Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 11:25 pm BST

PDB ID	:	8CJB / pdb_00008cjb
Title	:	A268M variant of the CODH/ACS complex of C. hydrogenoformans
Authors	:	Ruickoldt, J.; Jeoung, J.; Lennartz, F.; Dobbek, H.
Deposited on	:	2023-02-13
Resolution	:	2.50 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 (i) symbol.

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

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

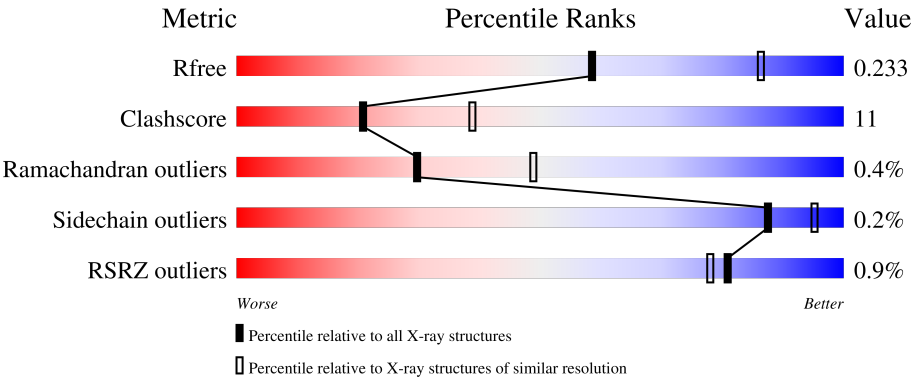
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

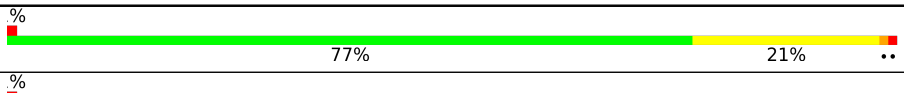
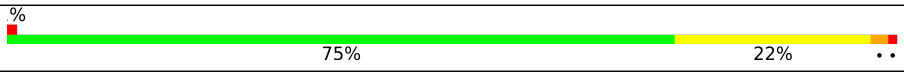
The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	669	
2	B	731	

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
6	OH	A	705	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11267 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 Carbon monoxide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	669	5147	3264	887	961	35	0	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ASP	GLU	conflict	UNP A0A1L8D0M5
A	29	ILE	THR	conflict	UNP A0A1L8D0M5
A	73	GLN	MET	conflict	UNP A0A1L8D0M5
A	120	ALA	THR	conflict	UNP A0A1L8D0M5
A	153	THR	ILE	conflict	UNP A0A1L8D0M5
A	159	MET	LEU	conflict	UNP A0A1L8D0M5
A	199	GLU	ASP	conflict	UNP A0A1L8D0M5
A	205	SER	ALA	conflict	UNP A0A1L8D0M5
A	220	ILE	MET	conflict	UNP A0A1L8D0M5
A	389	ILE	VAL	conflict	UNP A0A1L8D0M5
A	393	LEU	PHE	conflict	UNP A0A1L8D0M5
A	494	THR	ALA	conflict	UNP A0A1L8D0M5
A	602	THR	SER	conflict	UNP A0A1L8D0M5

- Molecule 2 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	730	5837	3744	981	1082	30	8	8	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	225	LEU	ALA	conflict	UNP Q3ACS4
B	268	MET	ALA	engineered mutation	UNP Q3ACS4
B	733	ARG	-	expression tag	UNP Q3ACS4

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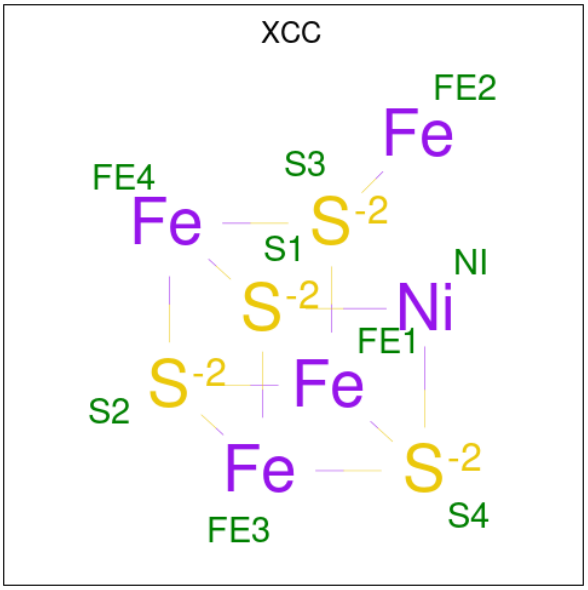
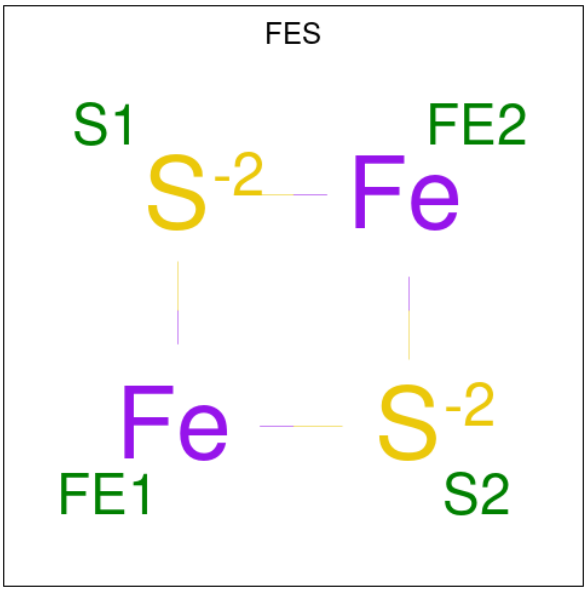
Chain	Residue	Modelled	Actual	Comment	Reference
B	734	SER	-	expression tag	UNP Q3ACS4
B	735	HIS	-	expression tag	UNP Q3ACS4

- Molecule 3 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



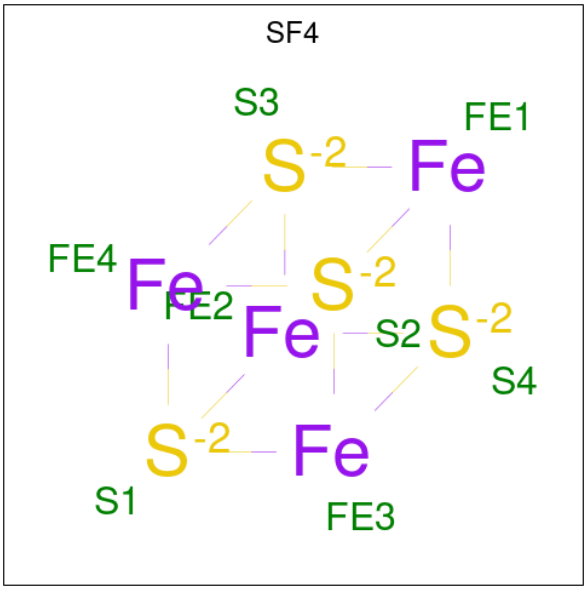
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
3	A	1	9	4	1	4	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		

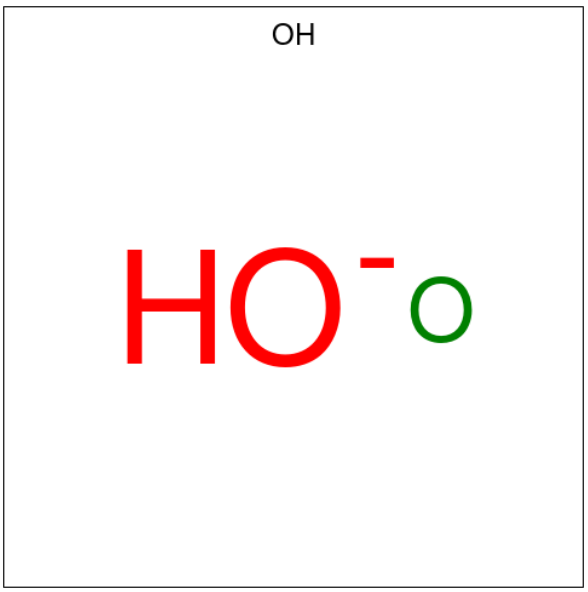
- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

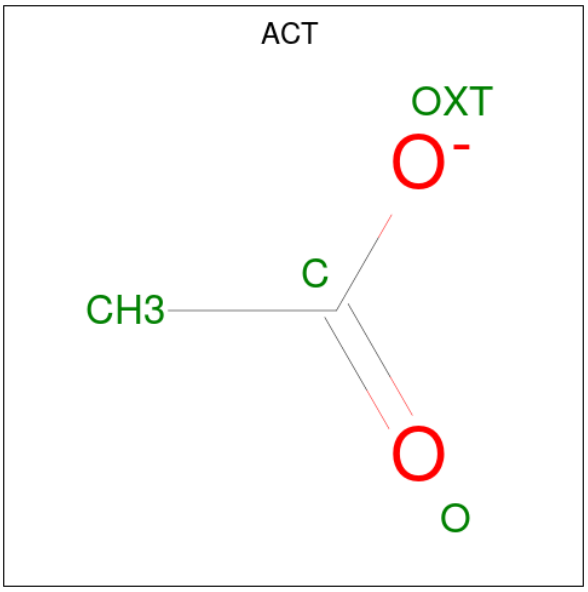
- Molecule 6 is HYDROXIDE ION (CCD ID: OH) (formula: HO) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	A	1	Total O 1 1	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Na 1 1	0	0

- Molecule 9 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Ni 2 2	0	1

- Molecule 10 is water.

