Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2026 – 03:09 pm BST

PDB ID	:	8CMW / pdb_00008cmw
Title	:	A225L variant of the CODH/ACS complex of C. hydrogenoformans
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Deposited on	:	2023-02-21
Resolution	:	2.60 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:

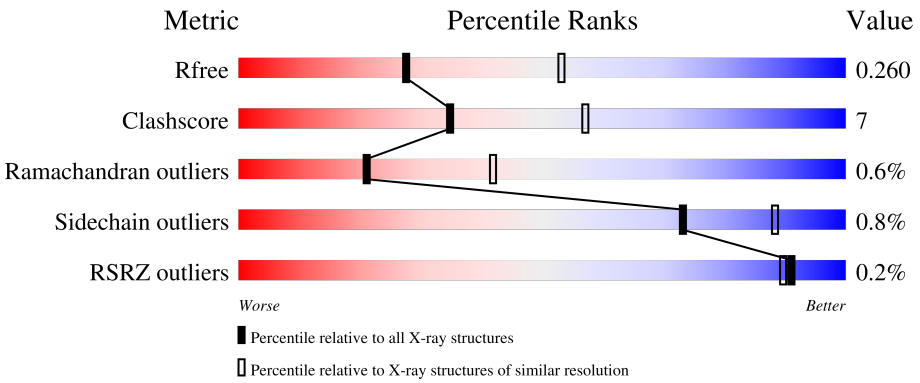
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	83% 17% •
2	B	730	83% 16% •

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	-
7	ACT	B	801	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11173 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	5153	3267	888	962	36	0	4	0

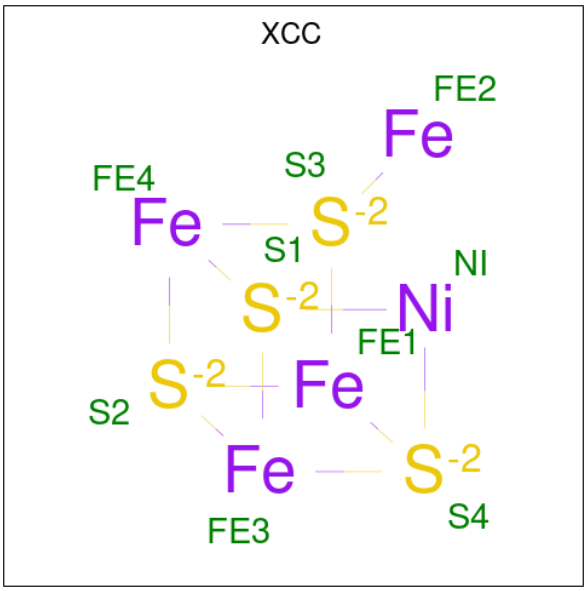
- Molecule 2 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	730	5837	3745	981	1082	29	8	8	0

There are 3 discrepancies between the modelled and reference sequences:

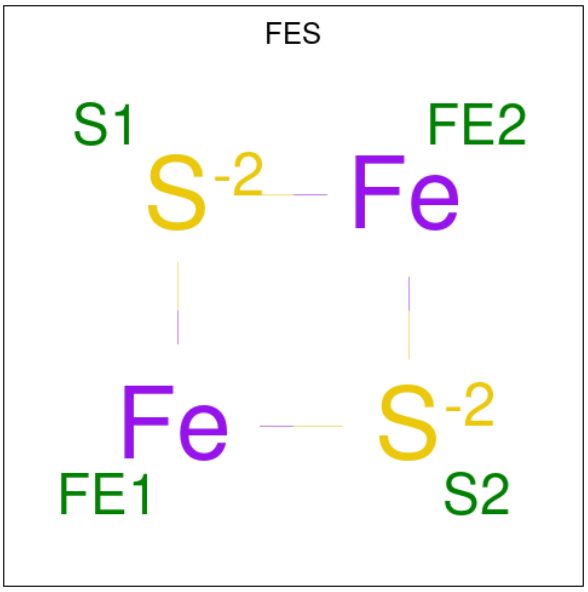
Chain	Residue	Modelled	Actual	Comment	Reference
B	225	LEU	ALA	engineered mutation	UNP Q3ACS4
B	733	ARG	-	expression tag	UNP Q3ACS4
B	734	SER	-	expression tag	UNP Q3ACS4

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



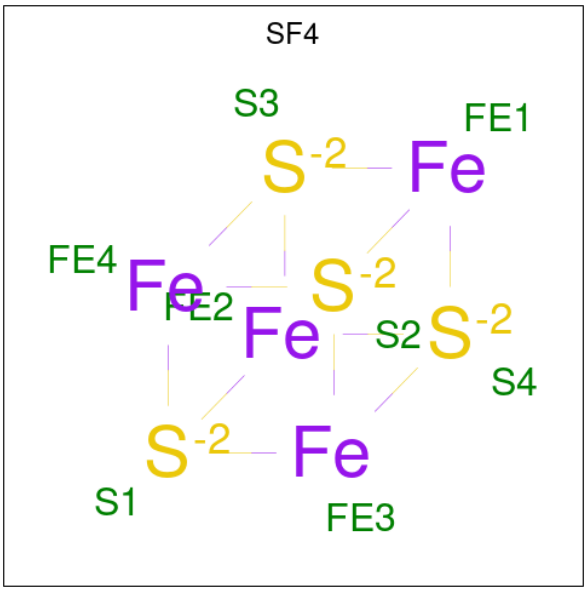
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
3	A	1	9	4	1	4	0	0

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



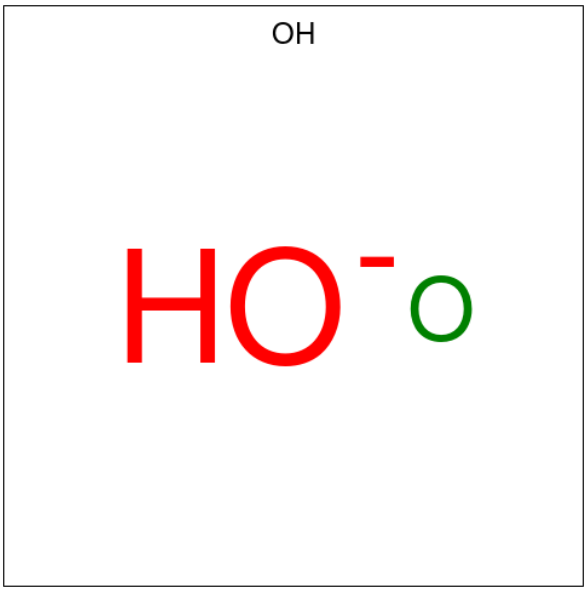
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0

