



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:21 PM BST

PDB ID : 6L8S  
Title : High resolution crystal structure of crustacean hemocyanin.  
Authors : Masuda, T.; Mikami, B.; Baba, S.  
Deposited on : 2019-11-07  
Resolution : 1.58 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

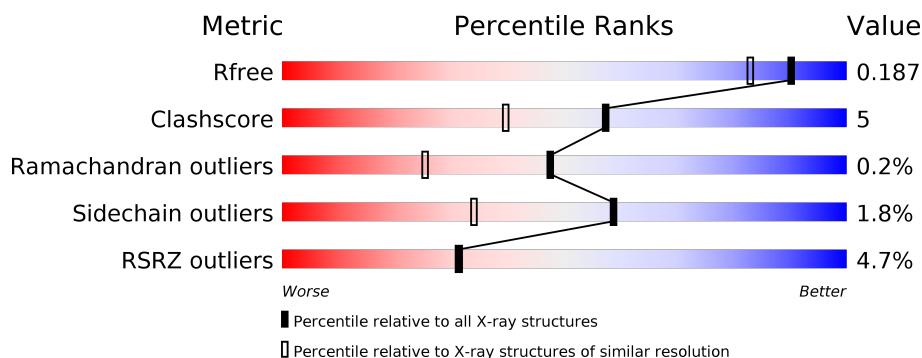
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	650	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	B	650	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
3	C	650	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>

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
5	NAG	B	703	-	-	-	X
9	EDO	B	711	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18043 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 Hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	45	0
			5524	3532	938	1029	25			

- Molecule 2 is a protein called Hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	650	Total	C	N	O	S	0	45	0
			5518	3527	935	1031	25			

- Molecule 3 is a protein called Hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	650	Total	C	N	O	S	0	50	0
			5539	3541	937	1035	26			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by author).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Mg	0	0
			2	2		
8	A	1	Total	Mg	0	0
			1	1		
8	C	2	Total	Mg	0	0
			2	2		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

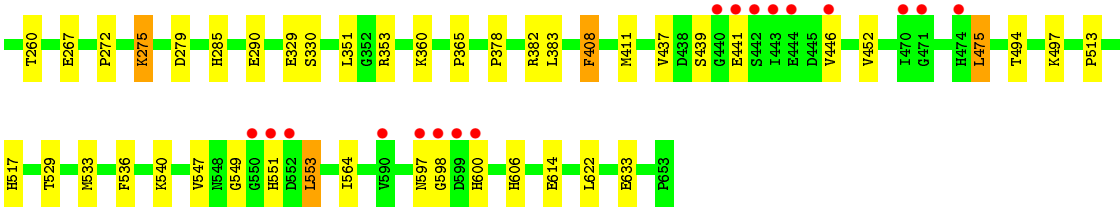
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	376	Total	O	0	0
			376	376		
11	B	509	Total	O	0	0
			509	509		
11	C	448	Total	O	0	0
			448	448		







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.45Å 207.60Å 187.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 1.58 45.31 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.70-1.58) 99.9 (45.31-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.149 , 0.186 0.149 , 0.187	Depositor DCC
$R_{free}$ test set	15490 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, CL, EDO, O, SO4, CU

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	0.34	0/5816	0.52	1/7875 (0.0%)
2	B	0.37	0/5808	0.54	0/7861
3	C	0.36	0/5846	0.54	0/7917
All	All	0.36	0/17470	0.53	1/23653 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ARG	NE-CZ-NH1	-5.17	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5524	0	5347	48	0
2	B	5518	0	5348	60	0
3	C	5539	0	5377	54	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
9	A	20	0	30	2	0
9	B	24	0	36	6	0
9	C	24	0	36	1	0
10	B	1	0	0	0	0
11	A	376	0	0	6	0
11	B	509	0	0	10	0
11	C	448	0	0	9	0
All	All	18043	0	16200	161	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 5.

