Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:32 PM EDT

PDB ID	:	7AQ8
Title	:	Pseudomonas stutzeri nitrous oxide reductase mutant, H583Y/D576A
Authors	:	Zhang, L.; Bill, E.; Kroneck, P.M.H.; Einsle, O.
Deposited on	:	2020-10-20
Resolution	:	1.79 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:

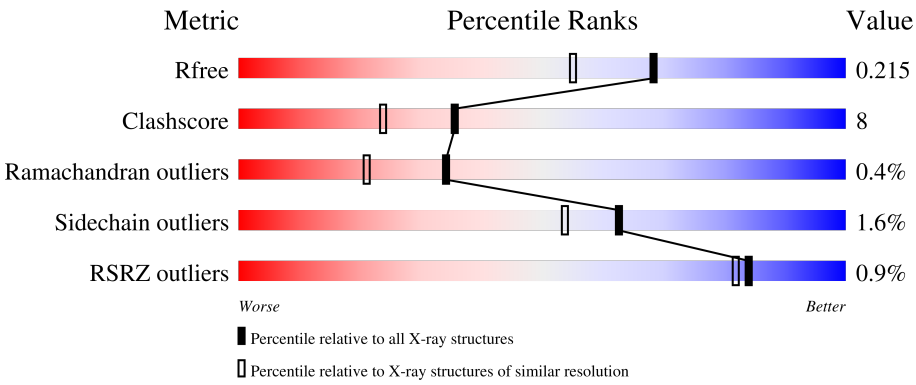
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	646	76% 12% • 11%
1	B	646	% 76% 14% • 9%

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	FMT	B	705	-	-	X	-
6	FMT	B	706	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10021 atoms, of which 4 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.

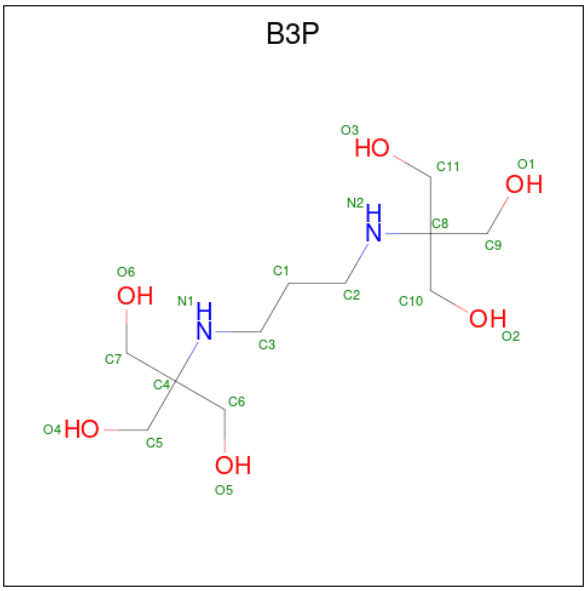
- Molecule 1 is a protein called Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	576	4552	2882	779	860	31	0	5	0
1	B	586	4617	2923	794	868	32	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	ALA	ASP	conflict	UNP P19573
A	583	TYR	HIS	conflict	UNP P19573
A	639	TRP	-	expression tag	UNP P19573
A	640	SER	-	expression tag	UNP P19573
A	641	HIS	-	expression tag	UNP P19573
A	642	PRO	-	expression tag	UNP P19573
A	643	GLN	-	expression tag	UNP P19573
A	644	PHE	-	expression tag	UNP P19573
A	645	GLU	-	expression tag	UNP P19573
A	646	LYS	-	expression tag	UNP P19573
B	576	ALA	ASP	conflict	UNP P19573
B	583	TYR	HIS	conflict	UNP P19573
B	639	TRP	-	expression tag	UNP P19573
B	640	SER	-	expression tag	UNP P19573
B	641	HIS	-	expression tag	UNP P19573
B	642	PRO	-	expression tag	UNP P19573
B	643	GLN	-	expression tag	UNP P19573
B	644	PHE	-	expression tag	UNP P19573
B	645	GLU	-	expression tag	UNP P19573
B	646	LYS	-	expression tag	UNP P19573