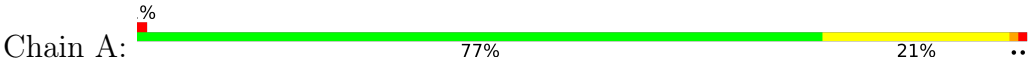
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	96	Total O 96 96	0	0
10	B	149	Total O 149 149	0	0

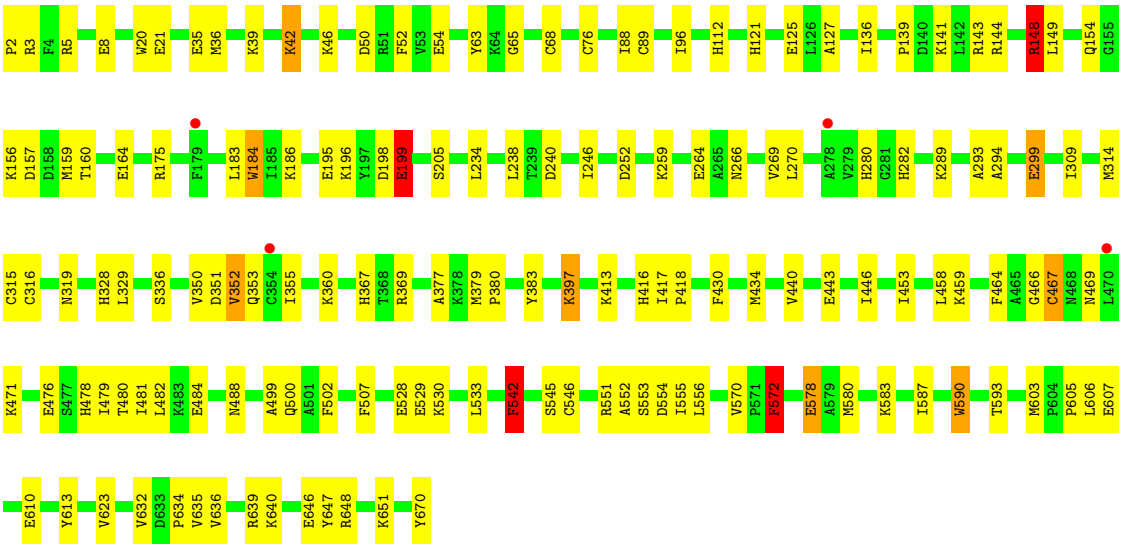
3 Residue-property plots (i)

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: Carbon monoxide dehydrogenase

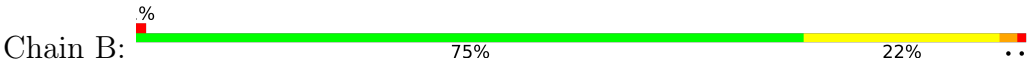
Chain A:

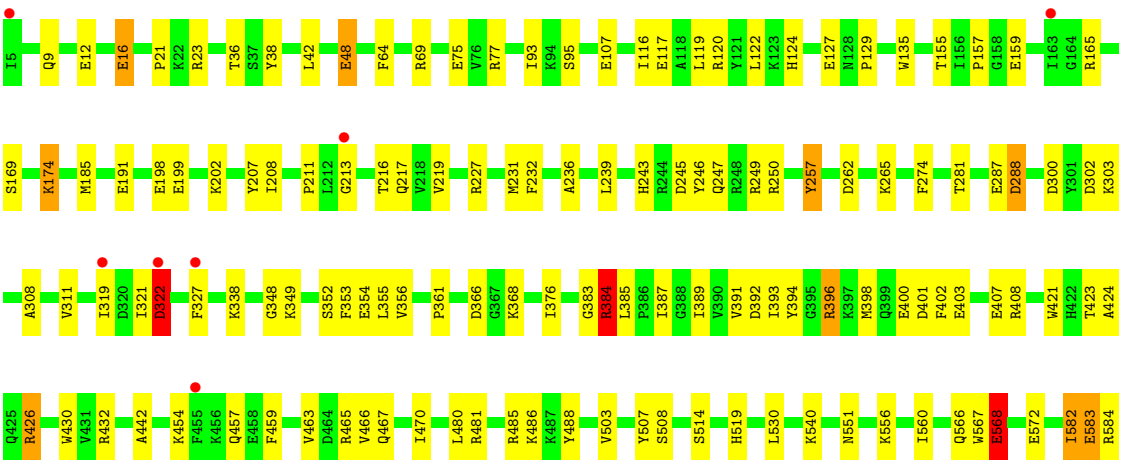


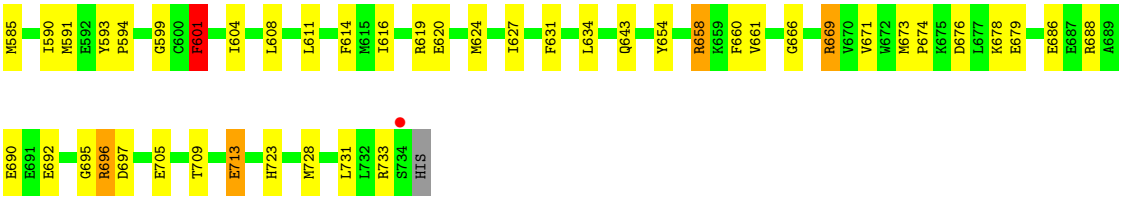


• Molecule 2: CO-methylating acetyl-CoA synthase

Chain B:






M585
I590
M591
E592
Y593
P594
G599
C600
F601
I604
L608
L611
F614
M615
I616
R619
E620
M624
I627
F631
L634
Q643
Y654
R658
K659
F660
V661
G666
R669
V670
V671
W672
M673
P674
K675
D676
L677
K678
E679
E686
E687
R688
A689
E690
E691
E692
G695
R696
D697
E705
T709
E713
H723
M728
L731
L732
R733
S734
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.12Å 142.12Å 290.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.02 – 2.50 45.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.02-2.50) 100.0 (45.02-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.235 0.208 , 0.233	Depositor DCC
R_{free} test set	1117 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11267	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: OH, ACT, FES, NI, NA, XCC, SF4

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	0.61	2/5259 (0.0%)	1.04	25/7118 (0.4%)
2	B	0.67	6/5995 (0.1%)	1.09	51/8111 (0.6%)
All	All	0.64	8/11254 (0.1%)	1.07	76/15229 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
2	B	0	11
All	All	0	21