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



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

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



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

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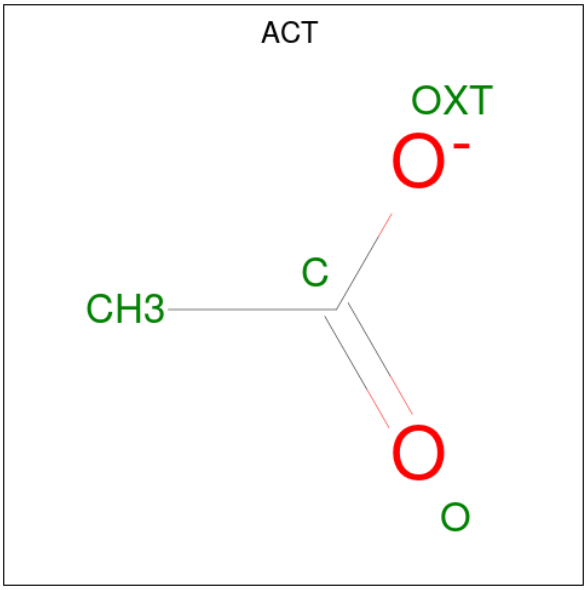
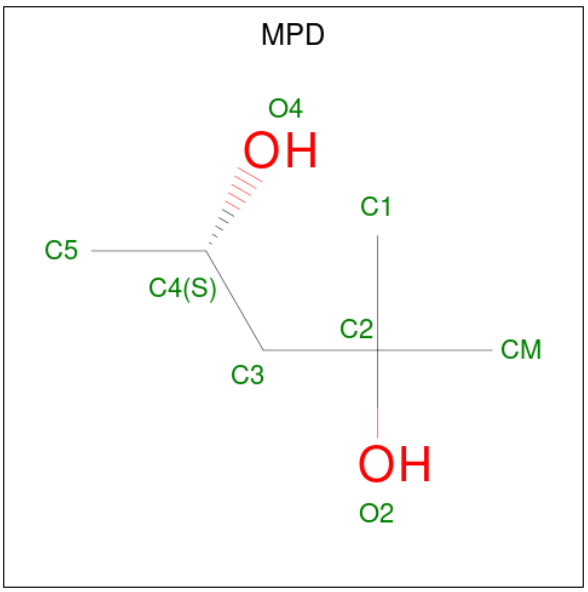
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

- 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 (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	8	6	2	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 10 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	53	53	53	0	0
			Total	O		
11	B	84	84	84	0	0

3 Residue-property plots (i)

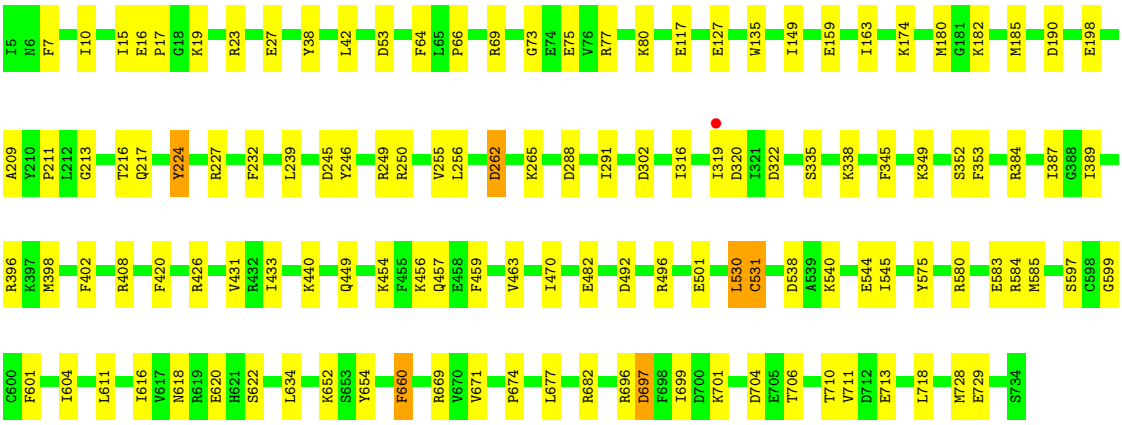
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 83% 17%

• Molecule 2: CO-methylating acetyl-CoA synthase

Chain B: 83% 16%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	141.72Å 141.72Å 290.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.94 – 2.60 22.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (22.94-2.60) 99.6 (22.94-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.203 , 0.264 0.208 , 0.260	Depositor DCC
R_{free} test set	2100 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11173	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, NA, OH, ACT, MPD, 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	0.41	0/5265	0.65	3/7126 (0.0%)
2	B	0.41	0/5995	0.63	0/8112
All	All	0.41	0/11260	0.64	3/15238 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	544	GLY	N-CA-C	6.44	120.01	110.60
1	A	184	TRP	N-CA-CB	6.44	120.25	110.28
1	A	590	TRP	CA-CB-CG	5.24	123.56	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	530	LEU	Peptide
2	B	696	ARG	Peptide

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	5153	0	5173	81	0
2	B	5837	0	5832	87	1
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	1	0
6	A	2	0	0	2	0
7	B	4	0	3	2	0
8	B	8	0	14	1	0
9	B	1	0	0	0	0
10	B	2	0	0	0	0
11	A	53	0	0	6	1
11	B	84	0	0	12	1
All	All	11173	0	11022	165	2

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 7.