All (161) 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:530:VAL:HG12	1:A:559:GLU:HG2	1.41	1.00
3:C:494:THR:H	3:C:497:LYS:HZ3	1.26	0.84
2:B:131:GLY:O	2:B:555:LEU:HD11	1.83	0.79
1:A:250:ARG:NH2	2:B:279:ASP:OD2	2.16	0.79
2:B:440:GLY:HA3	2:B:443:ILE:HD12	1.65	0.77
2:B:494:THR:H	2:B:497[B]:LYS:HZ3	1.33	0.76
1:A:559:GLU:OE2	11:A:801:HOH:O	2.03	0.76
3:C:86:LEU:HD22	3:C:110[B]:MET:HE1	1.70	0.73
1:A:218:GLU:HG2	1:A:622[B]:LEU:HD22	1.73	0.71
1:A:147:ASN:HA	1:A:260[B]:THR:HG22	1.73	0.70
2:B:150:VAL:HG21	2:B:168:VAL:HG22	1.74	0.70
2:B:566[B]:GLU:OE1	11:B:801:HOH:O	2.11	0.68
1:A:163:ALA:HB2	1:A:446:VAL:HG22	1.75	0.67
3:C:127[A]:LYS:HZ3	3:C:127[A]:LYS:H	1.43	0.67
1:A:191:ASN:O	1:A:195[A]:VAL:HG23	1.95	0.67
1:A:150:VAL:HG21	1:A:168:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD23	1:A:622[B]:LEU:HD21	1.77	0.66
3:C:147:ASN:HA	3:C:260[B]:THR:HG22	1.78	0.65
2:B:317[A]:GLN:OE1	11:B:802:HOH:O	2.13	0.65
3:C:179[B]:GLN:OE1	11:C:801:HOH:O	2.14	0.65
2:B:127[A]:LYS:HE2	2:B:128:LEU:HG	1.79	0.64
1:A:24:ASP:OD1	11:A:802:HOH:O	2.15	0.64
3:C:24:ASP:OD1	11:C:802:HOH:O	2.15	0.63
1:A:353[A]:ARG:NH2	11:A:806:HOH:O	2.32	0.63
2:B:147:ASN:HA	2:B:260[B]:THR:HG22	1.80	0.62
3:C:606:HIS:NE2	9:C:713:EDO:H11	2.14	0.62
2:B:191:ASN:O	2:B:195[B]:VAL:HG13	2.00	0.62
3:C:244:ASP:OD2	3:C:253[A]:ARG:NH2	2.33	0.62
3:C:163:ALA:HB2	3:C:446:VAL:HG22	1.82	0.61
2:B:171:THR:O	2:B:179[B]:GLN:NE2	2.33	0.61
2:B:353[A]:ARG:NH2	11:B:806:HOH:O	2.33	0.61
2:B:179[B]:GLN:OE1	11:B:803:HOH:O	2.16	0.60
2:B:250:ARG:NH2	3:C:279:ASP:OD2	2.34	0.60
3:C:353[B]:ARG:NH2	11:C:806:HOH:O	2.35	0.59
2:B:423[B]:ILE:HG23	2:B:458:LYS:HG3	1.85	0.58
3:C:437:VAL:HG23	11:C:840:HOH:O	2.03	0.57
3:C:475:LEU:HD11	3:C:598:GLY:HA3	1.86	0.57
1:A:513:PRO:HG2	1:A:517:HIS:CD2	2.39	0.57
1:A:127[A]:LYS:HZ3	1:A:127[A]:LYS:H	1.52	0.56
1:A:127[A]:LYS:NZ	1:A:127[A]:LYS:H	2.04	0.56
3:C:150:VAL:HG21	3:C:168[A]:VAL:HG23	1.87	0.56
1:A:131:GLY:O	1:A:555:LEU:HD23	2.06	0.56
2:B:152[B]:ASP:OD1	11:B:804:HOH:O	2.18	0.56
3:C:250[B]:ARG:NH2	11:C:804:HOH:O	2.34	0.56
2:B:543:ALA:HA	2:B:553:LEU:HD12	1.88	0.56
1:A:376:ARG:HD2	11:A:877:HOH:O	2.05	0.55
2:B:604:GLY:O	9:B:711:EDO:O2	2.24	0.55
3:C:127[A]:LYS:NZ	3:C:127[A]:LYS:H	2.04	0.55
2:B:178[B]:GLU:HG3	2:B:254:GLU:HG2	1.89	0.54
3:C:95:VAL:HG22	11:C:882:HOH:O	2.08	0.54
1:A:606:HIS:NE2	9:A:712:EDO:H11	2.23	0.54
1:A:256[B]:PHE:HB2	1:A:378:PRO:HD2	1.91	0.53
3:C:29:ASP:O	3:C:32[A]:GLU:HG2	2.08	0.53
1:A:409:ALA:O	1:A:470:ILE:HD11	2.08	0.53
1:A:633[B]:GLU:CD	1:A:633[B]:GLU:H	2.12	0.53
3:C:633[B]:GLU:H	3:C:633[B]:GLU:CD	2.12	0.53
3:C:150:VAL:HG21	3:C:168[B]:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:LYS:HD2	3:C:163:ALA:N	2.23	0.52
1:A:168:VAL:HB	1:A:452:VAL:HG12	1.91	0.52
2:B:168:VAL:HB	2:B:452:VAL:HG12	1.89	0.52
3:C:8:ALA:HB2	3:C:553:LEU:HB2	1.91	0.52
1:A:367[B]:VAL:HG22	1:A:373:THR:HB	1.92	0.52
3:C:12:GLN:OE1	3:C:547[A]:VAL:HG21	2.10	0.52
3:C:549:GLY:HA3	3:C:551:HIS:NE2	2.25	0.52
3:C:600:HIS:HE1	3:C:614:GLU:OE2	1.92	0.52
3:C:290[B]:GLU:OE2	11:C:803:HOH:O	2.19	0.51
3:C:222:TRP:CD1	3:C:622:LEU:HD12	2.45	0.51
1:A:133:VAL:HG21	1:A:558:TYR:CD2	2.46	0.51
2:B:555:LEU:C	2:B:557:ALA:H	2.14	0.50
1:A:555:LEU:C	1:A:557:ALA:H	2.14	0.50
1:A:261[A]:SER:OG	1:A:267:GLU:OE1	2.27	0.50
1:A:272[B]:PRO:HG2	1:A:275:ILE:HG21	1.92	0.50
1:A:195[A]:VAL:CG2	1:A:372[A]:GLU:HA	2.41	0.50
2:B:536:PHE:CZ	2:B:540:LYS:HE3	2.47	0.49
9:B:711:EDO:H21	11:B:1257:HOH:O	2.13	0.49
2:B:16:HIS:HD2	11:B:861:HOH:O	1.96	0.48
2:B:82:GLU:HA	2:B:85:MET:HE2	1.95	0.48
1:A:133:VAL:HG21	1:A:558:TYR:HD2	1.78	0.48
1:A:222:TRP:CD1	1:A:622[A]:LEU:HD12	2.49	0.48
3:C:513:PRO:HG2	3:C:517:HIS:CD2	2.48	0.48
3:C:191:ASN:O	3:C:195[A]:VAL:HG13	2.14	0.47
3:C:494:THR:N	3:C:497:LYS:HZ3	2.03	0.47
2:B:178[B]:GLU:HG3	2:B:254:GLU:CG	2.45	0.47
3:C:86:LEU:HD22	3:C:110[B]:MET:CE	2.41	0.47
2:B:247:HIS:HB2	2:B:250:ARG:HB2	1.97	0.47
2:B:191:ASN:O	2:B:195[A]:VAL:HG12	2.14	0.47
