17	30, 84, 190, 265	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	GLY	5.2
1	D	437	VAL	5.1
1	D	454	GLU	4.7
1	D	423	GLY	4.6
1	D	442	GLU	4.5
1	D	424	GLU	4.5
1	D	333	ALA	4.2
1	D	438	VAL	4.2
1	D	419	LEU	4.1
1	A	420	LYS	4.0
1	D	338	VAL	4.0
1	A	345	VAL	4.0
1	A	394	GLY	3.9
1	D	582	GLY	3.8
1	D	420	LYS	3.6
1	A	317	ALA	3.6
1	D	334	ASP	3.6
1	D	365	LEU	3.6
1	D	441	CYS	3.5
1	A	352	THR	3.5
1	D	316	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	409	GLY	3.4
1	D	373	MET	3.4
1	D	354	ASP	3.4
1	A	674	PHE	3.4
1	A	408	ILE	3.3
1	D	418	ARG	3.2
1	D	368	VAL	3.2
1	D	533	GLU	3.1
1	D	484	SER	3.1
1	D	376	ASP	3.1
1	D	479	VAL	3.1
1	D	317	ALA	3.1
1	A	546	VAL	3.0
1	D	310	ILE	3.0
1	D	345	VAL	3.0
1	A	422	PHE	3.0
1	D	482	PHE	3.0
1	D	674	PHE	3.0
1	A	444	THR	2.9
1	D	471	LEU	2.9
1	A	545	LYS	2.9
1	D	364	MET	2.8
1	D	339	GLU	2.7
1	A	643	LEU	2.7
1	A	419	LEU	2.6
1	A	673	ASN	2.6
1	D	358	GLY	2.6
1	D	445	ILE	2.6
1	A	417	PHE	2.6
1	A	638	LYS	2.6
1	A	318	GLU	2.6
1	A	344	GLU	2.6
1	D	662	ASN	2.6
1	A	564	TYR	2.5
1	A	539	ASN	2.5
1	D	529	ALA	2.5
1	A	535	VAL	2.5
2	C	326	GLY	2.5
1	D	685	THR	2.5
1	D	322	ASN	2.5
1	A	407	ARG	2.5
1	A	349	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	346	ILE	2.5
1	D	351	ASP	2.5
1	D	356	ALA	2.4
1	D	483	TYR	2.4
1	D	434	PHE	2.4
1	A	482	PHE	2.4
1	D	311	ARG	2.3
1	D	443	VAL	2.3
1	A	457	GLY	2.3
1	A	563	LEU	2.3
1	A	316	LEU	2.3
1	A	445	ILE	2.3
2	C	523	CYS	2.3
1	A	351	ASP	2.2
1	A	446	ILE	2.2
1	D	369	SER	2.2
1	A	541	GLY	2.2
1	D	394	GLY	2.2
1	D	312	LYS	2.2
1	D	513	LEU	2.2
1	D	408	ILE	2.2
1	A	310	ILE	2.2
1	D	421	HIS	2.2
1	D	300	SER	2.1
1	D	530	VAL	2.1
1	D	673	ASN	2.1
1	A	540	LEU	2.1
1	D	512	TRP	2.1
1	A	530	VAL	2.1
1	D	366	ILE	2.1
1	A	676	ASP	2.1
1	D	499	VAL	2.0
1	D	587	ALA	2.0
1	D	444	THR	2.0
1	D	473	SER	2.0
1	D	474	LEU	2.0
1	D	435	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NA	B	711	1/1	0.49	0.92	121,121,121,121	0
3	GOL	C	1001	6/6	0.69	0.42	117,127,128,134	0
3	GOL	B	705	6/6	0.69	0.41	86,100,119,126	0
3	GOL	C	1003	6/6	0.76	0.41	73,88,121,126	0
6	F	C	1007	1/1	0.76	0.52	76,76,76,76	0
3	GOL	B	706	6/6	0.76	0.47	99,110,111,113	0
3	GOL	C	1002	6/6	0.77	0.35	120,130,132,133	0
4	PE4	A	803	20/24	0.78	0.32	102,127,145,152	0
3	GOL	A	802	6/6	0.78	0.33	96,109,116,119	0
6	F	A	806	1/1	0.80	0.43	88,88,88,88	0
3	GOL	A	801	6/6	0.81	0.26	104,105,115,122	0
3	GOL	D	1001	6/6	0.81	0.19	111,127,136,153	0
3	GOL	B	701	6/6	0.81	0.23	83,99,110,119	0
9	NA	C	1013	1/1	0.86	0.55	84,84,84,84	0
4	PE4	B	703	11/24	0.86	0.31	82,113,123,124	0
6	F	C	1009	1/1	0.88	0.37	51,51,51,51	0
3	GOL	B	704	6/6	0.89	0.26	110,115,116,121	0
6	F	C	1011	1/1	0.89	0.20	70,70,70,70	0
9	NA	C	1014	1/1	0.90	0.07	80,80,80,80	0
6	F	C	1008	1/1	0.90	0.19	52,52,52,52	0
6	F	C	1010	1/1	0.93	0.14	41,41,41,41	0
3	GOL	B	702	6/6	0.93	0.21	93,102,111,117	0
9	NA	C	1012	1/1	0.94	0.19	56,56,56,56	0
6	F	C	1006	1/1	0.94	0.42	39,39,39,39	0
9	NA	B	712	1/1	0.95	0.16	63,63,63,63	0
6	F	A	805	1/1	0.95	0.35	50,50,50,50	0
6	F	B	710	1/1	0.96	0.20	33,33,33,33	0
8	XCC	C	1005	9/9	0.96	0.24	108,115,150,151	0
7	NI	A	808	1/1	0.97	0.08	122,122,122,122	0
5	SF4	B	708	8/8	0.97	0.27	98,120,144,181	0
8	XCC	B	709	9/9	0.98	0.23	72,115,132,141	0
7	NI	A	807	1/1	0.98	0.13	94,94,94,94	0