All (165) 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:245:ASP:OD1	11:B:901:HOH:O	1.87	0.90
2:B:127:GLU:OE1	11:B:902:HOH:O	1.89	0.90
2:B:501:GLU:OE1	11:B:903:HOH:O	1.92	0.88
1:A:476:GLU:OE2	2:B:338:LYS:NZ	2.08	0.85
2:B:322:ASP:O	11:B:904:HOH:O	1.93	0.85
1:A:369:ARG:NH2	11:A:803:HOH:O	2.07	0.82
1:A:45:VAL:O	11:A:801:HOH:O	1.99	0.79
2:B:319:ILE:HG12	2:B:457:GLN:OE1	1.88	0.73
2:B:53:ASP:OD1	2:B:80:LYS:NZ	2.20	0.70
1:A:653:GLY:O	1:A:657:GLN:HG3	1.92	0.70
2:B:408:ARG:NH1	2:B:538:ASP:OD2	2.25	0.70
1:A:121:HIS:NE2	1:A:125:GLU:OE2	2.25	0.69
1:A:350:VAL:HB	1:A:355:ILE:HD13	1.75	0.68
1:A:186:LYS:NZ	11:A:802:HOH:O	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:OE1	1:A:325:ARG:NH1	2.28	0.67
2:B:245:ASP:O	2:B:249:ARG:HG2	1.95	0.67
2:B:583:GLU:OE1	2:B:584[B]:ARG:NH2	2.28	0.66
2:B:262:ASP:OD2	11:B:907:HOH:O	2.14	0.66
2:B:27:GLU:OE1	11:B:908:HOH:O	2.14	0.65
1:A:112:HIS:ND1	1:A:240:ASP:OD1	2.29	0.64
1:A:310:ASN:OD1	1:A:328:HIS:NE2	2.32	0.62
2:B:69:ARG:NH1	2:B:73:GLY:O	2.32	0.61
1:A:316:CYS:SG	1:A:546[C]:CYS:HB3	2.41	0.60
1:A:565:VAL:O	11:A:804:HOH:O	2.15	0.60
1:A:271:ASP:HB3	1:A:274:LYS:HB2	1.84	0.60
2:B:232:PHE:CG	7:B:801:ACT:H3	2.37	0.59
1:A:428:PHE:O	1:A:543:MET:HG2	2.03	0.59
1:A:401:ARG:O	1:A:405:GLU:HG2	2.03	0.58
2:B:23:ARG:HD3	2:B:288:ASP:OD2	2.03	0.57
1:A:167:GLU:O	1:A:171:GLU:HG3	2.04	0.57
1:A:340:ILE:HD13	1:A:345:MET:HG2	1.85	0.57
2:B:163:ILE:HG22	2:B:265:LYS:HD3	1.85	0.56
2:B:710:THR:OG1	2:B:713:GLU:HG3	2.05	0.56
1:A:36:MET:HE3	1:A:418:PRO:HD3	1.88	0.56
2:B:575:TYR:CE1	2:B:580:ARG:HG2	2.41	0.56
2:B:232:PHE:CD1	7:B:801:ACT:H3	2.41	0.55
1:A:112:HIS:NE2	1:A:583:LYS:HD2	2.21	0.55
2:B:75:GLU:OE1	2:B:77:ARG:NH1	2.27	0.55
2:B:352:SER:HA	2:B:387:ILE:O	2.06	0.55
2:B:345:PHE:HB2	2:B:431:VAL:HG22	1.88	0.55
2:B:616:ILE:O	2:B:674:PRO:HD3	2.07	0.55
1:A:583:LYS:HE2	3:A:701:XCC:S4	2.47	0.54
2:B:389:ILE:HG12	2:B:470:ILE:HG12	1.90	0.54
1:A:496:GLY:HA3	1:A:546[A]:CYS:SG	2.47	0.53
1:A:408:LYS:NZ	11:A:809:HOH:O	2.40	0.53
2:B:163:ILE:HD12	2:B:255:VAL:HG13	1.89	0.53
2:B:482:GLU:OE1	11:B:910:HOH:O	2.18	0.53
2:B:530:LEU:HD12	2:B:531:CYS:H	1.74	0.53
2:B:64:PHE:CZ	2:B:75:GLU:HG2	2.44	0.53
1:A:68:CYS:HB2	1:A:96:ILE:HG12	1.90	0.52
1:A:52:PHE:CZ	1:A:471:LYS:HA	2.44	0.52
1:A:572:PHE:C	1:A:572:PHE:CD2	2.88	0.52
2:B:530:LEU:HD13	2:B:601:PHE:HB3	1.91	0.52
2:B:198:GLU:OE1	11:B:909:HOH:O	2.18	0.52
2:B:611:LEU:HD12	2:B:718:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:HE2	1:A:289:LYS:HA	1.93	0.51
1:A:278:ALA:CB	1:A:314:MET:HE2	2.40	0.51
2:B:459:PHE:O	2:B:463:VAL:HG22	2.10	0.51
1:A:315[B]:CYS:SG	1:A:316:CYS:N	2.84	0.51
2:B:545:ILE:O	11:B:911:HOH:O	2.19	0.51
2:B:611:LEU:CD2	2:B:711:VAL:HG12	2.41	0.50
2:B:77:ARG:NE	11:B:917:HOH:O	2.37	0.50
2:B:135:TRP:HA	2:B:211:PRO:HB2	1.94	0.50
1:A:282:HIS:CD2	6:A:705:OH:O	2.65	0.50
1:A:440:VAL:HG22	1:A:530:LYS:HG3	1.94	0.50
1:A:292:ASP:OD1	1:A:325:ARG:NH2	2.34	0.49
1:A:353:GLN:HB3	1:A:583:LYS:NZ	2.27	0.49
2:B:611:LEU:HD21	2:B:711:VAL:HG12	1.94	0.49
1:A:351:ASP:OD1	1:A:352:VAL:N	2.43	0.49
2:B:398:MET:HE3	2:B:402:PHE:HB2	1.95	0.48
1:A:185:ILE:HB	1:A:203:MET:HE1	1.96	0.48
1:A:424:VAL:HG21	1:A:503:ALA:HB1	1.96	0.48
1:A:572:PHE:C	1:A:572:PHE:HD2	2.21	0.48
2:B:585:MET:HE3	2:B:585:MET:HB3	1.71	0.48
1:A:240:ASP:OD2	1:A:586[A]:SER:OG	2.21	0.47
1:A:438:ALA:HA	1:A:441:ASN:O	2.13	0.47
2:B:174:LYS:HE2	2:B:302:ASP:OD1	2.14	0.47
1:A:55:MET:O	1:A:55:MET:HG3	2.14	0.47
1:A:143:ARG:NH2	1:A:156:LYS:O	2.47	0.47
1:A:152:ASP:OD1	1:A:153:THR:N	2.47	0.47
1:A:358:GLY:O	1:A:362:VAL:HG23	2.13	0.47
2:B:127:GLU:N	2:B:127:GLU:CD	2.72	0.47
2:B:597:SER:HB3	2:B:601:PHE:HD1	1.78	0.47
2:B:697:ASP:OD2	2:B:701:LYS:HE3	2.15	0.47
2:B:420:PHE:CD1	2:B:433:ILE:HG12	2.49	0.47
1:A:369:ARG:HG2	1:A:383:TYR:CE1	2.50	0.47
2:B:669:ARG:NH2	2:B:728:MET:HE2	2.29	0.47
2:B:682:ARG:HG3	2:B:699:ILE:HD13	1.96	0.47
2:B:64:PHE:CE1	2:B:75:GLU:HG2	2.49	0.47
1:A:434:MET:HE1	1:A:446:ILE:HB	1.97	0.47
1:A:476:GLU:O	1:A:480:THR:HG23	2.15	0.46
1:A:635:VAL:HG13	2:B:384:ARG:HD3	1.97	0.46
2:B:213:GLY:HA3	2:B:217:GLN:OE1	2.15	0.46
1:A:278:ALA:HB1	1:A:314:MET:HE2	1.96	0.46
2:B:224:TYR:CD2	2:B:224:TYR:C	2.94	0.46
2:B:224:TYR:C	2:B:224:TYR:HD2	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ALA:O	1:A:222:ASN:ND2	2.48	0.46
2:B:420:PHE:CE1	2:B:433:ILE:HG12	2.51	0.46
1:A:33:ALA:O	1:A:37:LEU:HD12	2.16	0.45
2:B:622:SER:HA	11:B:923:HOH:O	2.15	0.45
1:A:597:PRO:HD3	1:A:648:ARG:NH2	2.32	0.45
1:A:112:HIS:CE1	1:A:583:LYS:HD2	2.52	0.45
1:A:635:VAL:HG11	2:B:349:LYS:HB3	1.98	0.45
2:B:159:GLU:HG3	2:B:185:MET:HB3	1.98	0.45
1:A:15:LYS:HA	1:A:15:LYS:HD3	1.73	0.44
2:B:671:VAL:HB	2:B:718:LEU:HD11	1.98	0.44
2:B:16:GLU:OE2	2:B:19:LYS:HE3	2.17	0.44
2:B:16:GLU:HA	2:B:17:PRO:HD3	1.85	0.44
2:B:66:PRO:HB3	2:B:227:ARG:HG3	1.99	0.44
1:A:441:ASN:OD1	1:A:443:GLU:HG2	2.17	0.44
1:A:530:LYS:HB3	1:A:530:LYS:HE2	1.83	0.44
1:A:606:LEU:HD13	1:A:613:TYR:CD2	2.52	0.44
2:B:654:TYR:CZ	2:B:660:PHE:HA	2.53	0.44
1:A:184:TRP:O	1:A:188:THR:HG23	2.18	0.44
2:B:540:LYS:NZ	2:B:544:GLU:OE2	2.39	0.44
2:B:704:ASP:OD1	2:B:706:THR:OG1	2.25	0.44
1:A:145:ILE:HD13	1:A:249:ASP:HB3	2.00	0.43
2:B:149:ILE:HD11	5:B:805:SF4:S2	2.58	0.43
1:A:20:TRP:O	1:A:21:GLU:C	2.61	0.43
2:B:7:PHE:CZ	2:B:10:ILE:HD11	2.53	0.43
1:A:147:GLN:OE1	1:A:153:THR:HG21	2.19	0.43
2:B:604:ILE:HG21	2:B:634:LEU:HG	2.00	0.43
2:B:182:LYS:HB3	2:B:316:ILE:HD12	2.01	0.43
2:B:185:MET:HE3	2:B:185:MET:HB2	1.79	0.43
2:B:652:LYS:HD3	2:B:677:LEU:CD1	2.49	0.43
2:B:353:PHE:HA	2:B:426:ARG:O	2.18	0.43
2:B:408:ARG:NH2	11:B:905:HOH:O	2.08	0.43
1:A:464:PHE:HZ	1:A:481:ILE:HG22	1.84	0.42
1:A:19:VAL:HG12	1:A:22:PRO:HG3	2.01	0.42
2:B:618:ASN:HD22	2:B:620:GLU:CD	2.27	0.42
1:A:136:ILE:HD13	1:A:136:ILE:HA	1.87	0.42
1:A:302:LYS:HA	1:A:306:ALA:O	2.20	0.42
1:A:556:LEU:HB2	1:A:572:PHE:CE1	2.54	0.42
2:B:163:ILE:CG2	2:B:265:LYS:HD3	2.49	0.42
1:A:408:LYS:HD3	11:A:809:HOH:O	2.19	0.42
1:A:606:LEU:HD13	1:A:613:TYR:HD2	1.85	0.42
1:A:175:ARG:HD2	1:A:205:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:GLU:OE1	2:B:127:GLU:N	2.53	0.42
1:A:125:GLU:CD	1:A:389:ILE:HD11	2.46	0.41
2:B:15:ILE:HD11	2:B:291:ILE:HG12	2.02	0.41
2:B:38:TYR:CZ	2:B:42:LEU:HD11	2.54	0.41
1:A:570:VAL:HA	1:A:571:PRO:HD3	1.93	0.41
2:B:669:ARG:NH1	2:B:729:GLU:O	2.49	0.41
2:B:398:MET:CE	2:B:402:PHE:HB2	2.49	0.41
1:A:115:HIS:CD2	1:A:115:HIS:C	2.98	0.41
2:B:7:PHE:O	2:B:10:ILE:HG12	2.20	0.41
2:B:454:LYS:NZ	2:B:457:GLN:HE22	2.18	0.41
1:A:482:LEU:HD22	1:A:502:PHE:CD1	2.55	0.41
1:A:591:PHE:O	1:A:596:VAL:HG22	2.20	0.41
2:B:180:MET:HE3	2:B:209:ALA:HB2	2.03	0.41
1:A:151:LEU:HD21	1:A:168:LEU:HD11	2.03	0.41
1:A:583:LYS:HE3	6:A:705:OH:O	2.20	0.41
2:B:335:SER:OG	8:B:802:MPD:H31	2.21	0.41
2:B:456:LYS:HE3	2:B:456:LYS:HB3	1.86	0.41
1:A:269:VAL:HG11	1:A:328:HIS:HB2	2.03	0.41
1:A:273:ASN:O	1:A:307:GLU:HB2	2.21	0.41
1:A:597:PRO:HD3	1:A:648:ARG:CZ	2.51	0.41
2:B:209:ALA:O	2:B:211:PRO:HD3	2.20	0.41
2:B:492:ASP:O	2:B:496:ARG:HG3	2.20	0.40
1:A:257:THR:HA	1:A:258:PRO:HD3	1.93	0.40
1:A:416:HIS:CD2	1:A:416:HIS:C	3.00	0.40
2:B:117:GLU:OE2	2:B:216:THR:OG1	2.30	0.40
2:B:256:LEU:HD23	2:B:256:LEU:HA	1.89	0.40
2:B:246:TYR:CE2	2:B:250:ARG:HD2	2.56	0.40