2:B:597:ASN:HB3	2:B:600[A]:HIS:CG	2.50	0.46
3:C:246[B]:LEU:HG	3:C:382:ARG:HB3	1.96	0.46
3:C:168[B]:VAL:HB	3:C:452:VAL:HG12	1.98	0.46
2:B:423[B]:ILE:HG12	2:B:424:THR:N	2.31	0.46
2:B:530:VAL:C	2:B:566[A]:GLU:HG3	2.36	0.46
2:B:8:ALA:HA	2:B:553:LEU:HD13	1.98	0.46
3:C:408:PHE:CE2	3:C:411[B]:MET:HG3	2.51	0.46
1:A:355:GLY:O	11:A:803:HOH:O	2.21	0.45
1:A:42:ASP:O	1:A:45:MET:HG2	2.16	0.45
2:B:494:THR:N	2:B:497[B]:LYS:HZ3	2.08	0.45
3:C:110[B]:MET:HE2	3:C:110[B]:MET:HB2	1.82	0.45
3:C:23:GLU:OE2	3:C:439[A]:SER:OG	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ALA:HA	2:B:553:LEU:CD1	2.46	0.45
1:A:367[B]:VAL:HG13	1:A:373:THR:O	2.16	0.45
2:B:555:LEU:C	2:B:555:LEU:HD12	2.37	0.45
1:A:138:TYR:HA	1:A:145:PHE:CD1	2.52	0.44
2:B:222:TRP:CD1	2:B:622:LEU:HD12	2.52	0.44
2:B:529:THR:O	9:B:711:EDO:O2	2.34	0.44
3:C:150:VAL:HG21	3:C:168[A]:VAL:CG2	2.45	0.44
1:A:279:ASP:OD2	3:C:250[B]:ARG:NH2	2.51	0.44
1:A:192:ILE:HA	1:A:195[B]:VAL:HG12	2.00	0.44
2:B:566[B]:GLU:HG2	11:B:981:HOH:O	2.17	0.44
3:C:441:GLU:H	3:C:441:GLU:CD	2.21	0.44
2:B:195[B]:VAL:CG1	2:B:372:GLU:HA	2.46	0.44
2:B:82:GLU:HA	2:B:85:MET:CE	2.48	0.44
2:B:222:TRP:CH2	2:B:623:GLY:HA2	2.53	0.44
3:C:162:LYS:HD2	3:C:163:ALA:H	1.82	0.44
1:A:475:LEU:HD11	1:A:598:GLY:HA3	2.00	0.44
2:B:329:GLU:N	2:B:330:SER:HA	2.32	0.43
3:C:536:PHE:CZ	3:C:540:LYS:HE3	2.53	0.43
2:B:463[B]:LYS:HD3	2:B:520:HIS:ND1	2.33	0.43
3:C:251[B]:ILE:HG13	11:C:1177:HOH:O	2.17	0.43
2:B:419:ASP:HB2	2:B:463[B]:LYS:HE3	2.00	0.43
3:C:329:GLU:N	3:C:330:SER:HA	2.34	0.43
2:B:131:GLY:O	2:B:555:LEU:CD1	2.60	0.43
1:A:329:GLU:N	1:A:330:SER:HA	2.34	0.43
2:B:600[B]:HIS:CG	2:B:601:ASP:N	2.86	0.43
2:B:485:ILE:HG22	2:B:486[B]:GLU:HG3	2.01	0.43
2:B:411[B]:MET:HE1	2:B:512:VAL:HG11	2.01	0.43
2:B:555:LEU:C	2:B:557:ALA:N	2.72	0.43
3:C:275[A]:LYS:HB2	3:C:275[A]:LYS:HE2	1.67	0.43
2:B:566[A]:GLU:OE2	9:B:711:EDO:O1	2.34	0.42
3:C:129:GLY:HA2	3:C:132:ILE:HD12	2.01	0.42
3:C:529:THR:HA	3:C:564:ILE:O	2.19	0.42
1:A:419:ASP:CG	1:A:463[A]:LYS:HD2	2.40	0.42
2:B:138:TYR:HA	2:B:145:PHE:CD1	2.55	0.42
1:A:412:VAL:CG1	1:A:467:SER:HB2	2.50	0.42
2:B:566[B]:GLU:OE2	11:B:805:HOH:O	2.21	0.42
3:C:351[B]:LEU:HD12	3:C:383:LEU:HD22	2.01	0.41
2:B:147:ASN:ND2	2:B:168:VAL:HG13	2.35	0.41
1:A:463[B]:LYS:HG3	1:A:518:THR:CG2	2.50	0.41
1:A:222:TRP:HB2	1:A:622[B]:LEU:HD23	2.02	0.41
3:C:272:PRO:HG2	3:C:275[B]:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376[A]:ARG:HD2	11:B:903:HOH:O	2.20	0.41
2:B:529:THR:HA	2:B:564:ILE:O	2.20	0.41
3:C:192:ILE:HA	3:C:195[B]:VAL:HG12	2.01	0.41
1:A:529:THR:HA	1:A:564:ILE:O	2.21	0.41
3:C:178[A]:GLU:HG2	3:C:378:PRO:HG3	2.03	0.41
1:A:559:GLU:HB3	1:A:560:ARG:H	1.42	0.41
2:B:195[B]:VAL:HG12	2:B:371:PHE:C	2.41	0.41
1:A:6:SER:O	1:A:10:LYS:HG3	2.21	0.41
3:C:360:LYS:HE3	3:C:360:LYS:HB3	1.86	0.41
2:B:133:VAL:HG23	2:B:555:LEU:HD22	2.02	0.41
2:B:566[A]:GLU:HG2	9:B:711:EDO:O1	2.21	0.41
3:C:275[A]:LYS:NZ	11:C:810:HOH:O	2.42	0.41
2:B:530:VAL:O	2:B:566[A]:GLU:HG3	2.21	0.41
3:C:600:HIS:CE1	3:C:614:GLU:OE2	2.73	0.41
1:A:367[A]:VAL:CG2	1:A:377:ASP:HB2	2.51	0.40
2:B:172:GLY:HA3	2:B:179[B]:GLN:HG3	2.02	0.40
1:A:459[B]:GLU:HG3	11:A:1068:HOH:O	2.21	0.40
1:A:185:GLY:HA3	9:A:710:EDO:H22	2.03	0.40
2:B:546:ALA:CB	2:B:553:LEU:HB2	2.52	0.40
3:C:353[B]:ARG:HH21	3:C:365:PRO:HG3	1.85	0.40
1:A:195[A]:VAL:HG22	1:A:372[A]:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	693/650 (107%)	674 (97%)	17 (2%)	2 (0%)	41	21
2	B	693/650 (107%)	677 (98%)	15 (2%)	1 (0%)	51	28
3	C	699/650 (108%)	685 (98%)	12 (2%)	2 (0%)	41	21
All	All	2085/1950 (107%)	2036 (98%)	44 (2%)	5 (0%)	47	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	GLU
1	A	556	SER
3	C	597[A]	ASN
3	C	597[B]	ASN
2	B	170	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	616/571 (108%)	604 (98%)	12 (2%)	57	31
2	B	614/569 (108%)	598 (97%)	16 (3%)	46	19
3	C	619/568 (109%)	604 (98%)	15 (2%)	49	22
All	All	1849/1708 (108%)	1806 (98%)	43 (2%)	59	23