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	384	ARG	CG-CD	9.26	1.80	1.52
2	B	384	ARG	CB-CG	-8.86	1.25	1.52
1	A	89	CYS	CB-SG	-8.59	1.52	1.81
1	A	184	TRP	CG-CD1	-7.17	1.19	1.36
2	B	384	ARG	CA-CB	7.05	1.66	1.53
2	B	696	ARG	CD-NE	6.96	1.55	1.46
2	B	384	ARG	CZ-NH1	6.01	1.41	1.32
2	B	396	ARG	CA-C	5.27	1.59	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	384	ARG	CA-CB-CG	-24.26	65.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	GLU	CG-CD-OE1	17.99	159.78	118.40
1	A	299	GLU	OE1-CD-OE2	-15.39	85.97	122.90
1	A	299	GLU	CG-CD-OE2	-14.38	85.31	118.40
2	B	601	PHE	CB-CG-CD2	-13.54	97.68	120.70
2	B	322	ASP	CB-CG-OD1	13.19	148.73	118.40
1	A	184	TRP	N-CA-CB	12.65	131.03	110.40
2	B	396	ARG	CD-NE-CZ	12.01	141.22	124.40
2	B	396	ARG	NE-CZ-NH1	-10.58	110.92	121.50
2	B	322	ASP	OD1-CG-OD2	-10.53	97.63	122.90
2	B	384	ARG	NE-CZ-NH1	-10.43	111.07	121.50
1	A	183	LEU	CA-C-N	-10.34	103.05	121.14
1	A	183	LEU	C-N-CA	-10.34	103.05	121.14
2	B	582	ILE	CA-C-N	-10.14	105.48	122.11
2	B	582	ILE	C-N-CA	-10.14	105.48	122.11
2	B	396	ARG	CA-CB-CG	-10.10	93.91	114.10
2	B	384	ARG	CB-CG-CD	-9.57	89.29	111.30
2	B	322	ASP	CB-CG-OD2	-9.54	96.47	118.40
2	B	384	ARG	CG-CD-NE	-9.50	91.09	112.00
1	A	184	TRP	CA-CB-CG	9.27	131.22	113.60
2	B	384	ARG	CD-NE-CZ	9.14	137.20	124.40
2	B	601	PHE	N-CA-CB	-8.86	95.88	110.23
1	A	352	VAL	CA-C-N	8.26	137.31	121.54
1	A	352	VAL	C-N-CA	8.26	137.31	121.54
2	B	601	PHE	CD1-CG-CD2	-7.93	106.70	118.60
1	A	397	LYS	CG-CD-CE	7.71	129.02	111.30
2	B	48	GLU	OE1-CD-OE2	-7.53	104.83	122.90
2	B	567	TRP	CA-C-N	-7.50	108.47	121.66
2	B	567	TRP	C-N-CA	-7.50	108.47	121.66
1	A	572	PHE	CB-CG-CD2	-7.42	108.09	120.70
2	B	601	PHE	CB-CA-C	7.25	121.50	109.53
1	A	8	GLU	CA-CB-CG	7.05	128.20	114.10
2	B	48	GLU	CG-CD-OE1	6.97	134.43	118.40
2	B	384	ARG	N-CA-C	-6.96	96.38	108.69
1	A	148	ARG	CB-CG-CD	-6.95	95.32	111.30
1	A	572	PHE	CB-CA-C	6.77	121.31	109.80
2	B	23	ARG	CG-CD-NE	6.58	126.48	112.00
2	B	396	ARG	NE-CZ-NH2	6.41	124.97	119.20
2	B	48	GLU	CG-CD-OE2	-6.36	103.77	118.40
1	A	89	CYS	N-CA-CB	-6.19	100.03	110.49
1	A	542	PHE	CB-CA-C	6.14	120.94	110.81
2	B	384	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	A	184	TRP	CB-CA-C	-6.03	97.39	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	321	ILE	CA-C-N	-5.97	114.31	123.14
2	B	321	ILE	C-N-CA	-5.97	114.31	123.14
1	A	8	GLU	CB-CG-CD	5.93	122.69	112.60
2	B	265	LYS	CG-CD-CE	-5.93	97.66	111.30
2	B	583	GLU	N-CA-C	-5.78	106.57	113.97
2	B	396	ARG	CG-CD-NE	-5.77	99.32	112.00
2	B	696	ARG	N-CA-C	-5.73	105.39	112.38
1	A	529	GLU	CA-CB-CG	-5.70	102.71	114.10
2	B	696	ARG	CD-NE-CZ	5.62	132.27	124.40
2	B	696	ARG	CA-C-N	5.61	128.07	120.38
2	B	696	ARG	C-N-CA	5.61	128.07	120.38
2	B	174	LYS	CB-CG-CD	-5.58	98.46	111.30
2	B	426	ARG	CB-CA-C	-5.48	110.28	116.63
2	B	620	GLU	CA-CB-CG	5.47	125.03	114.10
1	A	186	LYS	CB-CG-CD	-5.45	98.77	111.30
2	B	16	GLU	OE1-CD-OE2	-5.40	109.93	122.90
1	A	154	GLN	CA-CB-CG	5.38	124.85	114.10
2	B	287[A]	GLU	CA-C-N	-5.33	114.71	122.86
2	B	287[A]	GLU	C-N-CA	-5.33	114.71	122.86
2	B	287[B]	GLU	CA-C-N	-5.33	114.71	122.86
2	B	287[B]	GLU	C-N-CA	-5.33	114.71	122.86
2	B	288	ASP	CA-CB-CG	-5.32	107.28	112.60
2	B	568	GLU	N-CA-CB	5.32	118.73	110.44
2	B	583	GLU	OE1-CD-OE2	-5.27	110.25	122.90
2	B	658	ARG	CD-NE-CZ	5.14	131.60	124.40
1	A	590	TRP	CA-CB-CG	5.13	123.36	113.60
2	B	713	GLU	N-CA-C	5.12	116.54	111.07
1	A	42	LYS	CB-CA-C	-5.09	102.82	110.92
2	B	16	GLU	CG-CD-OE2	-5.04	106.80	118.40
1	A	529	GLU	CA-C-N	-5.01	111.80	121.58
1	A	529	GLU	C-N-CA	-5.01	111.80	121.58
2	B	384	ARG	N-CA-CB	5.01	119.23	110.81
2	B	669	ARG	CB-CG-CD	5.00	122.81	111.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	A	198	ASP	Peptide
1	A	199	GLU	Sidechain
1	A	299	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	A	466	GLY	Peptide
1	A	467	CYS	Peptide
1	A	542	PHE	Sidechain
1	A	572	PHE	Sidechain
1	A	578	GLU	Sidechain
1	A	610	GLU	Sidechain
2	B	16	GLU	Sidechain
2	B	257	TYR	Sidechain
2	B	322	ASP	Sidechain
2	B	384	ARG	Sidechain
2	B	408	ARG	Sidechain
2	B	48	GLU	Sidechain
2	B	568	GLU	Sidechain
2	B	583	GLU	Sidechain
2	B	601	PHE	Sidechain
2	B	658	ARG	Sidechain
2	B	713	GLU	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5147	0	5168	102	0
2	B	5837	0	5827	145	0
3	A	9	0	0	1	0
4	A	4	0	0	0	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
6	A	2	0	0	2	0
7	B	4	0	3	1	0
8	B	1	0	0	0	0
9	B	2	0	0	0	0
10	A	96	0	0	12	3
10	B	149	0	0	21	3
All	All	11267	0	10998	245	3