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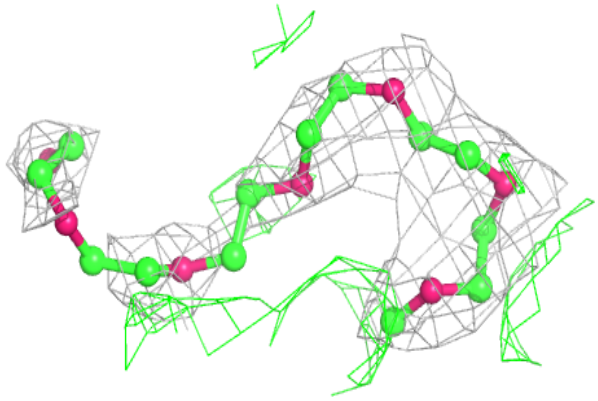
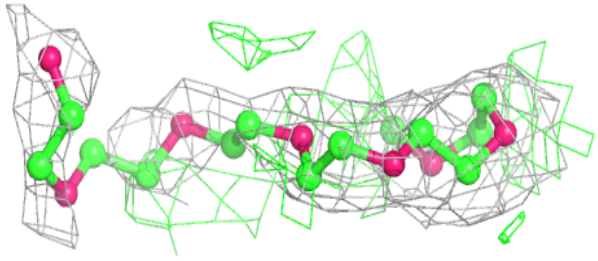
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NA	B	713	1/1	0.98	0.26	63,63,63,63	0
5	SF4	A	804	8/8	0.98	0.07	126,159,205,213	0
5	SF4	D	1002	8/8	0.99	0.13	144,160,197,199	0
5	SF4	C	1004	8/8	0.99	0.20	81,94,107,189	0
7	NI	D	1004	1/1	0.99	0.15	85,85,85,85	0
7	NI	D	1003	1/1	0.99	0.14	89,89,89,89	0
5	SF4	B	707	8/8	1.00	0.20	84,93,138,212	0

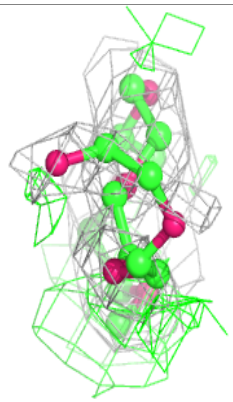
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PE4 A 803:

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

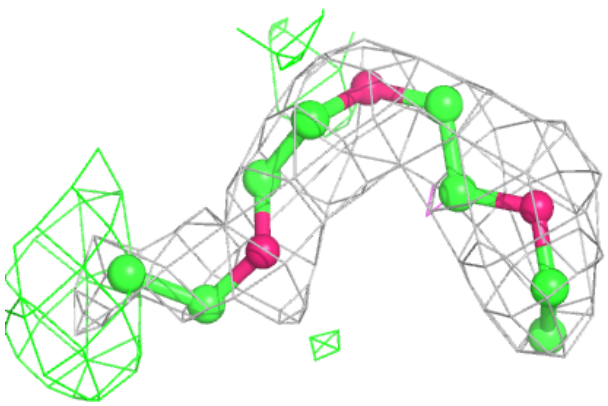


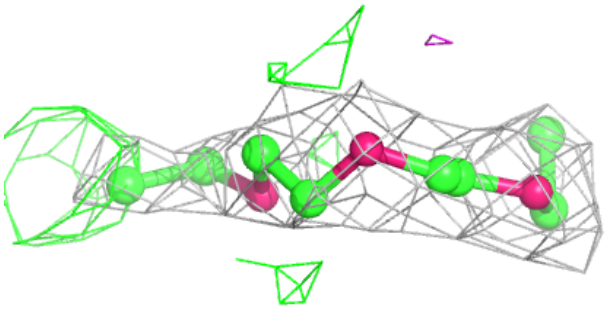


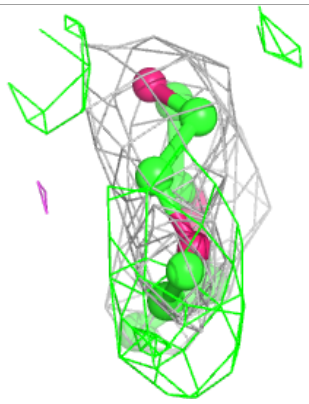


Electron density around PE4 B 703:

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

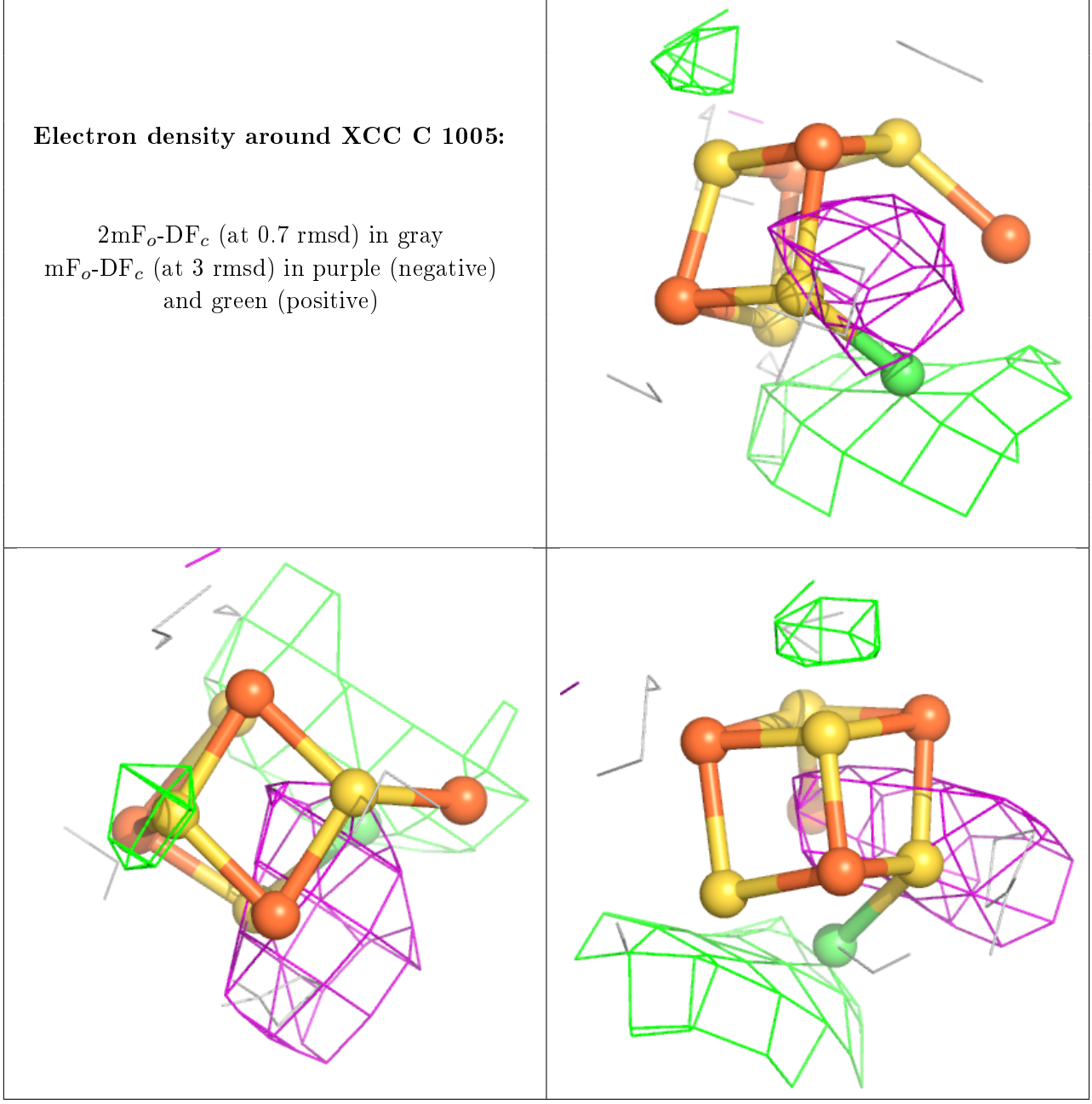






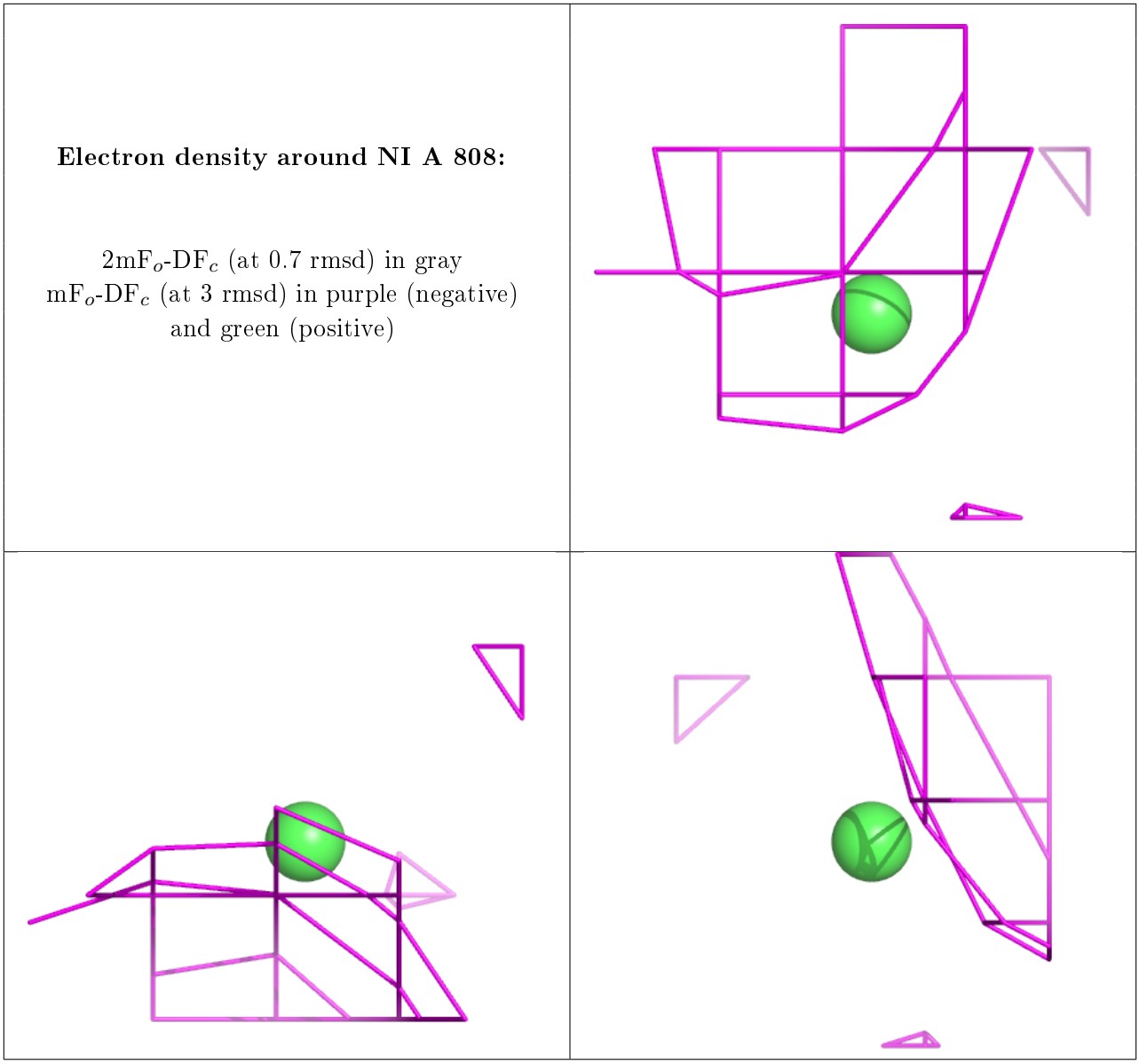
Electron density around XCC C 1005:

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



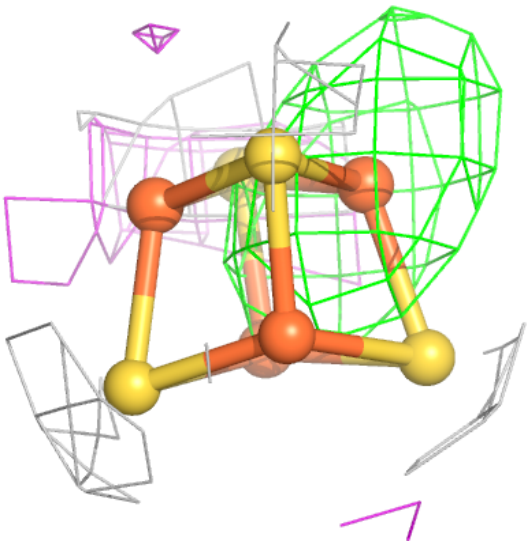
Electron density around NI A 808:

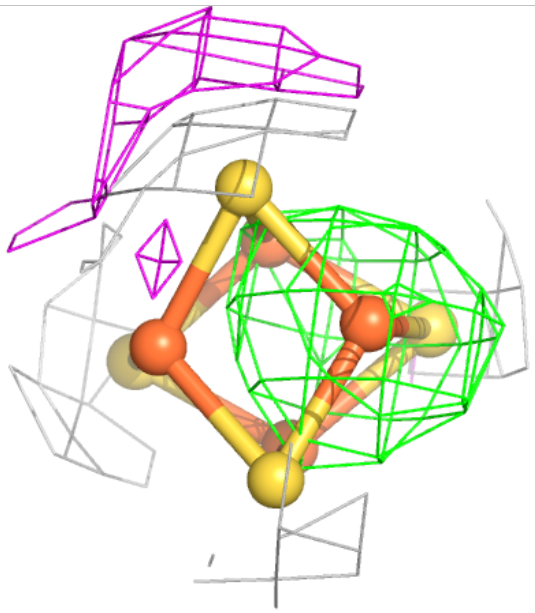
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

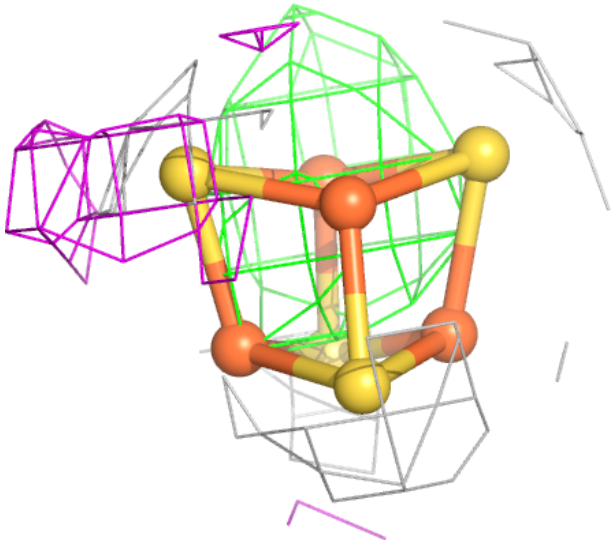


Electron density around SF4 B 708:

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

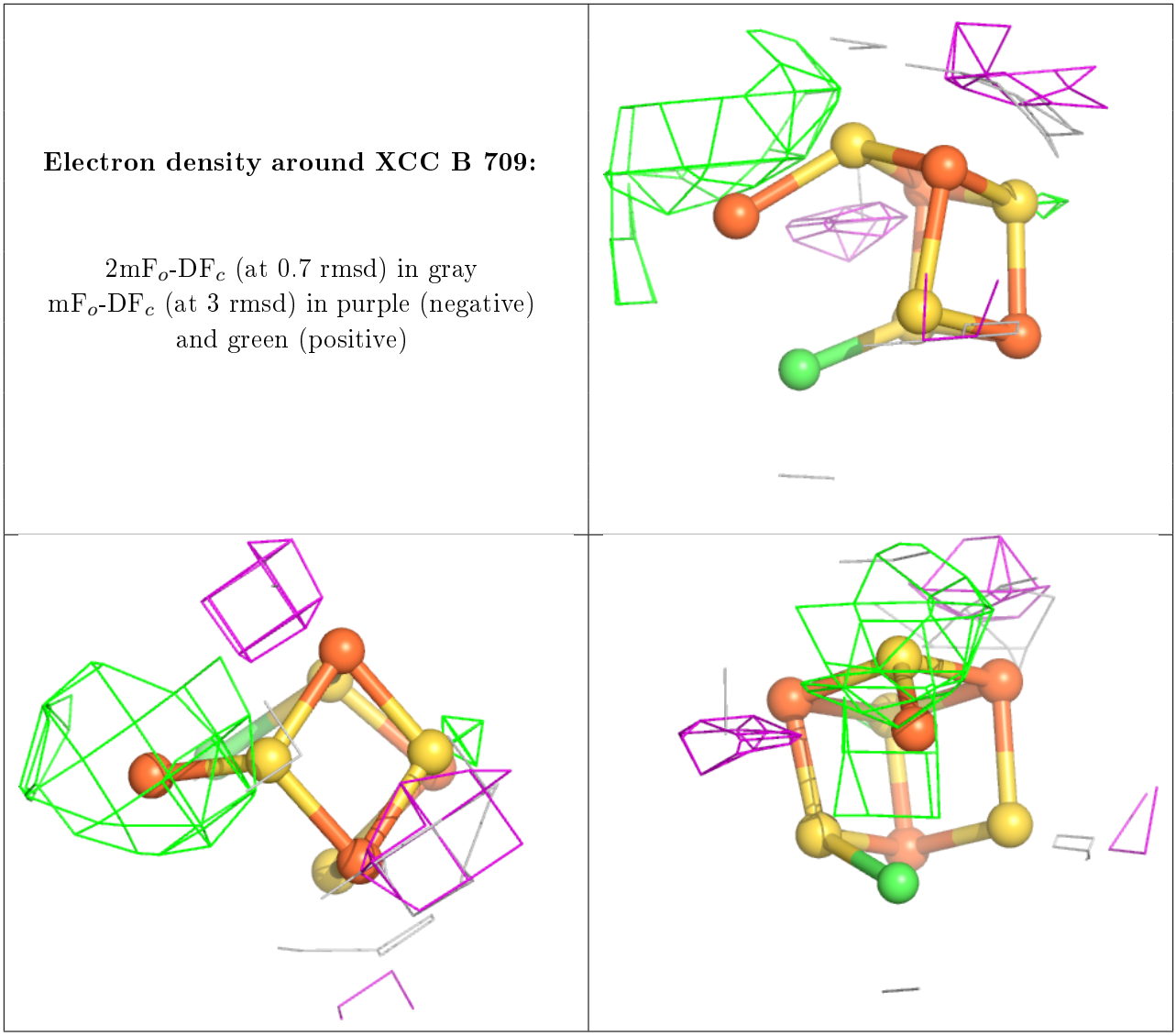






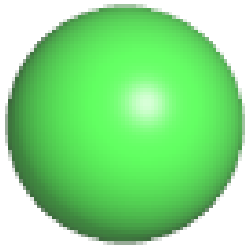
Electron density around XCC B 709:

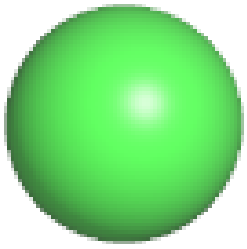
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

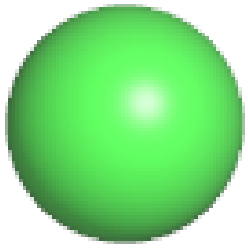


Electron density around NI A 807:

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

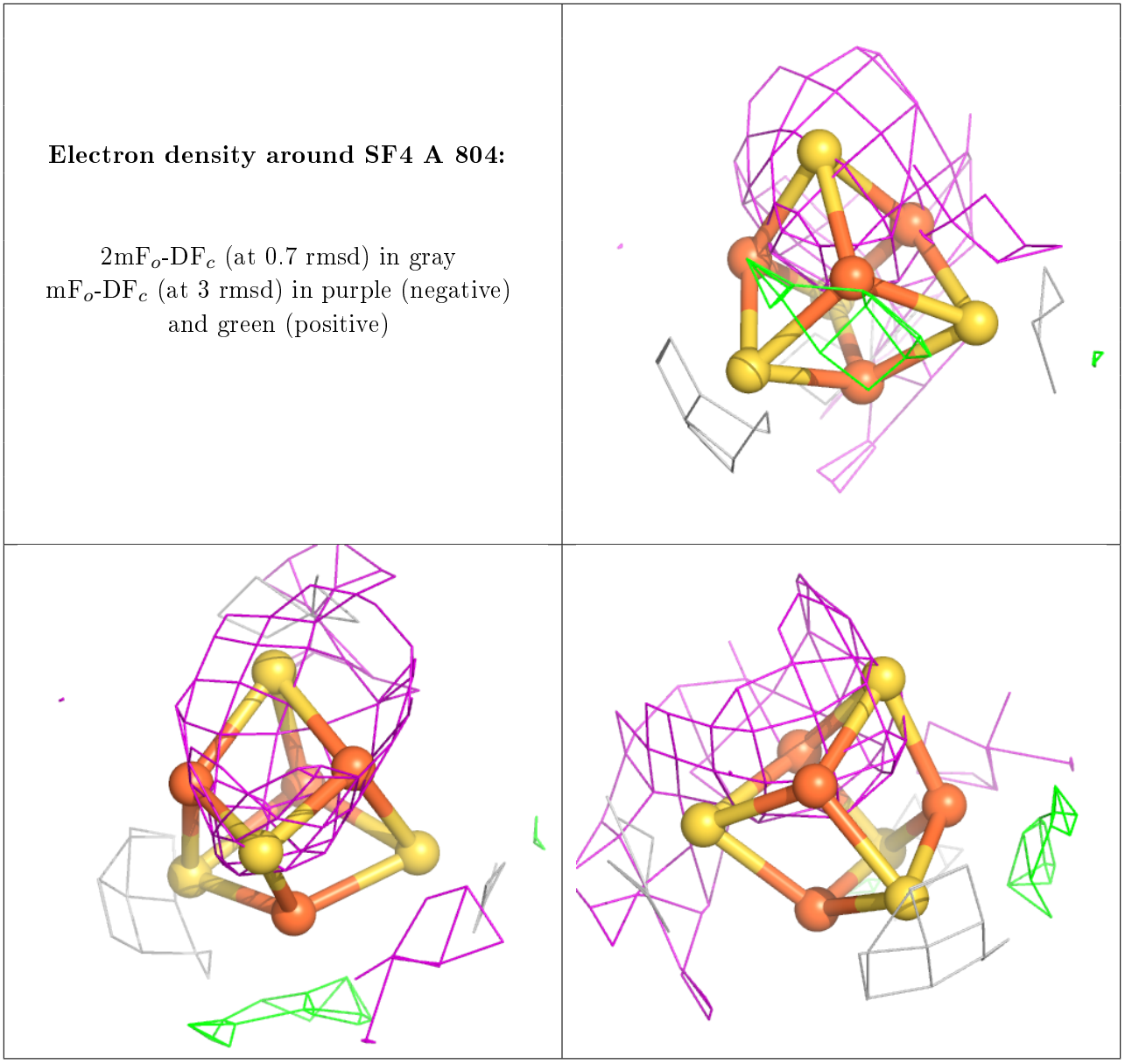






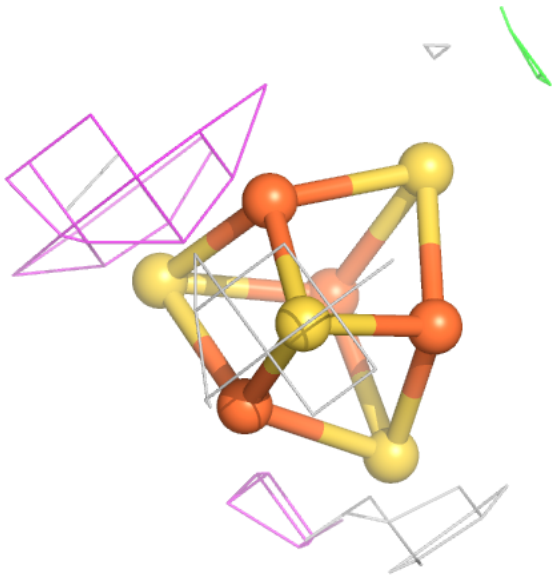
Electron density around SF4 A 804:

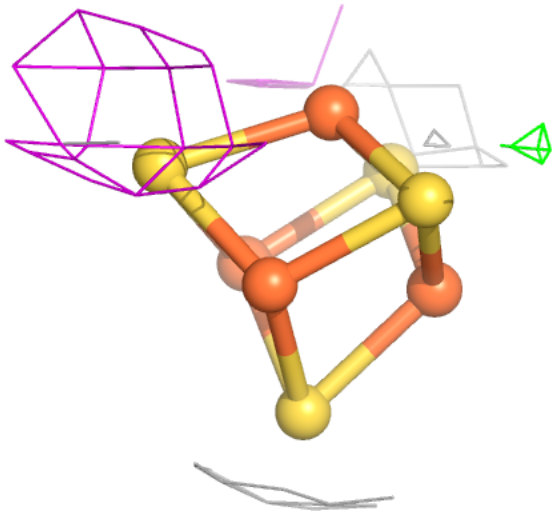
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

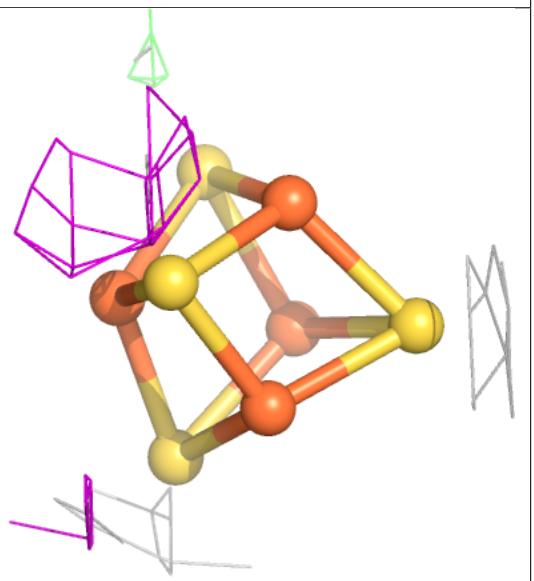


Electron density around SF4 D 1002:

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

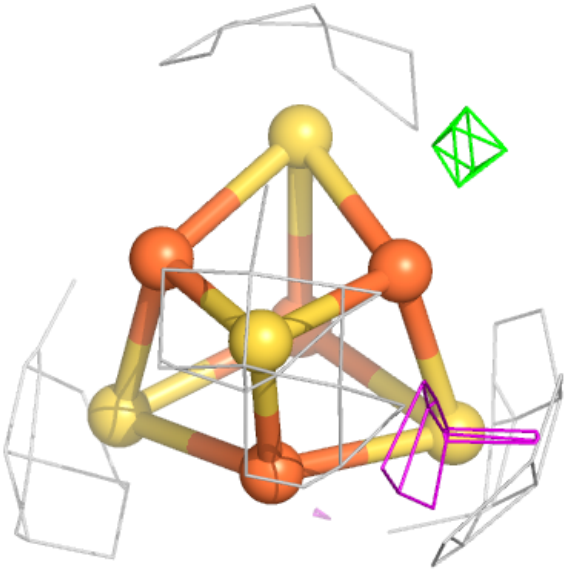


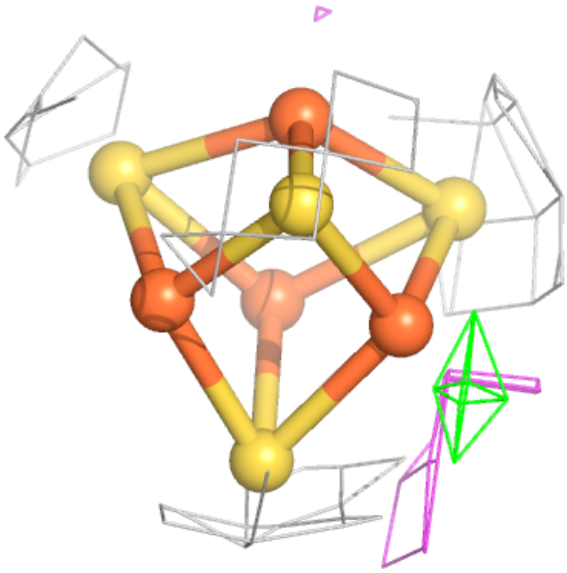


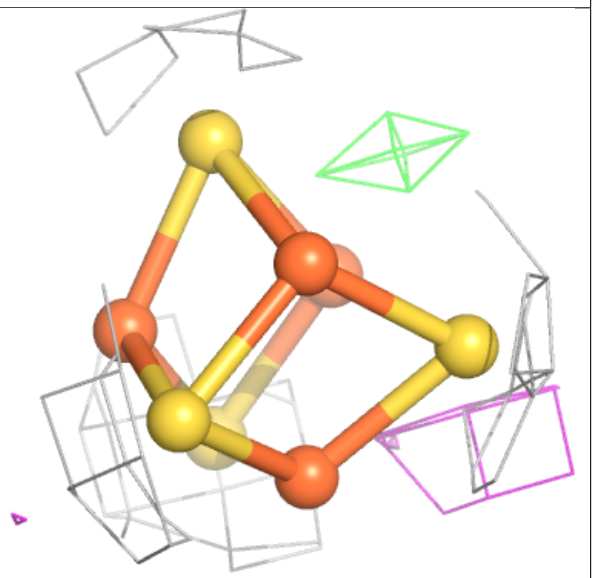


Electron density around SF4 C 1004:

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

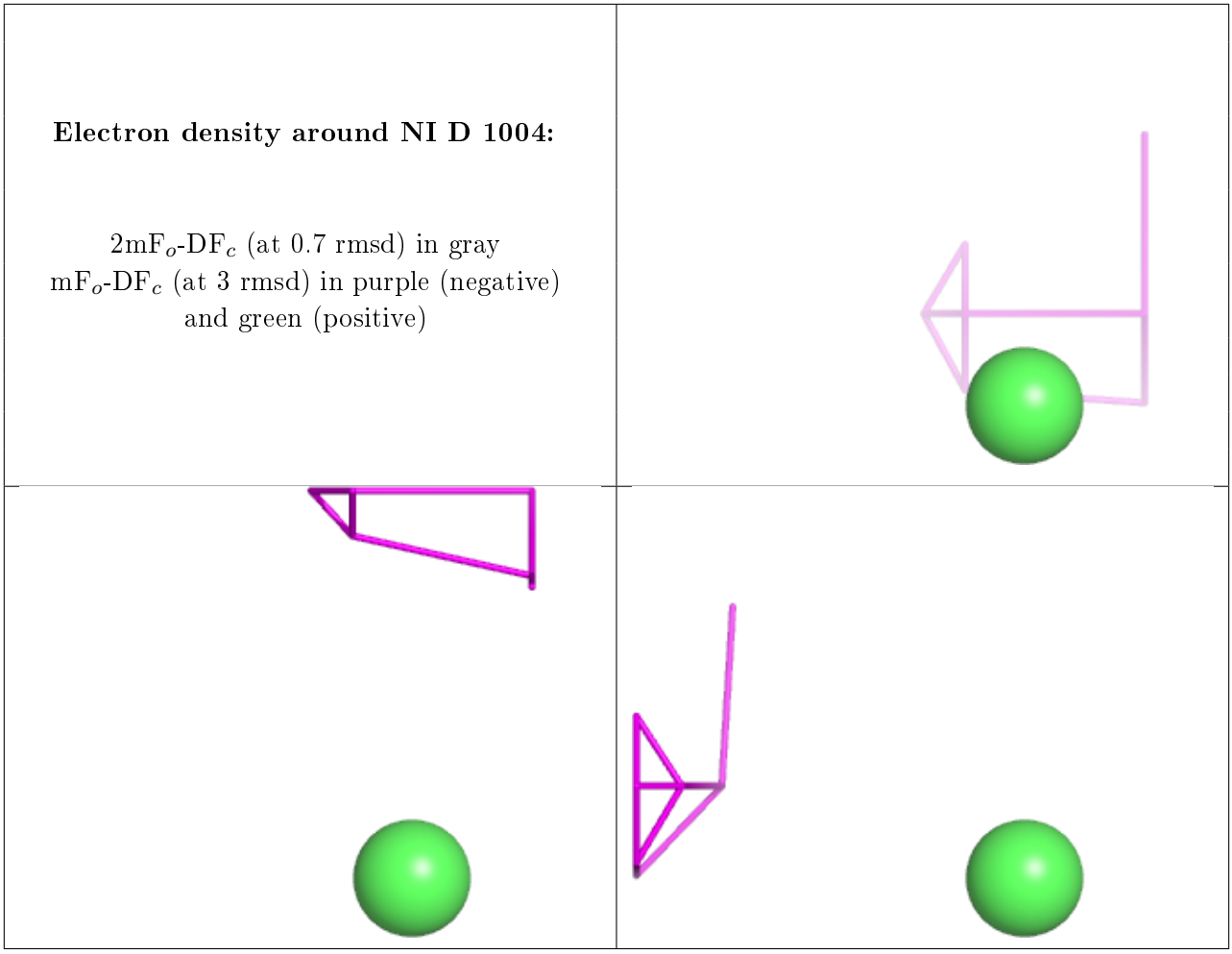






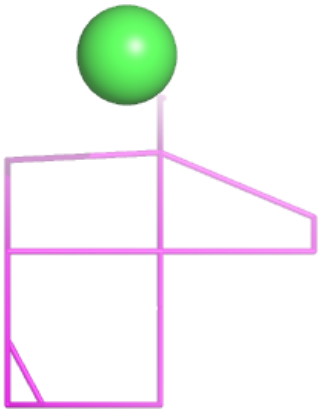
Electron density around NI D 1004:

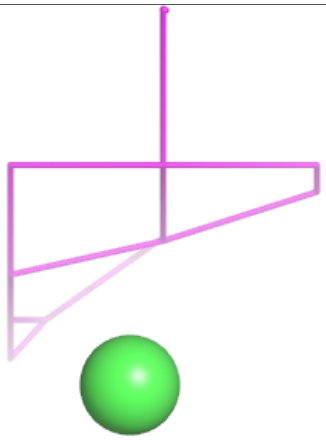
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

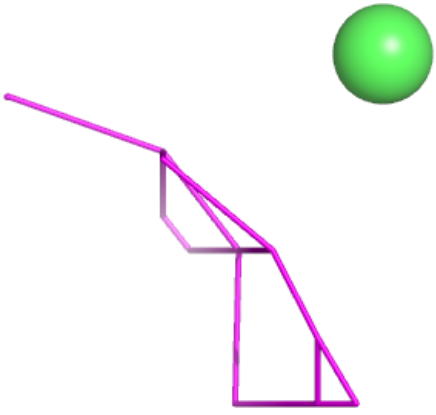


Electron density around NI D 1003:

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

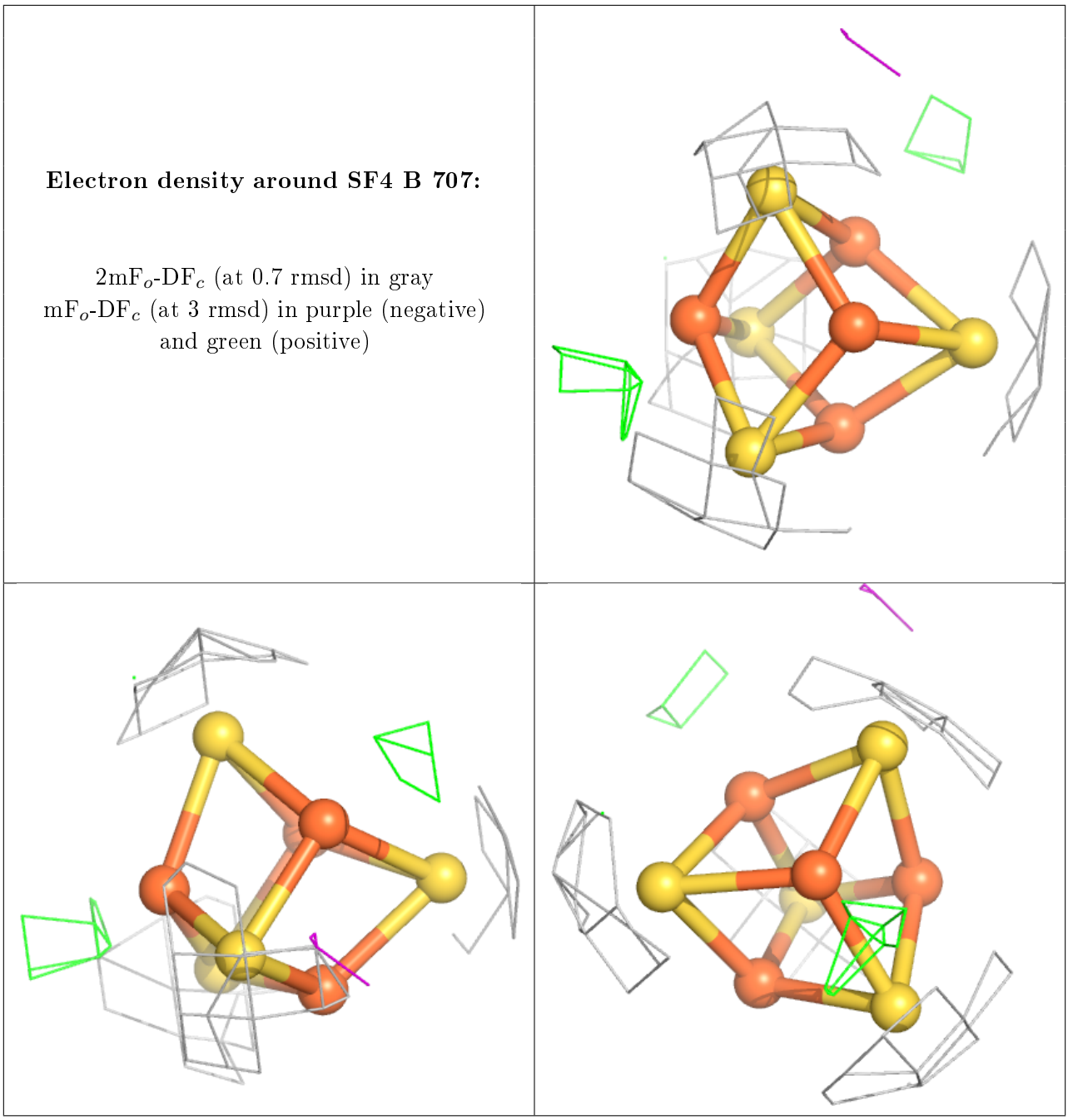






Electron density around SF4 B 707:

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



6.5 Other polymers

There are no such residues in this entry.