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127[A]	LYS
1	A	127[B]	LYS
1	A	221	PHE
1	A	233	PHE
1	A	252[A]	ILE
1	A	252[B]	ILE
1	A	278[A]	GLU
1	A	278[B]	GLU
1	A	317	GLN
1	A	475	LEU
1	A	533	MET
1	A	559	GLU
2	B	32[A]	GLU
2	B	32[B]	GLU
2	B	127[A]	LYS
2	B	127[B]	LYS

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Mol	Chain	Res	Type
2	B	152[A]	ASP
2	B	152[B]	ASP
2	B	221	PHE
2	B	233	PHE
2	B	278[A]	GLU
2	B	278[B]	GLU
2	B	317[A]	GLN
2	B	317[B]	GLN
2	B	408	PHE
2	B	533	MET
2	B	555	LEU
2	B	599	ASP
3	C	127[A]	LYS
3	C	127[B]	LYS
3	C	168[A]	VAL
3	C	168[B]	VAL
3	C	221	PHE
3	C	233	PHE
3	C	267[A]	GLU
3	C	267[B]	GLU
3	C	275[A]	LYS
3	C	275[B]	LYS
3	C	285	HIS
3	C	408	PHE
3	C	475	LEU
3	C	533	MET
3	C	553	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	600	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 18 are monoatomic - leaving 22 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	$\# Z  > 2$
9	EDO	C	711	-	3,3,3	0.51	0	2,2,2	0.26	0
9	EDO	A	711	-	3,3,3	0.54	0	2,2,2	0.21	0
9	EDO	B	711	-	3,3,3	0.36	0	2,2,2	0.49	0
9	EDO	A	710	-	3,3,3	0.50	0	2,2,2	0.32	0
9	EDO	C	710	-	3,3,3	0.48	0	2,2,2	0.32	0
9	EDO	B	714	-	3,3,3	0.32	0	2,2,2	0.66	0
9	EDO	B	710	-	3,3,3	0.43	0	2,2,2	0.79	0
9	EDO	C	708	-	3,3,3	0.45	0	2,2,2	0.72	0
9	EDO	A	712	-	3,3,3	0.43	0	2,2,2	0.42	0
9	EDO	B	712	-	3,3,3	0.52	0	2,2,2	0.21	0
9	EDO	B	713	-	3,3,3	0.57	0	2,2,2	0.13	0
9	EDO	C	712	-	3,3,3	0.52	0	2,2,2	0.16	0
9	EDO	B	709	-	3,3,3	0.48	0	2,2,2	0.27	0
9	EDO	A	709	-	3,3,3	0.44	0	2,2,2	0.46	0
7	SO4	B	706	-	4,4,4	0.22	0	6,6,6	0.48	0
5	NAG	A	703	1	14,14,15	0.59	1 (7%)	17,19,21	0.50	0
9	EDO	A	708	-	3,3,3	0.42	0	2,2,2	0.46	0
9	EDO	C	709	-	3,3,3	0.39	0	2,2,2	0.56	0
5	NAG	B	703	2	14,14,15	0.28	0	17,19,21	0.54	0
9	EDO	C	713	-	3,3,3	0.50	0	2,2,2	0.35	0
7	SO4	A	706	-	4,4,4	0.20	0	6,6,6	0.22	0
7	SO4	C	705	-	4,4,4	0.19	0	6,6,6	0.19	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
9	EDO	C	711	-	-	0/1/1/1	-
9	EDO	A	711	-	-	1/1/1/1	-
9	EDO	B	711	-	-	1/1/1/1	-
9	EDO	A	710	-	-	0/1/1/1	-
9	EDO	B	712	-	-	0/1/1/1	-
9	EDO	C	710	-	-	0/1/1/1	-
9	EDO	A	709	-	-	0/1/1/1	-
9	EDO	B	713	-	-	1/1/1/1	-
9	EDO	A	712	-	-	0/1/1/1	-
5	NAG	B	703	2	-	2/6/23/26	0/1/1/1
9	EDO	C	713	-	-	1/1/1/1	-
9	EDO	B	714	-	-	1/1/1/1	-
9	EDO	C	712	-	-	0/1/1/1	-
9	EDO	B	709	-	-	0/1/1/1	-
9	EDO	A	708	-	-	0/1/1/1	-
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
9	EDO	C	708	-	-	0/1/1/1	-
9	EDO	B	710	-	-	0/1/1/1	-
9	EDO	C	709	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	NAG	O5-C1	-2.07	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	NAG	O5-C5-C6-O6
5	A	703	NAG	C4-C5-C6-O6
5	B	703	NAG	O5-C5-C6-O6
5	B	703	NAG	C4-C5-C6-O6
9	A	711	EDO	O1-C1-C2-O2
9	B	711	EDO	O1-C1-C2-O2
9	B	714	EDO	O1-C1-C2-O2
9	B	713	EDO	O1-C1-C2-O2
9	C	713	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	711	EDO	6	0
9	A	710	EDO	1	0
9	A	712	EDO	1	0
9	C	713	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	650/650 (100%)	0.22	48 (7%)	14 14	17, 29, 56, 99	0
2	B	650/650 (100%)	-0.30	19 (2%)	51 53	15, 23, 45, 93	0
3	C	650/650 (100%)	-0.06	25 (3%)	40 41	17, 25, 44, 86	0
All	All	1950/1950 (100%)	-0.05	92 (4%)	31 31	15, 25, 49, 99	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	LEU	20.5
1	A	440	GLY	15.8
1	A	552	ASP	11.4
1	A	554	ASP	11.3
1	A	599	ASP	10.1
3	C	442	SER	9.4
1	A	555	LEU	9.3
1	A	556	SER	8.3
1	A	443	ILE	8.2
1	A	558	TYR	8.2
1	A	442	SER	6.9
1	A	470	ILE	6.9
2	B	549	GLY	6.9
3	C	599	ASP	6.8
3	C	170	PHE	6.8
1	A	597	ASN	6.3
3	C	171	THR	6.2
1	A	441	GLU	6.2
2	B	550	GLY	6.2
3	C	443	ILE	5.8
1	A	559	GLU	5.8
1	A	550	GLY	5.8
2	B	555	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	551	SER	5.7
2	B	557	ALA	5.7
1	A	41	GLY	5.7
1	A	549	GLY	5.4
2	B	599	ASP	5.3
1	A	598	GLY	5.3
3	C	440	GLY	5.1
2	B	553	LEU	5.1
2	B	170	PHE	4.9
1	A	600	HIS	4.7
3	C	172	GLY	4.7
3	C	552[A]	ASP	4.7
3	C	441	GLU	4.7
3	C	169	SER	4.6
1	A	557	ALA	4.5
2	B	169	SER	4.4
1	A	654	GLU	4.4
2	B	171	THR	4.2
3	C	470	ILE	4.1
2	B	597	ASN	4.0
3	C	550	GLY	3.9
3	C	5	SER	3.8
3	C	598	GLY	3.7
3	C	597[A]	ASN	3.7
2	B	558	TYR	3.6
1	A	473	ASP	3.6
2	B	162[A]	LYS	3.5
3	C	471	GLY	3.5
1	A	444	GLU	3.5
1	A	172	GLY	3.4
1	A	471	GLY	3.4
2	B	556	SER	3.4
3	C	600	HIS	3.4
1	A	162[A]	LYS	3.4
3	C	4	ALA	3.3
1	A	5	SER	3.2
1	A	513	PRO	3.2
1	A	170	PHE	3.1
2	B	554	ASP	2.9
1	A	596	HIS	2.9
1	A	517	HIS	2.9
1	A	601	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	511	LYS	2.8
1	A	35	LYS	2.7
3	C	444	GLU	2.7
1	A	472	SER	2.7
1	A	474	HIS	2.7
2	B	4	ALA	2.6
1	A	49[A]	GLN	2.6
1	A	595	GLY	2.5
1	A	512	VAL	2.5
1	A	36	ASN	2.4
1	A	412	VAL	2.4
3	C	195[A]	VAL	2.3
3	C	590	VAL	2.3
3	C	474	HIS	2.3
3	C	551	HIS	2.2
1	A	32[A]	GLU	2.2
1	A	97	HIS	2.2
3	C	446	VAL	2.1
2	B	600[A]	HIS	2.1
3	C	162	LYS	2.1
1	A	594[A]	GLU	2.1
1	A	171	THR	2.1
2	B	172	GLY	2.1
1	A	519	ILE	2.1
1	A	514	SER	2.0
2	B	552	ASP	2.0
2	B	441	GLU	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,