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 (245) 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)
2:B:384:ARG:CD	2:B:384:ARG:CG	1.80	1.60
2:B:384:ARG:CD	2:B:384:ARG:CB	2.18	1.22
2:B:384:ARG:CD	2:B:384:ARG:N	2.16	1.08
2:B:384:ARG:CG	2:B:384:ARG:NE	2.32	0.93
2:B:384:ARG:CD	2:B:384:ARG:HB2	2.00	0.91
2:B:384:ARG:CD	2:B:384:ARG:CA	2.48	0.91
2:B:733:ARG:NH2	10:B:907:HOH:O	2.04	0.89
2:B:384:ARG:N	2:B:384:ARG:HD2	1.87	0.88
2:B:127:GLU:OE1	10:B:901:HOH:O	1.93	0.85
1:A:528:GLU:OE2	10:A:801:HOH:O	1.95	0.84
2:B:560:ILE:HD11	2:B:568:GLU:HG2	1.59	0.84
2:B:338:LYS:O	10:B:902:HOH:O	1.95	0.84
2:B:21:PRO:HA	2:B:288:ASP:HB2	1.57	0.83
1:A:63:TYR:O	10:A:802:HOH:O	1.96	0.82
3:A:701:XCC:S4	10:A:811:HOH:O	2.40	0.80
2:B:705:GLU:OE2	10:B:903:HOH:O	1.97	0.80
2:B:236:ALA:HB3	2:B:239:LEU:HD12	1.63	0.80
2:B:624:MET:O	10:B:904:HOH:O	1.99	0.80
1:A:556:LEU:HB2	1:A:572:PHE:CE2	2.19	0.78
2:B:75:GLU:OE1	2:B:77:ARG:NH2	2.15	0.77
1:A:440:VAL:HG22	1:A:530:LYS:HD2	1.67	0.77
2:B:566:GLN:OE1	2:B:584[A]:ARG:NH1	2.17	0.76
2:B:383:GLY:HA2	2:B:384:ARG:HD2	1.67	0.75
2:B:690:GLU:OE2	2:B:696:ARG:HG2	1.87	0.74
2:B:709:THR:OG1	10:B:905:HOH:O	1.99	0.74
1:A:635:VAL:HG22	2:B:384:ARG:NH1	2.02	0.74
2:B:245:ASP:OD1	10:B:908:HOH:O	2.05	0.74
1:A:377:ALA:O	10:A:804:HOH:O	2.05	0.73
2:B:383:GLY:CA	2:B:384:ARG:HD2	2.19	0.73
2:B:383:GLY:C	2:B:384:ARG:HD2	2.15	0.72
2:B:198:GLU:OE2	10:B:909:HOH:O	2.08	0.72
1:A:269:VAL:HB	1:A:328:HIS:CD2	2.24	0.71
2:B:384:ARG:HB2	2:B:384:ARG:HD3	1.71	0.70
2:B:384:ARG:CG	2:B:384:ARG:HE	2.04	0.70
2:B:403:GLU:OE2	10:B:910:HOH:O	2.10	0.69
1:A:264:GLU:HB2	1:A:328:HIS:HB3	1.74	0.69
2:B:368:LYS:HD3	2:B:467:GLN:HE21	1.55	0.69
2:B:481:ARG:O	2:B:485:ARG:HG3	1.91	0.69
1:A:651:LYS:NZ	10:A:807:HOH:O	2.18	0.68
2:B:679:GLU:OE1	10:B:911:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:ARG:O	2:B:692:GLU:HG3	1.95	0.67
1:A:632:VAL:O	10:A:805:HOH:O	2.11	0.67
2:B:300:ASP:HB3	2:B:303:LYS:HG2	1.77	0.66
1:A:553:SER:OG	10:A:806:HOH:O	2.12	0.66
2:B:117:GLU:OE2	10:B:913:HOH:O	2.13	0.66
1:A:369:ARG:HD3	1:A:383:TYR:CE1	2.30	0.66
1:A:360:LYS:HE3	1:A:380:PRO:O	1.97	0.65
1:A:583:LYS:HE3	10:A:811:HOH:O	1.96	0.65
2:B:213:GLY:HA3	2:B:217:GLN:OE1	1.97	0.64
1:A:289:LYS:HE2	1:A:289:LYS:HA	1.81	0.63
1:A:434:MET:HE1	1:A:446:ILE:HB	1.81	0.63
2:B:159:GLU:HG3	2:B:185:MET:HB3	1.81	0.63
1:A:459:LYS:HG3	1:A:488:ASN:O	1.98	0.62
2:B:383:GLY:C	2:B:384:ARG:CD	2.72	0.61
2:B:245:ASP:O	2:B:249:ARG:HG3	2.01	0.61
2:B:421:TRP:CE3	2:B:432:ARG:HD3	2.36	0.60
2:B:616:ILE:O	2:B:674:PRO:HD3	2.01	0.60
1:A:367:HIS:NE2	1:A:413:LYS:NZ	2.50	0.60
2:B:673:MET:HE2	2:B:678:LYS:HA	1.84	0.60
1:A:443:GLU:N	1:A:443:GLU:OE2	2.29	0.60
2:B:361:PRO:O	2:B:465:ARG:NH1	2.34	0.59
1:A:430:PHE:CZ	1:A:434:MET:HE2	2.38	0.58
1:A:141:LYS:NZ	1:A:252:ASP:OD2	2.36	0.58
1:A:157:ASP:N	1:A:157:ASP:OD1	2.28	0.58
2:B:389:ILE:HG12	2:B:470:ILE:HG12	1.85	0.58
2:B:591:MET:HE2	2:B:731:LEU:HB3	1.86	0.58
2:B:568:GLU:O	2:B:572:GLU:HG3	2.03	0.58
2:B:38:TYR:CZ	2:B:42:LEU:HD11	2.39	0.58
1:A:5:ARG:NH2	1:A:646:GLU:OE2	2.37	0.58
2:B:686:GLU:O	2:B:690:GLU:HG3	2.04	0.57
1:A:603:MET:HE3	1:A:607:GLU:OE1	2.03	0.57
2:B:530:LEU:HD13	2:B:601:PHE:HB3	1.86	0.57
1:A:329:LEU:HD22	1:A:500:GLN:HG2	1.87	0.57
2:B:361:PRO:HB3	2:B:394:TYR:CZ	2.39	0.57
2:B:392:ASP:OD2	10:B:915:HOH:O	2.17	0.56
2:B:366:ASP:OD2	2:B:465:ARG:HA	2.05	0.56
2:B:601:PHE:HD1	2:B:601:PHE:H	1.53	0.56
1:A:52:PHE:CZ	1:A:471:LYS:HA	2.40	0.56
1:A:157:ASP:OD1	1:A:160:THR:OG1	2.22	0.55
1:A:546[A]:CYS:HB2	6:A:705:OH:O	2.05	0.55
2:B:566:GLN:OE1	2:B:584[B]:ARG:NH1	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:HIS:CD2	1:A:578:GLU:OE1	2.60	0.55
2:B:202:LYS:HD3	2:B:207:TYR:CE1	2.41	0.55
2:B:116:ILE:O	2:B:120[A]:ARG:HG3	2.06	0.55
2:B:582:ILE:HD12	2:B:643:GLN:HG3	1.88	0.55
1:A:68:CYS:HB2	1:A:96:ILE:HG12	1.89	0.55
2:B:400:GLU:O	2:B:403:GLU:HG3	2.07	0.54
2:B:384:ARG:HE	2:B:384:ARG:HG2	1.72	0.54
1:A:76:CYS:SG	1:A:88:ILE:HD12	2.48	0.54
1:A:46:LYS:HE2	1:A:54:GLU:OE2	2.07	0.54
1:A:499:ALA:HB1	1:A:542:PHE:CD1	2.42	0.54
1:A:350:VAL:HB	1:A:355:ILE:HD13	1.89	0.54
1:A:280:HIS:HB3	1:A:350:VAL:HG12	1.90	0.54
1:A:351:ASP:OD1	1:A:352:VAL:N	2.38	0.54
2:B:508:SER:O	2:B:551:ASN:HA	2.08	0.53
2:B:319:ILE:HG12	2:B:457:GLN:OE1	2.08	0.53
1:A:36:MET:HA	1:A:36:MET:HE2	1.90	0.53
1:A:315[B]:CYS:SG	1:A:316:CYS:N	2.82	0.53
1:A:195:GLU:O	1:A:199:GLU:HB2	2.08	0.53
2:B:423:THR:HG22	2:B:430:TRP:HB3	1.91	0.52
2:B:185:MET:HG3	2:B:208:ILE:HG22	1.89	0.52
2:B:69:ARG:NH2	2:B:75:GLU:HG3	2.23	0.52
2:B:584[A]:ARG:HB2	2:B:593:TYR:CD1	2.45	0.52
2:B:590:ILE:HD11	2:B:614:PHE:CE2	2.44	0.52
1:A:480:THR:OG1	1:A:634:PRO:HB2	2.10	0.52
2:B:116:ILE:O	2:B:120[C]:ARG:HG3	2.09	0.52
2:B:95:SER:N	10:B:931:HOH:O	2.36	0.51
2:B:507:TYR:CZ	2:B:540:LYS:HG3	2.45	0.51
2:B:590:ILE:O	2:B:594:PRO:HG3	2.09	0.51
1:A:670:TYR:N	10:A:803:HOH:O	2.03	0.51
1:A:35:GLU:OE1	1:A:416:HIS:NE2	2.38	0.51
2:B:117:GLU:OE1	2:B:216:THR:OG1	2.26	0.51
2:B:354:GLU:OE1	10:B:916:HOH:O	2.18	0.51
2:B:64:PHE:CE2	2:B:75:GLU:HG2	2.46	0.50
1:A:469:ASN:OD1	1:A:471:LYS:HG3	2.12	0.50
2:B:322:ASP:OD1	2:B:322:ASP:O	2.30	0.50
2:B:368:LYS:HD3	2:B:467:GLN:NE2	2.23	0.50
2:B:459:PHE:O	2:B:463:VAL:HG22	2.10	0.50
1:A:570:VAL:O	1:A:648:ARG:HD3	2.11	0.50
2:B:9:GLN:HA	2:B:12:GLU:HG3	1.92	0.50
2:B:584[B]:ARG:HB2	2:B:593:TYR:CD1	2.46	0.50
2:B:355:LEU:HA	2:B:407:GLU:OE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:NE2	1:A:125:GLU:OE2	2.45	0.49
1:A:196:LYS:HE3	1:A:623:VAL:O	2.12	0.49
1:A:464:PHE:HZ	1:A:481:ILE:HG22	1.77	0.49
2:B:300:ASP:OD2	2:B:303:LYS:HE3	2.12	0.49
2:B:676:ASP:OD1	2:B:676:ASP:N	2.44	0.49
1:A:476:GLU:O	1:A:480:THR:HG23	2.13	0.49
1:A:112:HIS:ND1	1:A:240:ASP:OD1	2.44	0.49
1:A:479:ILE:HD12	1:A:507:PHE:CE2	2.48	0.49
2:B:503:VAL:O	2:B:556:LYS:HE2	2.14	0.48
1:A:184:TRP:CE2	1:A:246:ILE:HG12	2.47	0.48
1:A:234:LEU:HD22	1:A:593:THR:OG1	2.14	0.48
1:A:282:HIS:CD2	6:A:705:OH:O	2.66	0.48
1:A:603:MET:HE3	1:A:607:GLU:CD	2.38	0.48
2:B:356:VAL:HG22	2:B:391:VAL:HB	1.96	0.48
2:B:165:ARG:HG3	2:B:191:GLU:HB2	1.95	0.48
2:B:227:ARG:O	2:B:231:MET:HG3	2.14	0.48
1:A:112:HIS:NE2	1:A:583:LYS:HD2	2.29	0.48
2:B:124:HIS:ND1	2:B:129:PRO:HA	2.29	0.48
2:B:604:ILE:HG21	2:B:634:LEU:HG	1.95	0.48
2:B:556:LYS:NZ	10:B:936:HOH:O	2.47	0.47
1:A:149:LEU:HD21	1:A:184:TRP:CE3	2.50	0.47
2:B:398:MET:HE3	2:B:402:PHE:HB2	1.95	0.47
1:A:36:MET:HE3	1:A:418:PRO:HG3	1.95	0.47
1:A:639:ARG:NH1	2:B:348:GLY:O	2.48	0.47
2:B:288:ASP:N	2:B:288:ASP:OD2	2.32	0.47
2:B:257:TYR:O	2:B:281:THR:HA	2.14	0.46
2:B:507:TYR:OH	2:B:540:LYS:HG3	2.15	0.46
2:B:673:MET:HE2	2:B:678:LYS:CA	2.45	0.46
1:A:482:LEU:HD22	1:A:502:PHE:CD1	2.51	0.46
2:B:174:LYS:HE2	2:B:302:ASP:OD1	2.15	0.46
2:B:608:LEU:HD21	2:B:627:ILE:HB	1.96	0.46
1:A:269:VAL:HG11	1:A:328:HIS:HB2	1.97	0.46
1:A:355:ILE:HG22	1:A:379:MET:HE1	1.97	0.46
2:B:303:LYS:HA	10:B:991:HOH:O	2.14	0.46
1:A:50:ASP:O	1:A:54:GLU:HG3	2.16	0.45
2:B:322:ASP:O	2:B:322:ASP:CG	2.58	0.45
2:B:262:ASP:C	2:B:262:ASP:OD1	2.59	0.45
2:B:396:ARG:HD2	2:B:396:ARG:HA	1.42	0.45
1:A:294:ALA:HB1	1:A:309:ILE:HG21	1.98	0.45
1:A:587:ILE:HA	1:A:590:TRP:NE1	2.31	0.45
2:B:619:ARG:HA	2:B:631:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120[C]:ARG:NE	10:B:913:HOH:O	2.42	0.45
2:B:243:HIS:O	2:B:247:GLN:HG2	2.17	0.45
2:B:352:SER:HA	2:B:387:ILE:O	2.16	0.45
2:B:393:ILE:CD1	2:B:466:VAL:HG22	2.47	0.45
2:B:398:MET:CE	2:B:402:PHE:HB2	2.47	0.45
2:B:36:THR:HG21	2:B:93:ILE:HD11	1.99	0.45
1:A:443:GLU:N	1:A:443:GLU:CD	2.74	0.44
2:B:660:PHE:O	2:B:666:GLY:HA2	2.18	0.44
2:B:530:LEU:HD13	2:B:601:PHE:CB	2.46	0.44
1:A:264:GLU:HB2	1:A:328:HIS:CB	2.44	0.44
1:A:314:MET:HE3	1:A:336:SER:HB2	2.00	0.44
2:B:107:GLU:HG3	2:B:274:PHE:CE2	2.52	0.44
2:B:384:ARG:CB	2:B:384:ARG:HD3	2.23	0.44
2:B:169:SER:HB3	2:B:199:GLU:HG2	1.99	0.44
2:B:485:ARG:HA	2:B:488:TYR:CD2	2.53	0.44
2:B:608:LEU:HD12	2:B:611:LEU:HD12	2.00	0.44
1:A:329:LEU:CD2	1:A:500:GLN:HG2	2.48	0.44
2:B:349:LYS:NZ	10:B:941:HOH:O	2.51	0.44
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.83	0.43
2:B:232:PHE:CG	7:B:801:ACT:H3	2.53	0.43
2:B:585:MET:HB3	2:B:585:MET:HE3	1.73	0.43
2:B:480:LEU:HD23	2:B:480:LEU:HA	1.81	0.43
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.77	0.43
1:A:551:ARG:O	1:A:554:ASP:HB2	2.19	0.43
2:B:155:THR:O	2:B:157:PRO:HD3	2.19	0.43
1:A:484:GLU:O	1:A:488:ASN:ND2	2.51	0.43
1:A:587:ILE:HA	1:A:590:TRP:CD1	2.53	0.43
2:B:376:ILE:HD11	2:B:442:ALA:O	2.19	0.43
1:A:65:GLY:HA2	1:A:605:PRO:HB2	2.01	0.43
2:B:120[C]:ARG:NH1	10:B:913:HOH:O	2.37	0.43
1:A:453:ILE:HG13	1:A:458:LEU:HB2	2.00	0.43
2:B:671:VAL:HG12	2:B:723:HIS:CE1	2.52	0.43
1:A:2:PRO:N	10:A:827:HOH:O	2.51	0.43
1:A:636:VAL:CG1	1:A:640:LYS:HE3	2.49	0.43
2:B:308:ALA:O	2:B:311:VAL:HG12	2.19	0.43
1:A:160:THR:O	1:A:164:GLU:HG3	2.18	0.43
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.76	0.43
1:A:143:ARG:NH1	1:A:156:LYS:O	2.43	0.42
2:B:246:TYR:CE2	2:B:250:ARG:HD2	2.54	0.42
2:B:669:ARG:NH2	2:B:728:MET:HE2	2.34	0.42
1:A:148:ARG:HD2	1:A:148:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:VAL:HG11	2:B:349:LYS:HB3	2.01	0.42
1:A:139:PRO:O	1:A:143:ARG:HG3	2.19	0.42
2:B:591:MET:HE2	2:B:731:LEU:CB	2.49	0.42
2:B:327:PHE:CD2	2:B:327:PHE:C	2.97	0.42
1:A:319:ASN:HD22	1:A:545:SER:HA	1.84	0.42
2:B:135:TRP:HA	2:B:211:PRO:HB2	2.02	0.42
2:B:216:THR:O	2:B:219:VAL:HG12	2.19	0.42
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.85	0.42
2:B:619:ARG:HA	2:B:631:PHE:CE1	2.55	0.42
1:A:20:TRP:O	1:A:21:GLU:C	2.63	0.42
2:B:119:LEU:O	2:B:122:LEU:HB2	2.19	0.42
1:A:2:PRO:HB2	1:A:647:TYR:CE2	2.55	0.41
1:A:606:LEU:HD13	1:A:613:TYR:CD2	2.55	0.41
2:B:77:ARG:HH21	2:B:77:ARG:HD2	1.69	0.41
1:A:184:TRP:CD1	1:A:246:ILE:HG13	2.55	0.41
2:B:308:ALA:HA	2:B:311:VAL:HG12	2.02	0.41
2:B:669:ARG:CZ	2:B:728:MET:HE2	2.50	0.41
2:B:695:GLY:C	2:B:697:ASP:N	2.73	0.41
1:A:467:CYS:CB	1:A:580:MET:HB3	2.50	0.41
1:A:39:LYS:O	1:A:42:LYS:HB3	2.21	0.41
2:B:127:GLU:N	2:B:127:GLU:CD	2.78	0.41
2:B:393:ILE:HD12	2:B:466:VAL:HG22	2.02	0.41
2:B:454:LYS:HD2	2:B:454:LYS:HA	1.86	0.41
2:B:654:TYR:CZ	2:B:660:PHE:HA	2.55	0.41
1:A:127:ALA:HA	1:A:159:MET:SD	2.60	0.41
1:A:3:ARG:NH1	10:A:819:HOH:O	2.43	0.41
2:B:519:HIS:HA	10:B:963:HOH:O	2.21	0.41
1:A:293:ALA:HB1	1:A:397:LYS:HG3	2.03	0.41
1:A:528:GLU:HG2	1:A:533:LEU:O	2.21	0.41
2:B:353:PHE:HA	2:B:426:ARG:O	2.21	0.41
2:B:486:LYS:HB3	2:B:486:LYS:HE3	1.71	0.41
1:A:136:ILE:HD13	1:A:136:ILE:HA	1.87	0.41
1:A:148:ARG:HD3	10:A:816:HOH:O	2.21	0.40
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.75	0.40
1:A:270:LEU:HB2	1:A:417:ILE:HG21	2.03	0.40
1:A:196:LYS:HA	1:A:196:LYS:HD3	1.82	0.40
2:B:120[A]:ARG:NH1	10:B:913:HOH:O	2.38	0.40
1:A:144:ARG:HH21	1:A:144:ARG:HG3	1.86	0.40
1:A:175:ARG:HD2	1:A:205:SER:O	2.21	0.40
1:A:552:ALA:O	1:A:555:ILE:HB	2.22	0.40
2:B:250:ARG:NH2	2:B:514:SER:O	2.50	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:886:HOH:O	10:B:1040:HOH:O[5_554]	1.86	0.34
10:A:862:HOH:O	10:B:953:HOH:O[5_554]	1.88	0.32
10:A:858:HOH:O	10:B:939:HOH:O[5_554]	2.03	0.17