All (2) 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)
11:A:820:HOH:O	11:B:955:HOH:O[5_554]	1.84	0.36
2:B:320:ASP:O	2:B:396:ARG:NH1[9_554]	2.11	0.09

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	672/669 (100%)	635 (94%)	35 (5%)	2 (0%)	36	58
2	B	737/730 (101%)	711 (96%)	20 (3%)	6 (1%)	16	34
All	All	1409/1399 (101%)	1346 (96%)	55 (4%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	531	CYS
2	B	697	ASP
2	B	660	PHE
1	A	266	ASN
2	B	239	LEU
2	B	190	ASP
2	B	599	GLY
1	A	353	GLN

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	553/548 (101%)	547 (99%)	6 (1%)	65	84
2	B	622/613 (102%)	617 (99%)	5 (1%)	73	88
All	All	1175/1161 (101%)	1164 (99%)	11 (1%)	73	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	TRP
1	A	375[A]	ASN
1	A	375[B]	ASN
1	A	572	PHE
1	A	606	LEU
1	A	639	ARG
2	B	224	TYR
2	B	262	ASP
2	B	440	LYS
2	B	449[A]	GLN
2	B	449[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	58	GLN
1	A	115	HIS
1	A	280	HIS
1	A	367	HIS
1	A	388	HIS
1	A	391	ASN
2	B	306	GLN
2	B	457	GLN
2	B	552	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are modelled with single atom and 3 are monoatomic - leaving 6 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	B	805	2	0,12,12	-	-	-		
7	ACT	B	801	10	3,3,3	1.05	0	3,3,3	1.68	2 (66%)
3	XCC	A	701	6,1	0,12,12	-	-	-		
5	SF4	A	703	1	0,12,12	-	-	-		
4	FES	A	702	1	0,4,4	-	-	-		
8	MPD	B	802	-	7,7,7	0.36	0	9,10,10	0.54	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
5	SF4	B	805	2	-	-	0/6/5/5
3	XCC	A	701	6,1	-	-	0/4/4/4
5	SF4	A	703	1	-	-	0/6/5/5
4	FES	A	702	1	-	-	0/1/1/1
8	MPD	B	802	-	-	0/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	801	ACT	OXT-C-O	2.06	129.65	122.05
7	B	801	ACT	O-C-CH3	-2.04	114.39	122.33

There are no chirality outliers.

There are no torsion outliers.

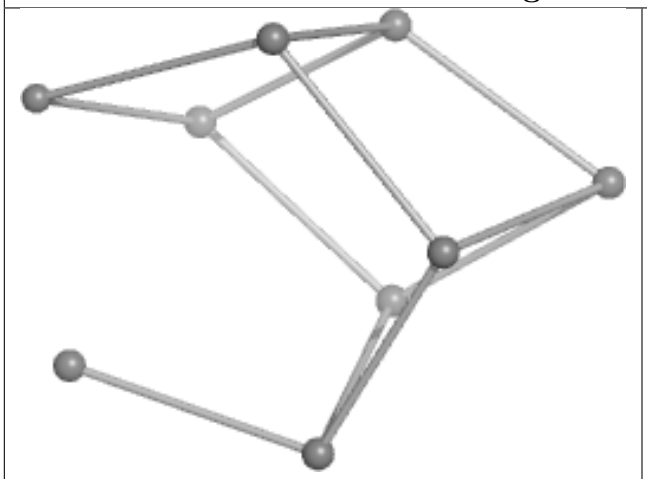
There are no ring outliers.