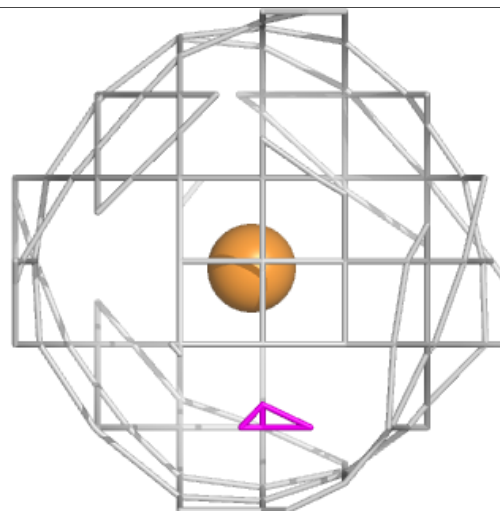
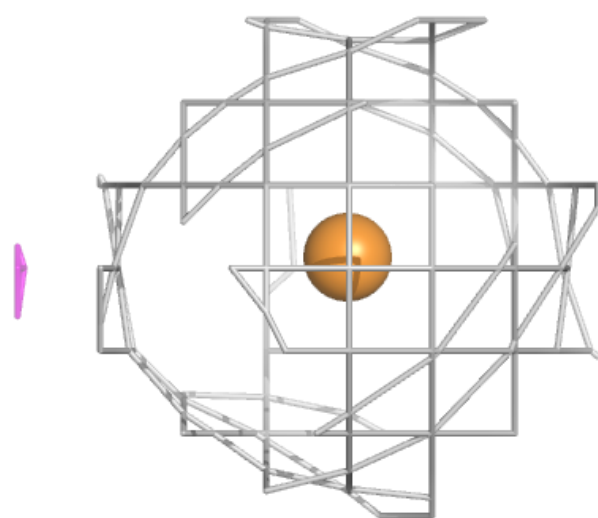
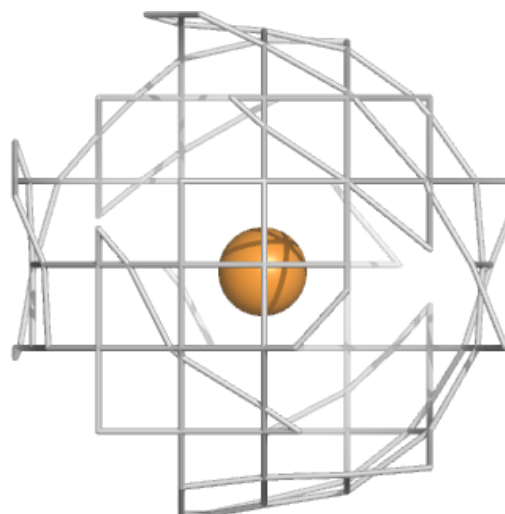
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	EDO	B	713	4/4	0.55	0.17	47,48,48,49	0
5	NAG	B	703	14/15	0.73	0.41	60,67,69,70	0
5	NAG	A	703	14/15	0.79	0.36	58,65,68,70	0
9	EDO	B	712	4/4	0.85	0.10	41,42,43,43	0
9	EDO	B	710	4/4	0.86	0.15	37,37,39,43	0
9	EDO	C	713	4/4	0.87	0.12	39,39,40,45	0
9	EDO	C	712	4/4	0.89	0.10	41,41,43,44	0
9	EDO	C	711	4/4	0.89	0.08	38,39,40,41	0
9	EDO	A	711	4/4	0.90	0.11	47,47,48,50	0
9	EDO	A	712	4/4	0.90	0.11	42,43,45,49	0
9	EDO	B	711	4/4	0.90	0.10	31,32,33,34	0
9	EDO	B	714	4/4	0.90	0.11	32,34,34,36	0
9	EDO	A	708	4/4	0.91	0.13	34,35,38,46	0
9	EDO	C	709	4/4	0.91	0.14	35,35,38,43	0
9	EDO	C	708	4/4	0.92	0.13	33,35,37,42	0
9	EDO	A	709	4/4	0.93	0.14	36,39,39,41	0
8	MG	A	707	1/1	0.93	0.25	65,65,65,65	0
9	EDO	C	710	4/4	0.95	0.10	28,30,30,31	0
9	EDO	A	710	4/4	0.95	0.14	25,31,34,35	0
6	O	C	704	1/1	0.96	0.10	43,43,43,43	0
8	MG	B	708	1/1	0.96	0.10	55,55,55,55	0
8	MG	C	707	1/1	0.96	0.05	51,51,51,51	0
6	O	A	704	1/1	0.97	0.15	49,49,49,49	0
10	CL	B	715	1/1	0.97	0.04	58,58,58,58	0
6	O	C	703	1/1	0.98	0.04	24,24,24,24	0
6	O	B	704	1/1	0.98	0.19	42,42,42,42	0
9	EDO	B	709	4/4	0.98	0.07	25,30,32,37	0
7	SO4	A	706	5/5	0.98	0.09	33,36,44,45	0
7	SO4	C	705	5/5	0.98	0.08	31,32,42,42	0
8	MG	C	706	1/1	0.99	0.06	42,42,42,42	0
6	O	B	705	1/1	0.99	0.06	24,24,24,24	0
7	SO4	B	706	5/5	0.99	0.08	28,30,34,37	0
8	MG	B	707	1/1	0.99	0.15	34,34,34,34	0
4	CU	A	701	1/1	1.00	0.08	21,21,21,21	0
4	CU	C	701	1/1	1.00	0.07	20,20,20,20	0
4	CU	C	702	1/1	1.00	0.06	21,21,21,21	0
4	CU	A	702	1/1	1.00	0.05	25,25,25,25	0
4	CU	B	701	1/1	1.00	0.05	20,20,20,20	0
4	CU	B	702	1/1	1.00	0.04	23,23,23,23	0
6	O	A	705	1/1	1.00	0.03	25,25,25,25	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.