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	671/669 (100%)	638 (95%)	30 (4%)	3 (0%)	30	49
2	B	737/731 (101%)	717 (97%)	17 (2%)	3 (0%)	30	49
All	All	1408/1400 (101%)	1355 (96%)	47 (3%)	6 (0%)	30	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	GLU
2	B	599	GLY
1	A	266	ASN
1	A	353	GLN
2	B	424	ALA
2	B	661	VAL

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	552/548 (101%)	552 (100%)	0	100 100
2	B	622/615 (101%)	619 (100%)	3 (0%)	81 92
All	All	1174/1163 (101%)	1171 (100%)	3 (0%)	87 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	384	ARG
2	B	401[A]	ASP
2	B	401[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	HIS
1	A	361	GLN
2	B	9	GLN
2	B	467	GLN
2	B	577	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are modelled with single atom and 3 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	SF4	A	703	1	0,12,12	-	-	-		
4	FES	A	702	1	0,4,4	-	-	-		
5	SF4	B	804	2	0,12,12	-	-	-		
3	XCC	A	701	1,10,6	0,12,12	-	-	-		
7	ACT	B	801	9	3,3,3	1.52	1 (33%)	3,3,3	1.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	702	1	-	-	0/1/1/1
5	SF4	A	703	1	-	-	0/6/5/5
3	XCC	A	701	1,10,6	-	-	0/4/4/4
5	SF4	B	804	2	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	ACT	CH3-C	2.45	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

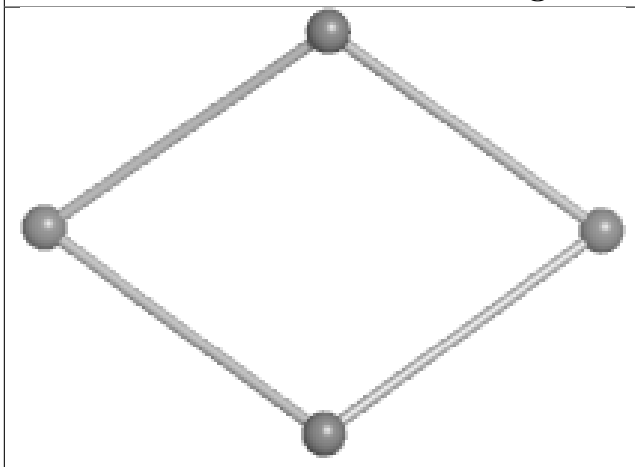
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	XCC	1	0
7	B	801	ACT	1	0

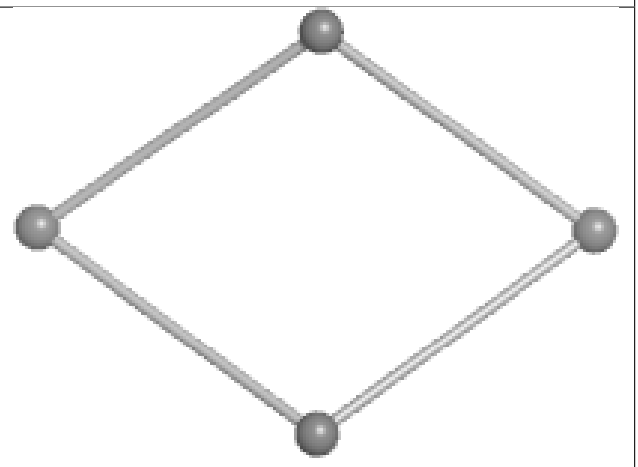
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