4 monomers are involved in 5 short contacts:

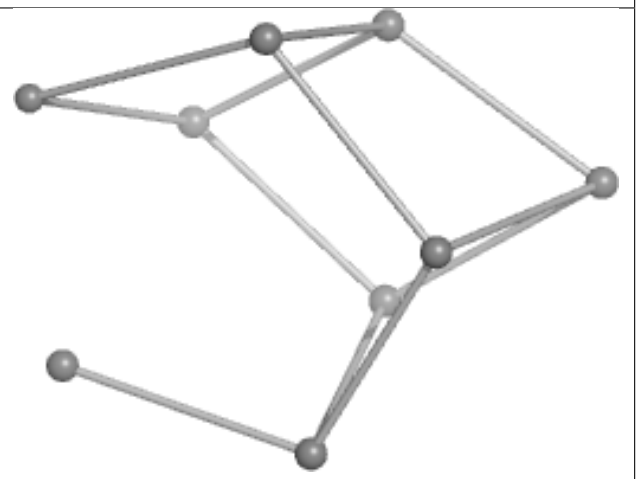
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	805	SF4	1	0
7	B	801	ACT	2	0
3	A	701	XCC	1	0
8	B	802	MPD	1	0

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.

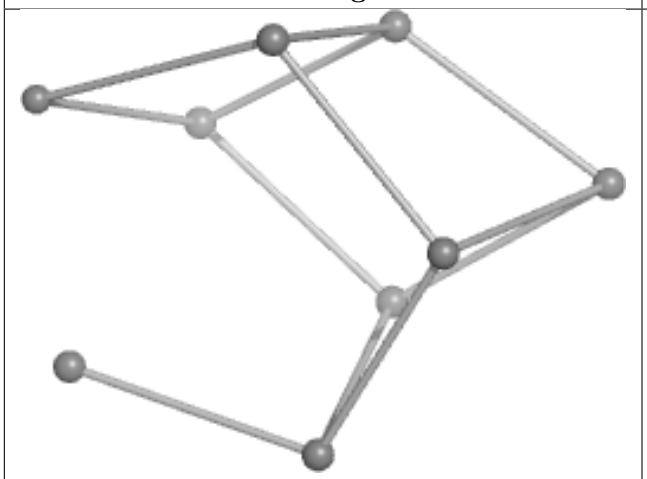
Ligand XCC A 701



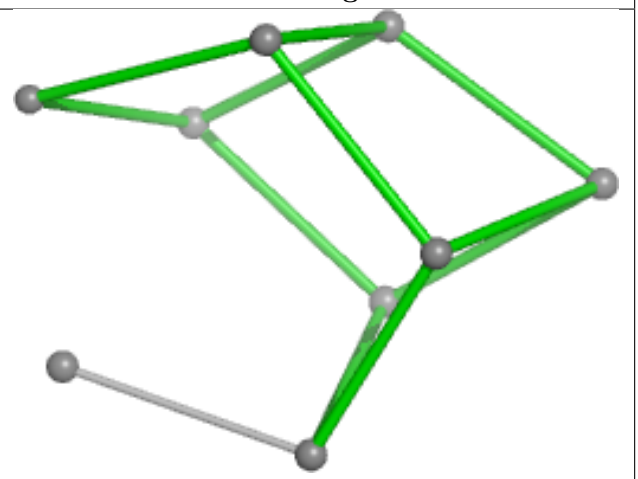
Bond lengths



Bond angles

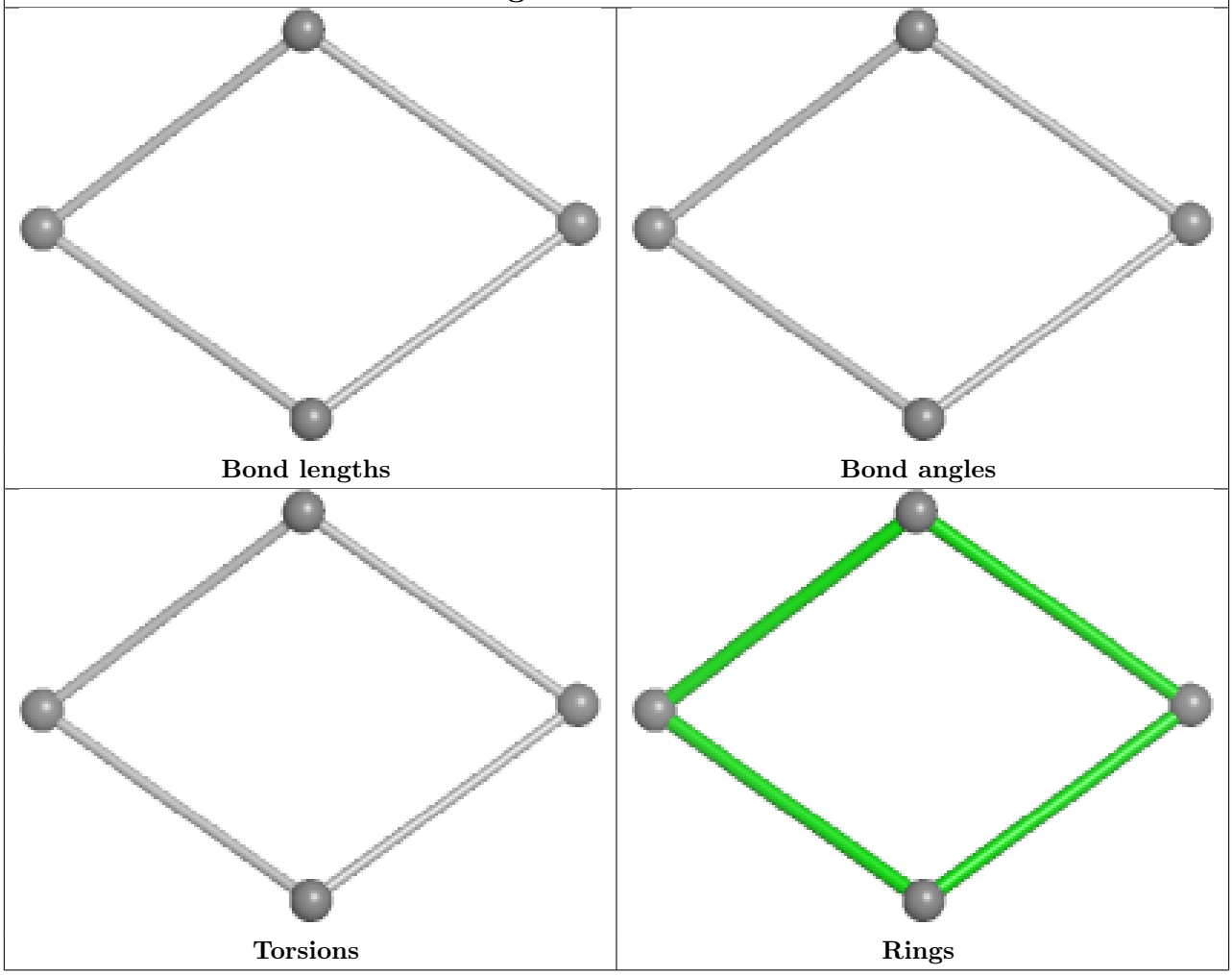


Torsions



Rings

Ligand FES A 702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.34	2 (0%)	90	88	15, 45, 63, 84	4 (0%)
2	B	730/730 (100%)	-0.35	1 (0%)	92	90	17, 46, 62, 86	8 (1%)
All	All	1399/1399 (100%)	-0.35	3 (0%)	91	90	15, 46, 63, 86	12 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	319	ILE	2.4
1	A	546[A]	CYS	2.2
1	A	466	GLY	2.2