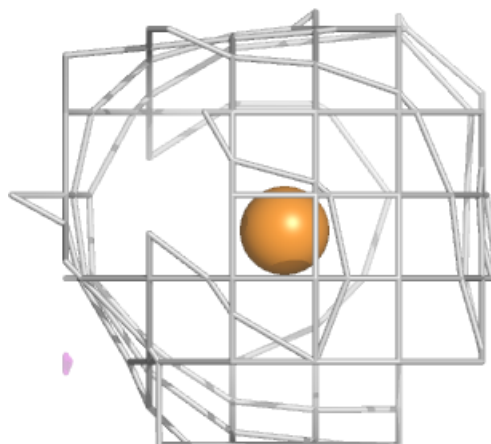
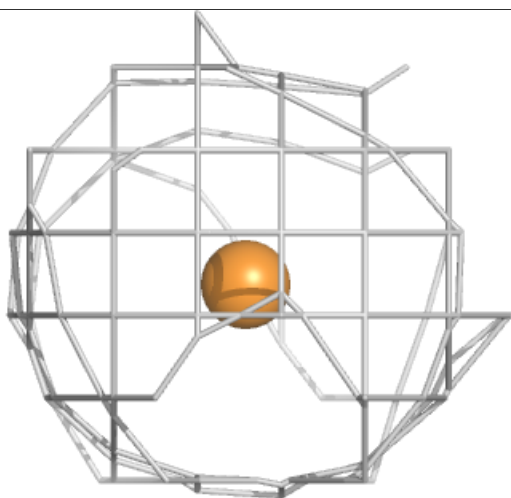
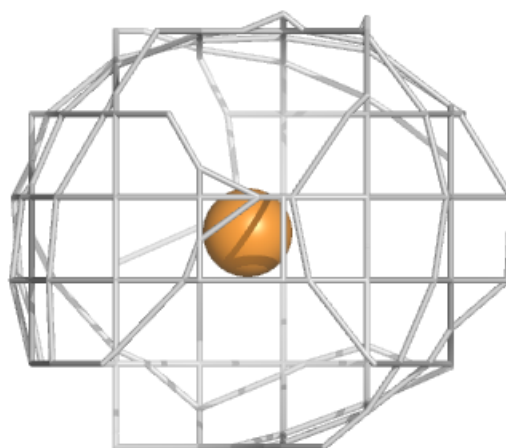
**Electron density around CU A 701:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