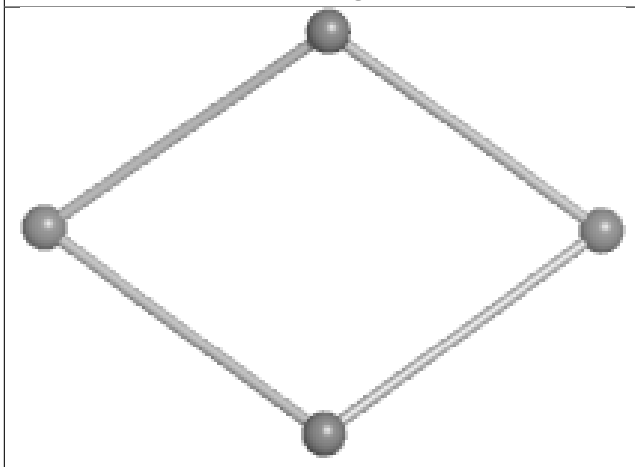
Ligand FES A 702



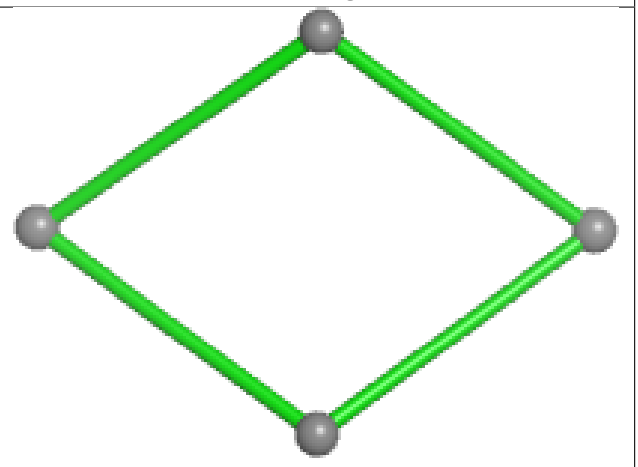
Bond lengths



Bond angles

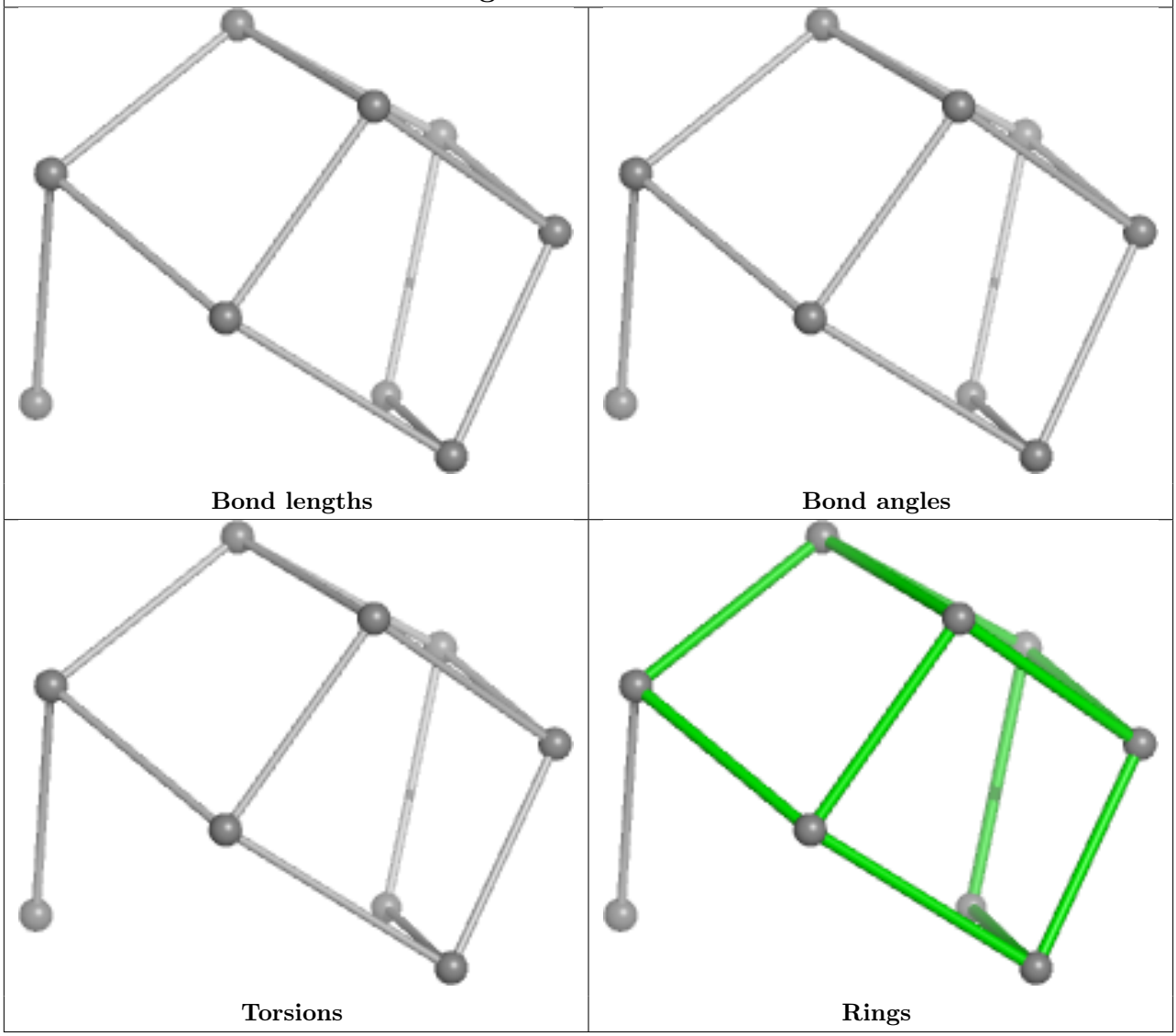


Torsions



Rings

Ligand XCC A 701



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	669/669 (100%)	-0.04	4 (0%)	85	83	25, 52, 71, 92	4 (0%)
2	B	730/731 (99%)	-0.08	8 (1%)	78	75	17, 52, 65, 81	8 (1%)
All	All	1399/1400 (99%)	-0.06	12 (0%)	81	78	17, 52, 68, 92	12 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	CYS	3.3
2	B	319	ILE	3.0
2	B	213	GLY	2.7
2	B	322	ASP	2.5
2	B	5	ILE	2.5
2	B	327	PHE	2.5
1	A	179	PHE	2.4
1	A	278	ALA	2.4
2	B	163	ILE	2.4
2	B	455	PHE	2.2
2	B	734	SER	2.2
1	A	470	LEU	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 oligosaccharides in this entry.

6.4 Ligands (i)

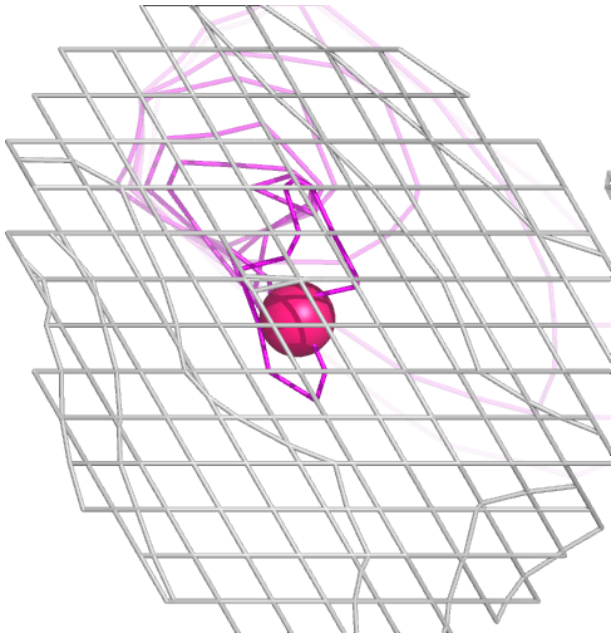
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

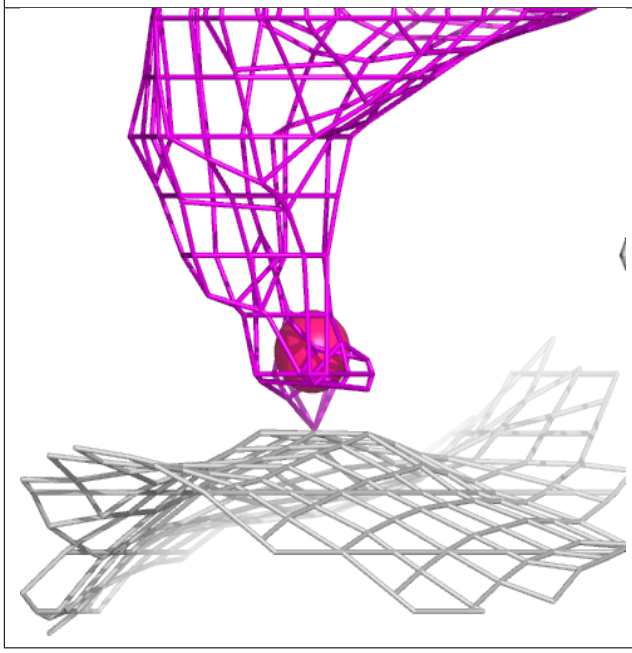
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OH	A	704	1/1	0.87	0.59	67,67,67,67	0
7	ACT	B	801	4/4	0.94	0.13	51,51,51,51	0
6	OH	A	705	1/1	0.96	0.05	56,56,56,56	0
3	XCC	A	701	9/9	0.96	0.06	63,75,76,79	7
8	NA	B	802	1/1	0.96	0.04	53,53,53,53	0
4	FES	A	702	4/4	0.98	0.04	43,43,43,44	0
5	SF4	A	703	8/8	0.99	0.04	42,43,44,45	0
5	SF4	B	804	8/8	0.99	0.03	48,50,51,52	0
9	NI	B	803	1/1	0.99	0.03	57,57,57,57	0
9	NI	B	805[A]	1/1	0.99	0.04	72,72,72,72	0