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 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
8	MPD	B	802	8/8	0.69	0.19	53,61,75,77	0
6	OH	A	705	1/1	0.81	0.28	43,43,43,43	1

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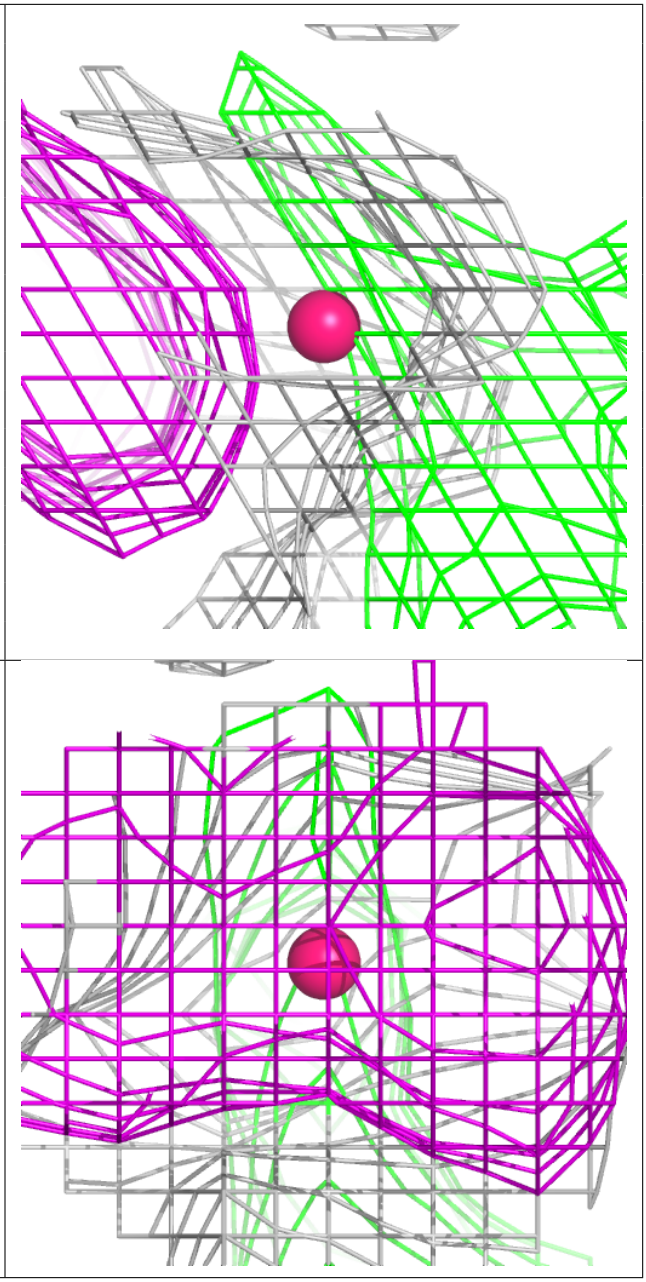
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OH	A	704	1/1	0.91	0.47	46,46,46,46	0
9	NA	B	803	1/1	0.91	0.04	42,42,42,42	0
3	XCC	A	701	9/9	0.94	0.15	38,46,49,54	5
7	ACT	B	801	4/4	0.94	0.15	41,44,44,46	0
4	FES	A	702	4/4	0.97	0.08	20,21,27,31	0
5	SF4	B	805	8/8	0.98	0.07	24,28,34,38	0
5	SF4	A	703	8/8	0.98	0.06	18,20,30,32	0
10	NI	B	806[A]	1/1	0.98	0.18	28,28,28,28	0
10	NI	B	804	1/1	0.99	0.13	24,24,24,24	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.

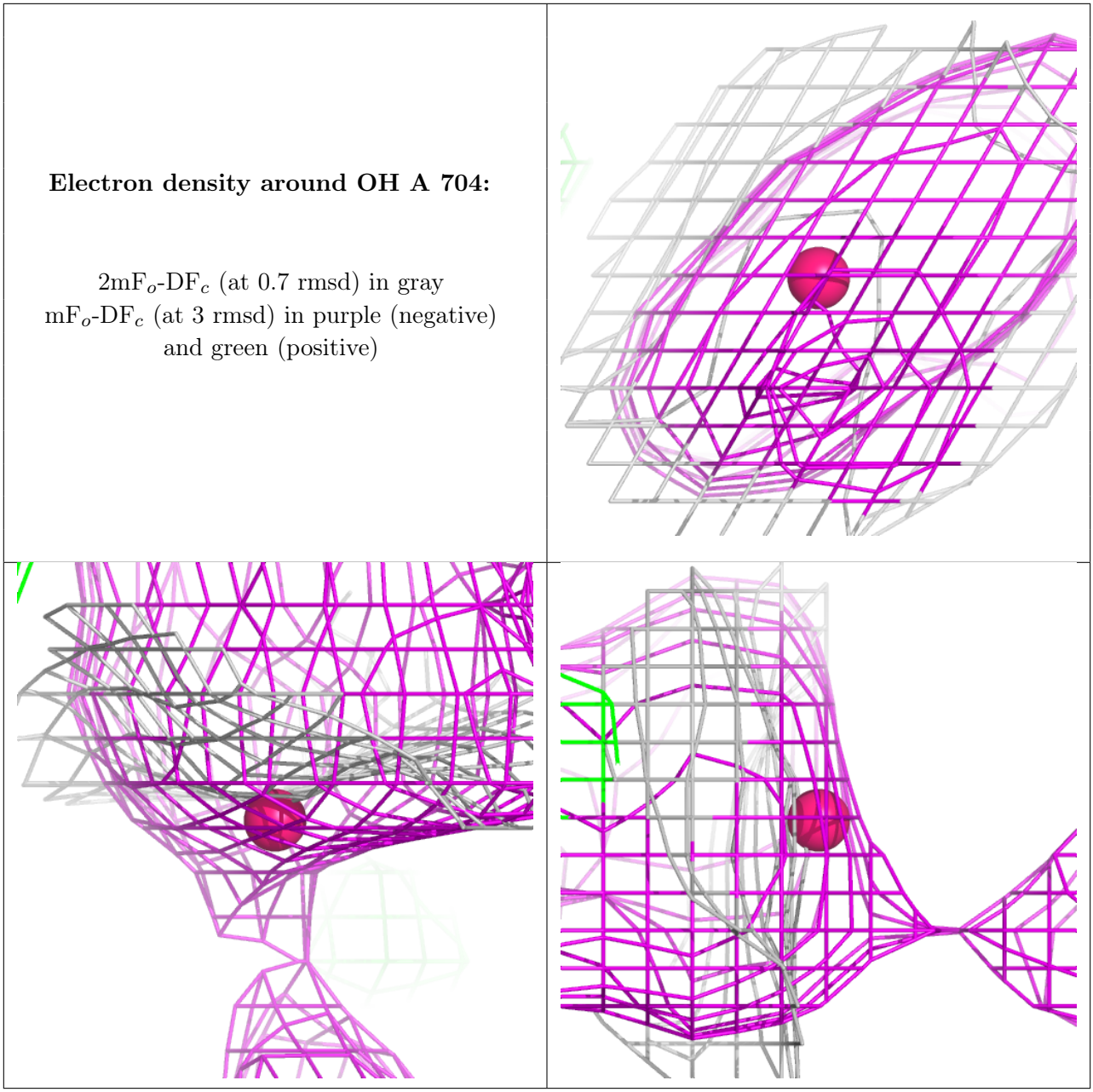
Electron density around OH A 705:

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



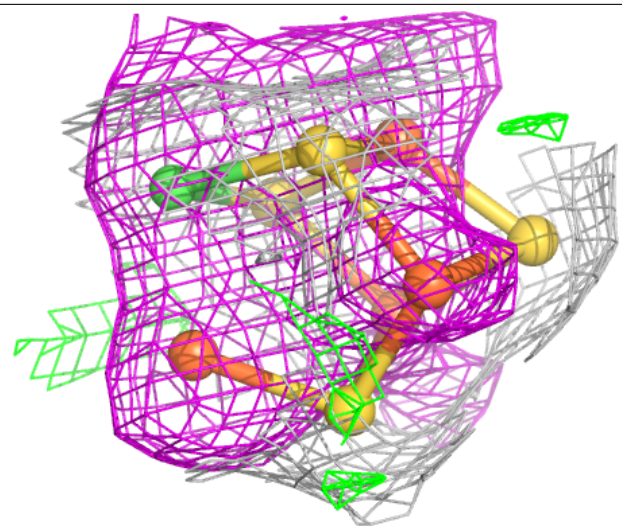
Electron density around OH A 704:

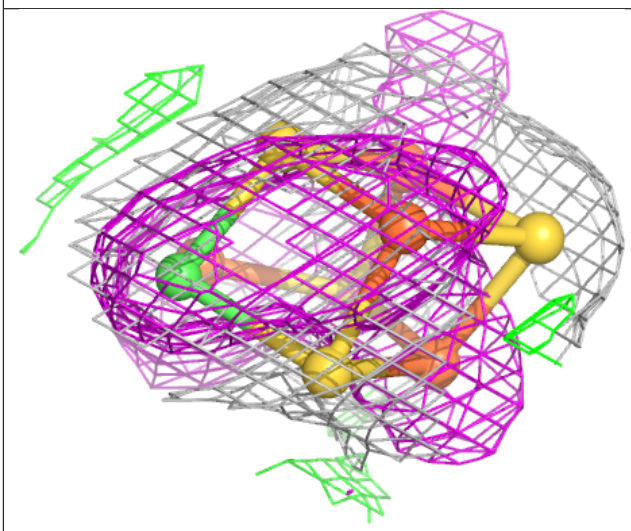
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

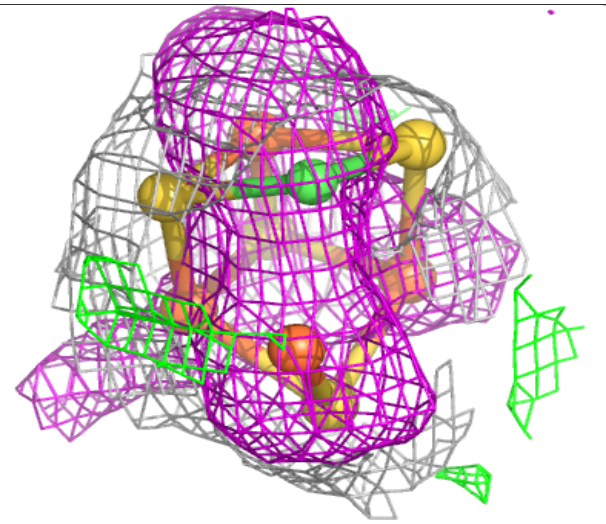


Electron density around XCC A 701:

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

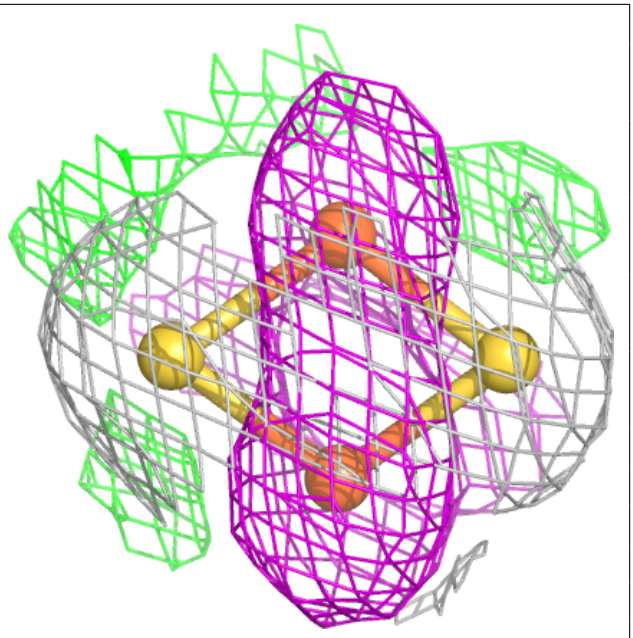


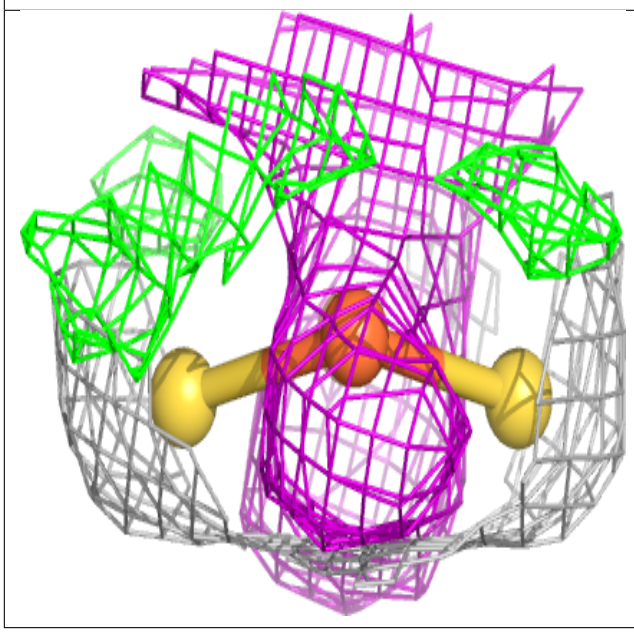


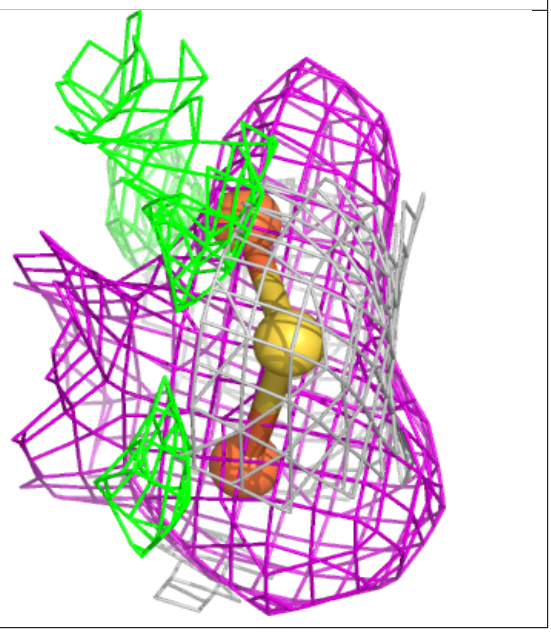


Electron density around FES A 702:

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

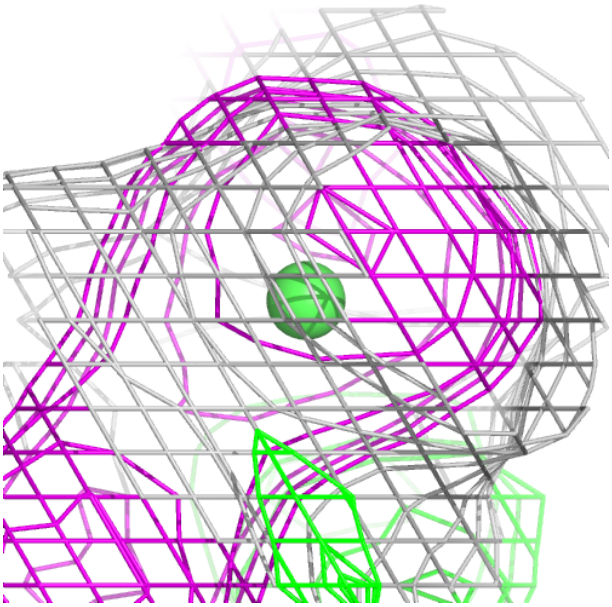


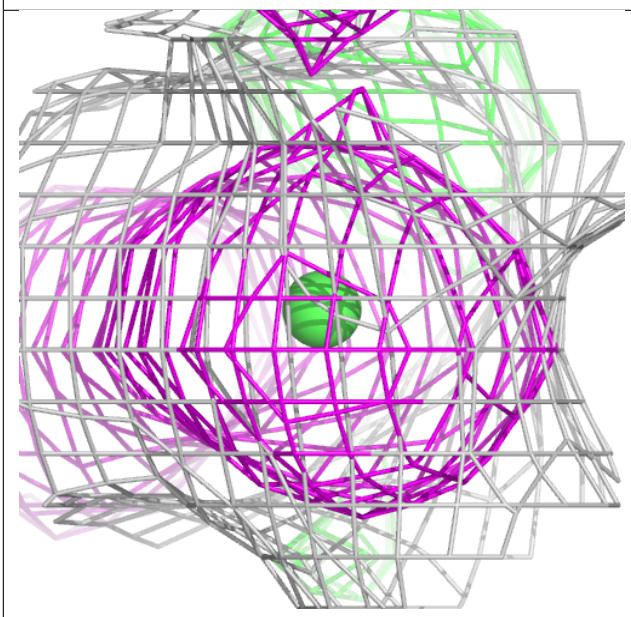


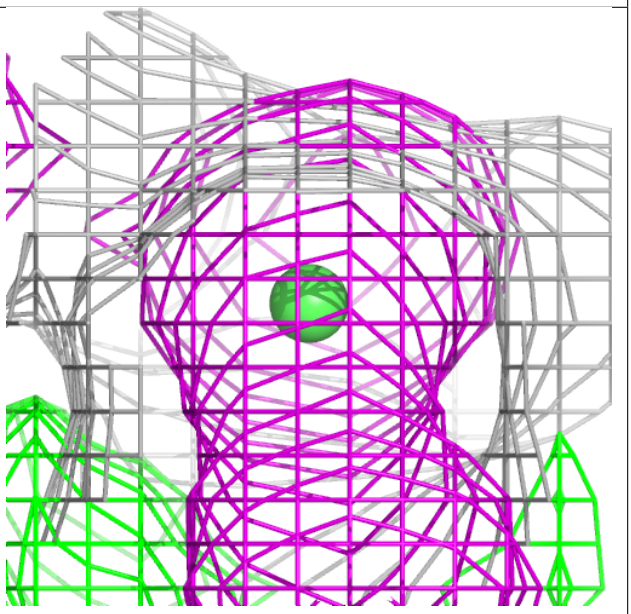


Electron density around NI B 806 (A):

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

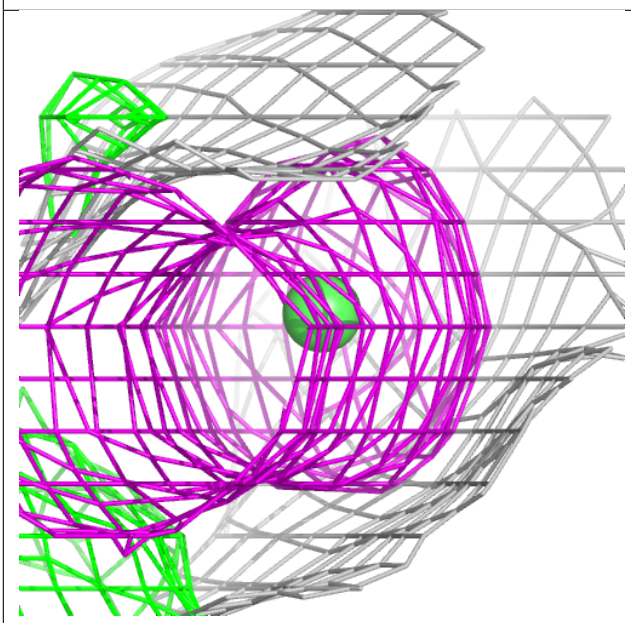


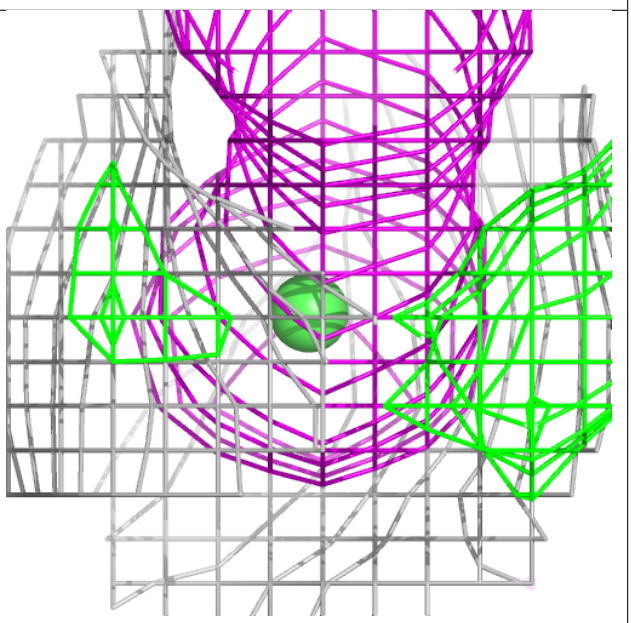




Electron density around NI B 804:

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





6.5 Other polymers (i)

There are no such residues in this entry.