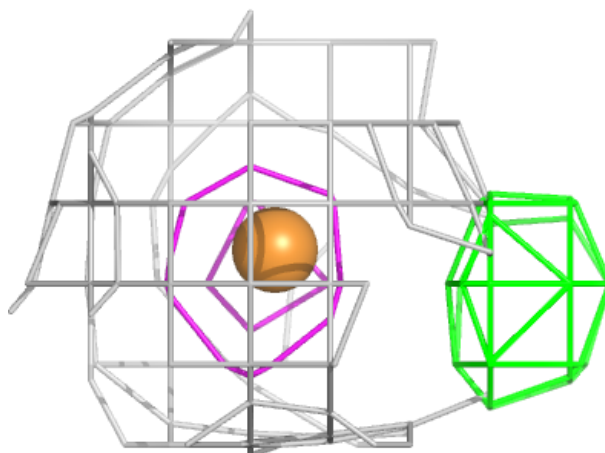
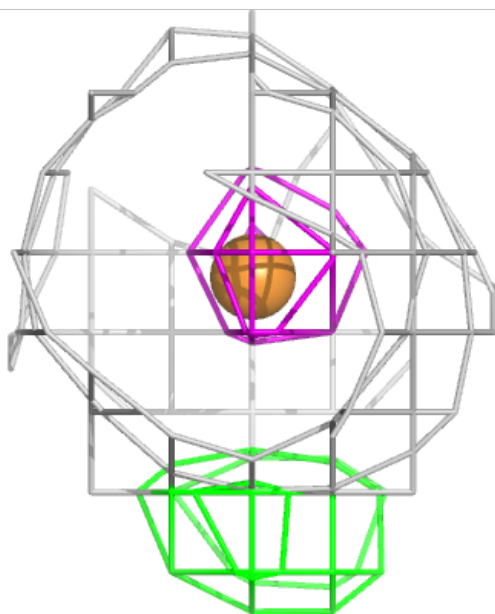
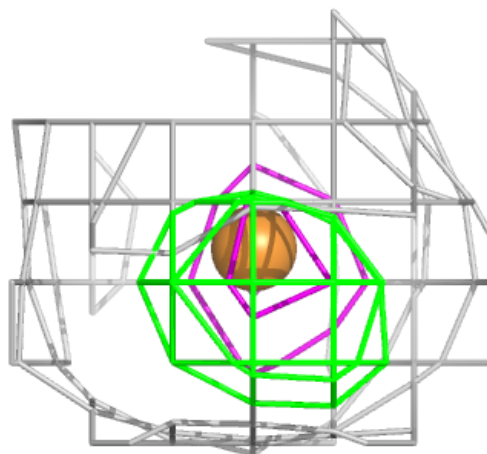
**Electron density around CU C 701:**

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



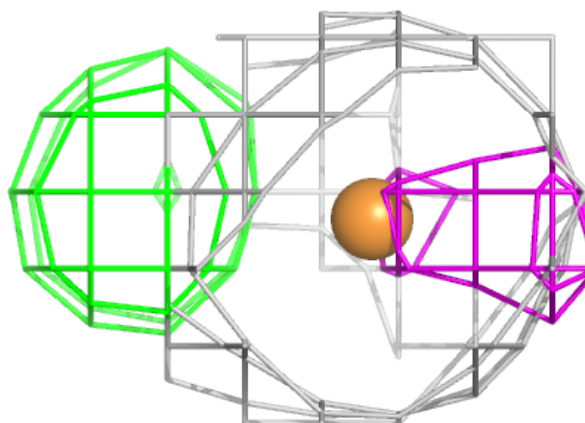
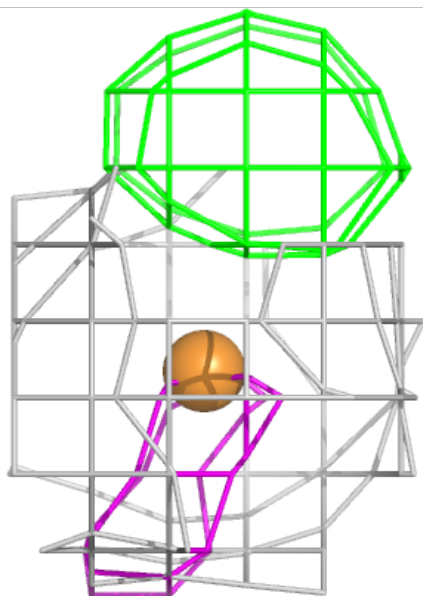
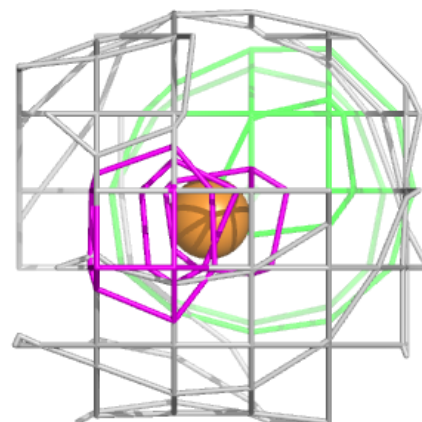
**Electron density around CU C 702:**