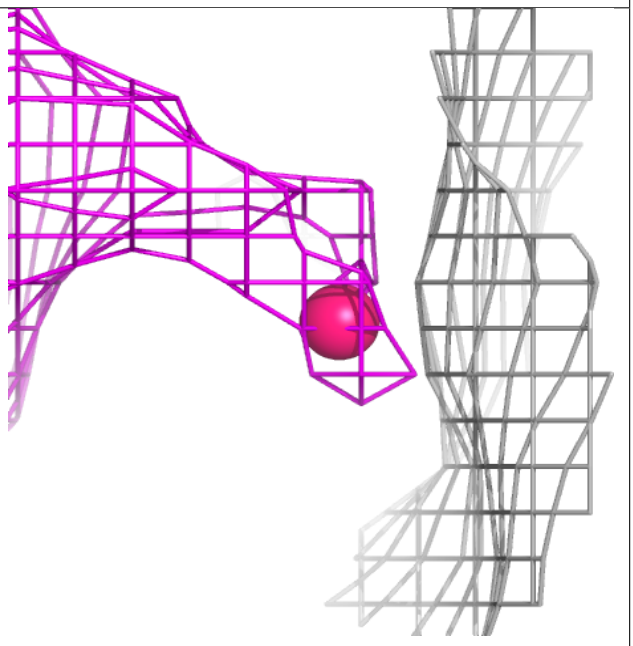
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OH A 704:

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

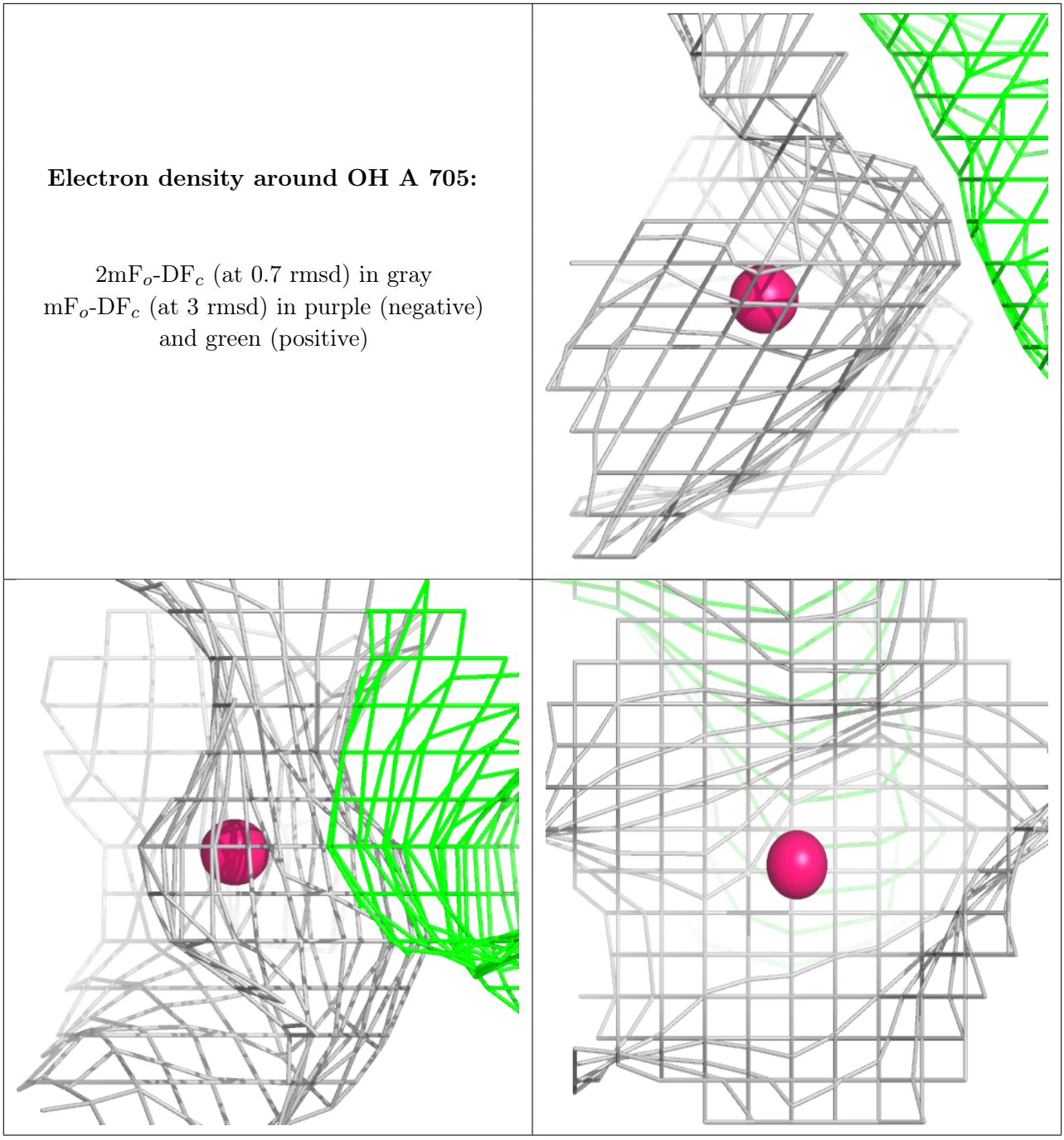






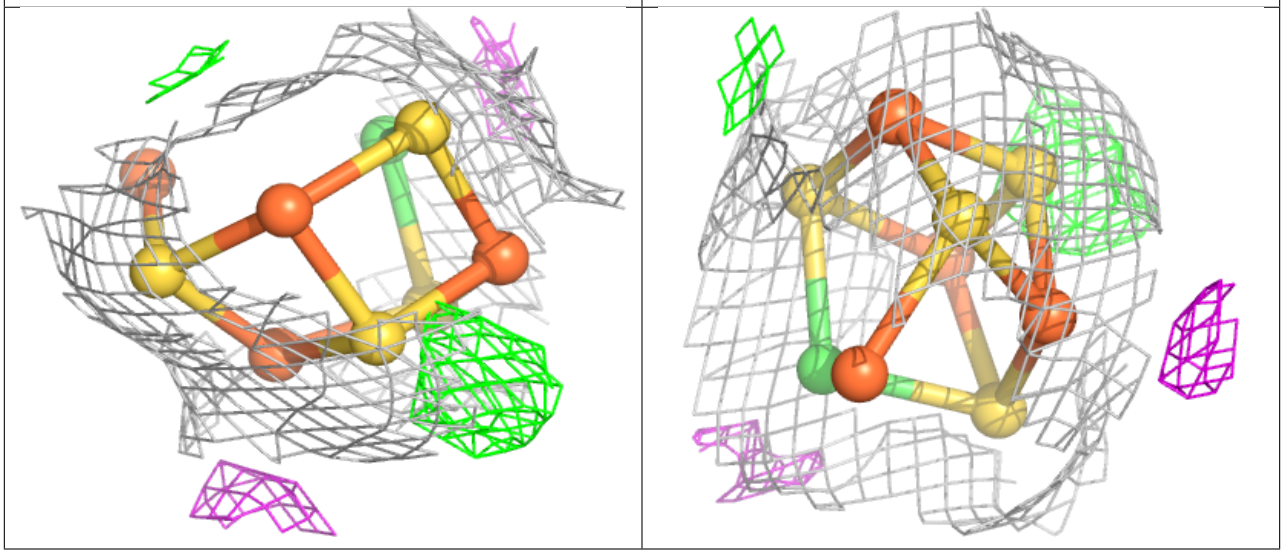
Electron density around OH A 705:

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



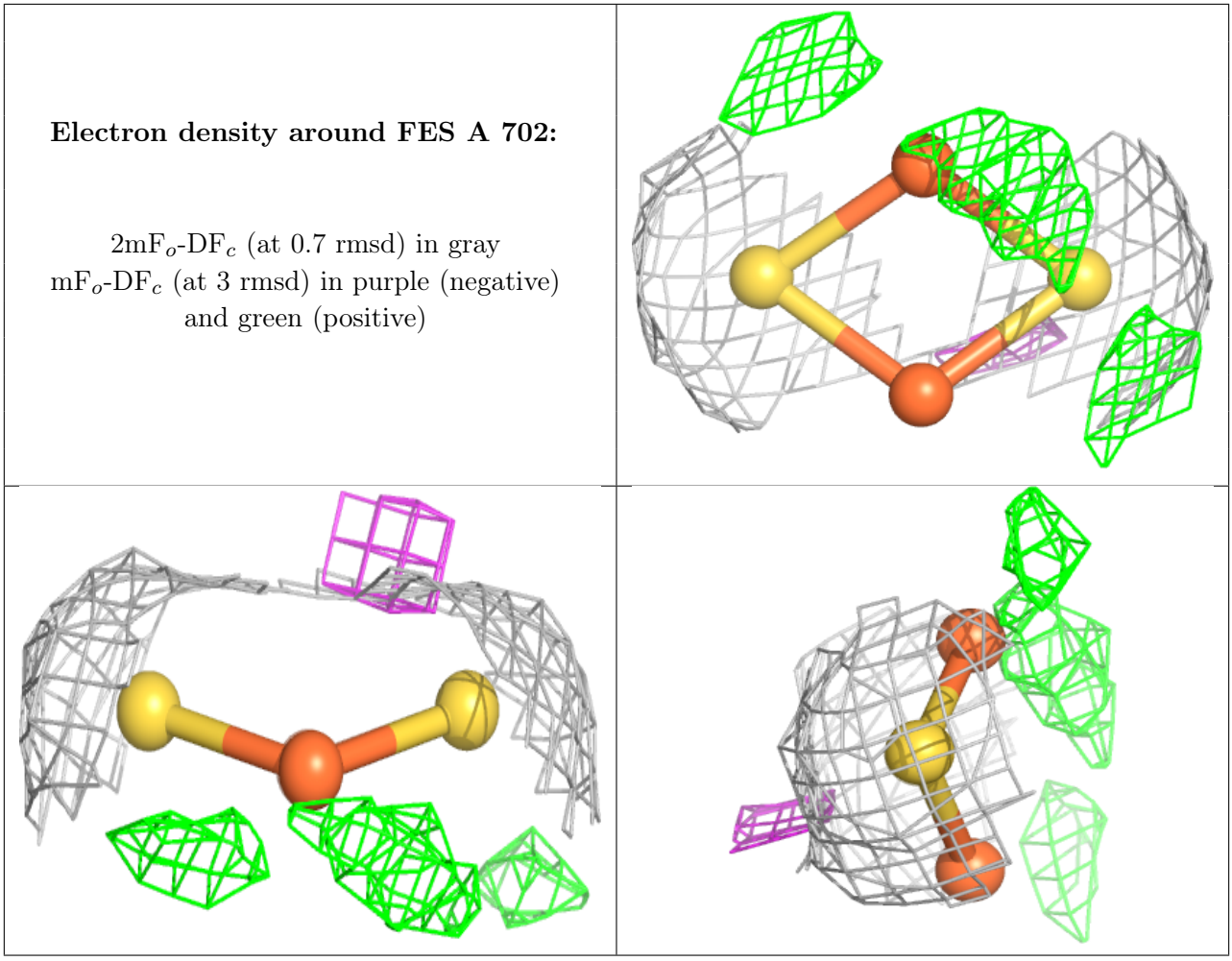
Electron density around XCC A 701:

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



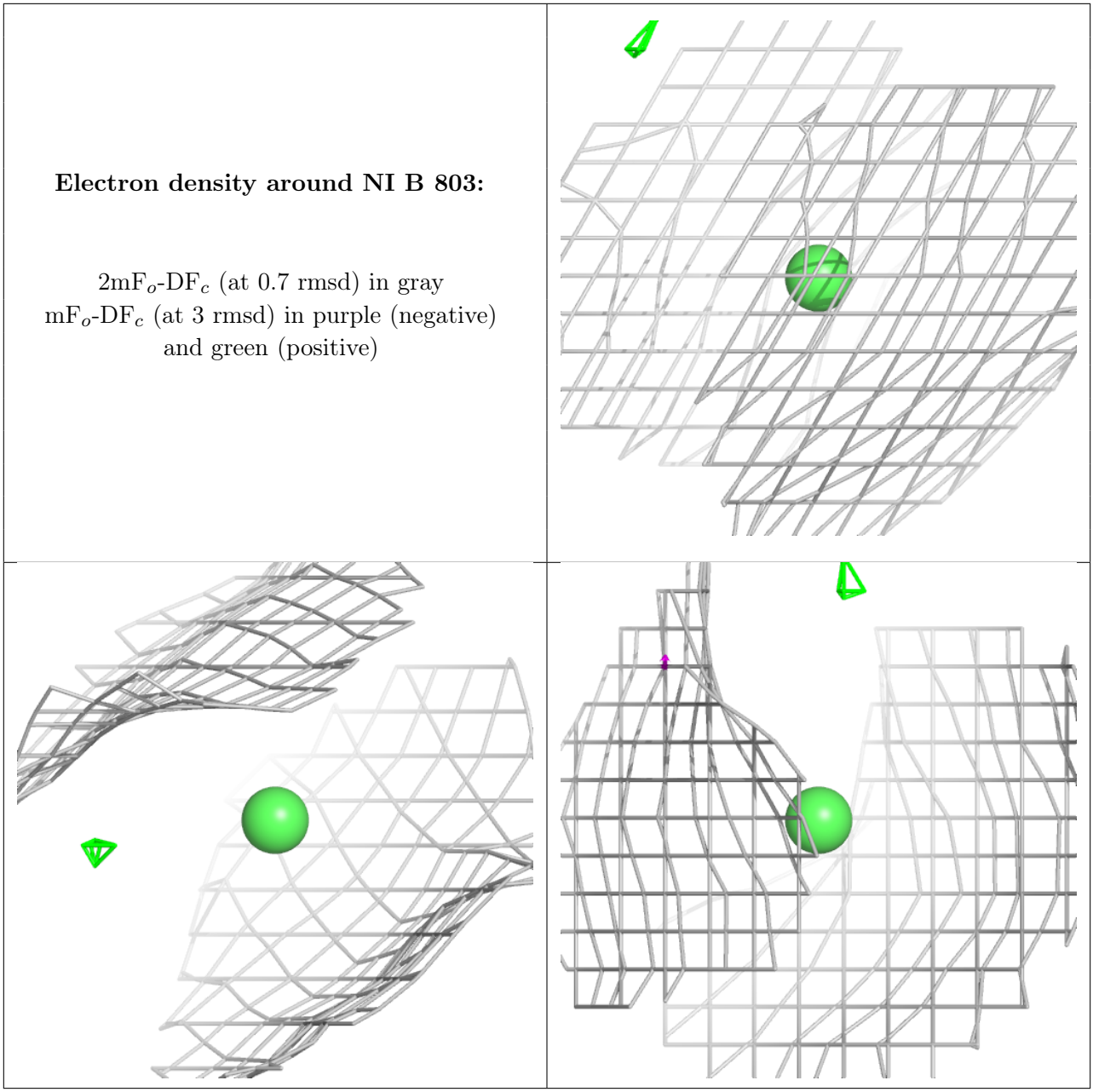
Electron density around FES A 702:

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



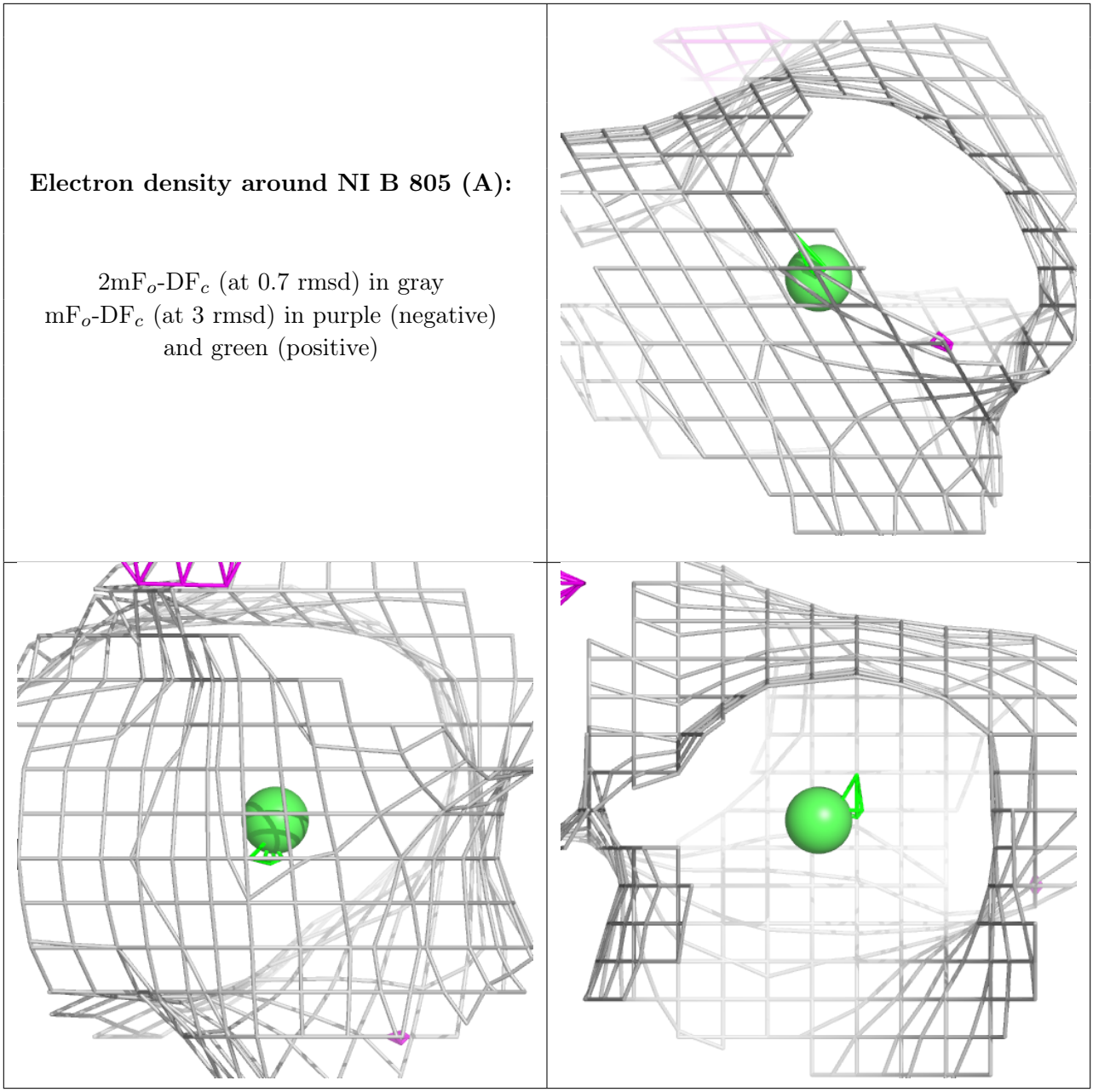
Electron density around NI B 803:

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



Electron density around NI B 805 (A):

$2mF_o$-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.