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



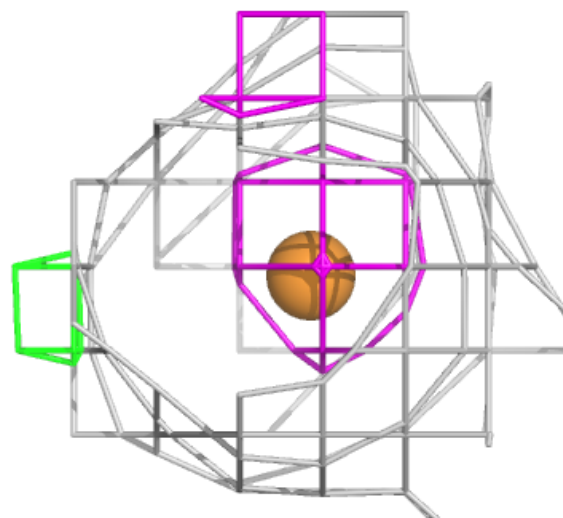
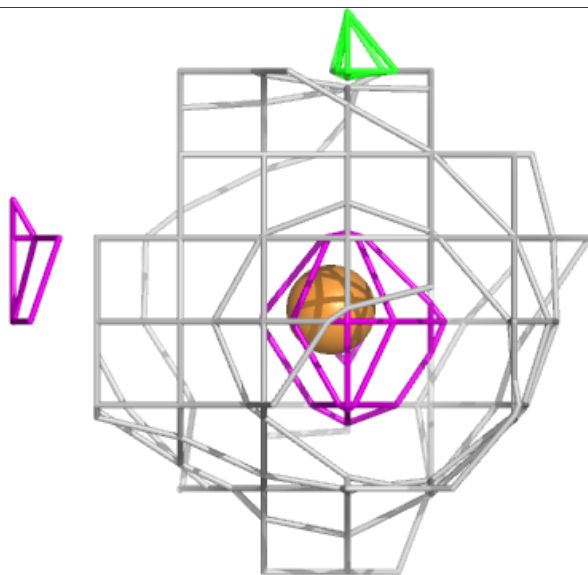
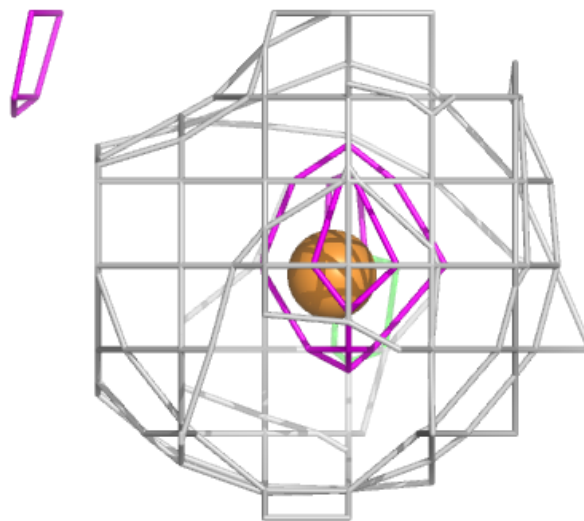
**Electron density around CU A 702:**

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



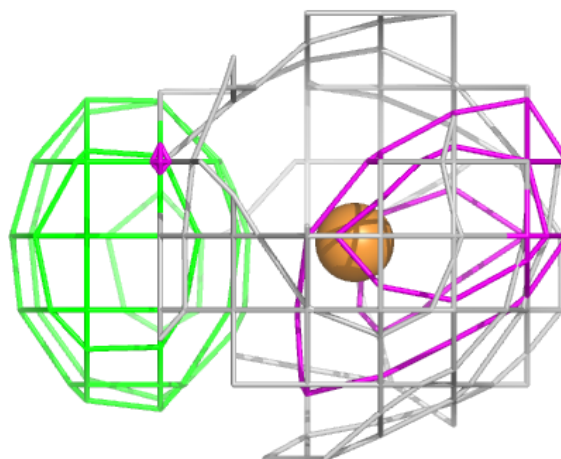
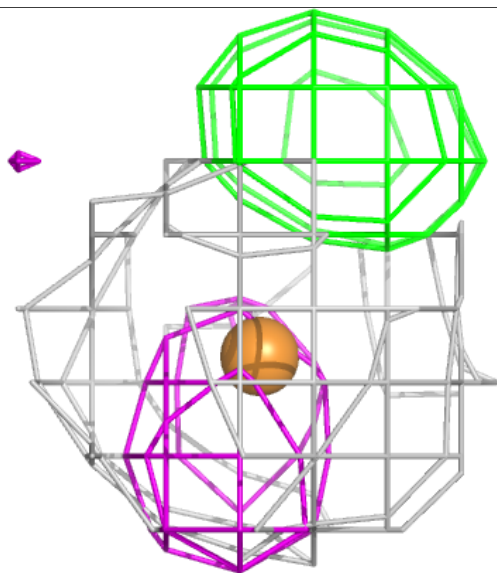
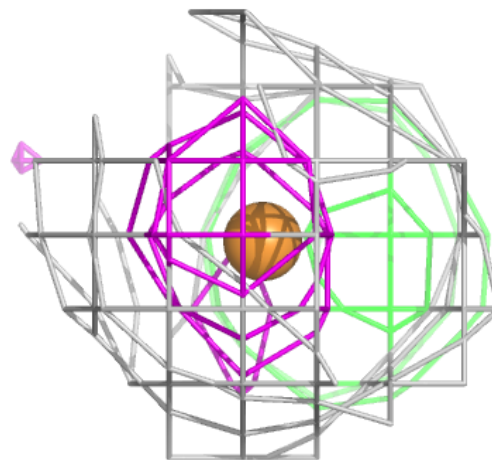
**Electron density around CU B 701:**

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



**Electron density around CU B 702:**

$2mF_o-DF_c$  (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.