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 19 11 2 6	0	0
2	B	1	Total C N O 19 11 2 6	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

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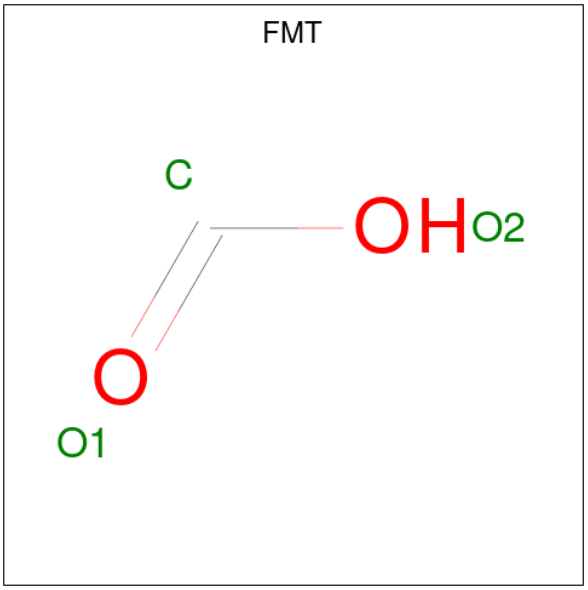
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

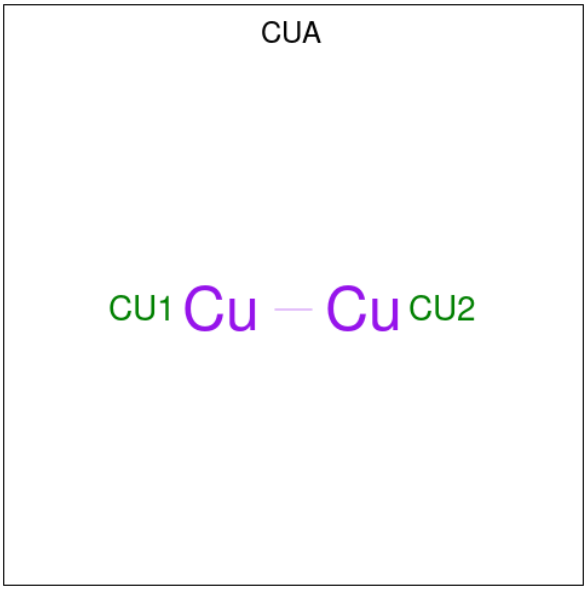


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C H O 5 1 2 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C H O 5 1 2 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).

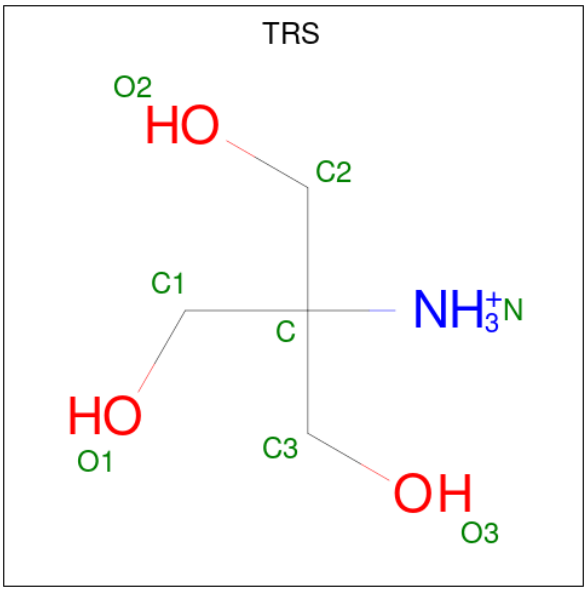


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cu 2 2	0	0
8	B	1	Total Cu 2 2	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

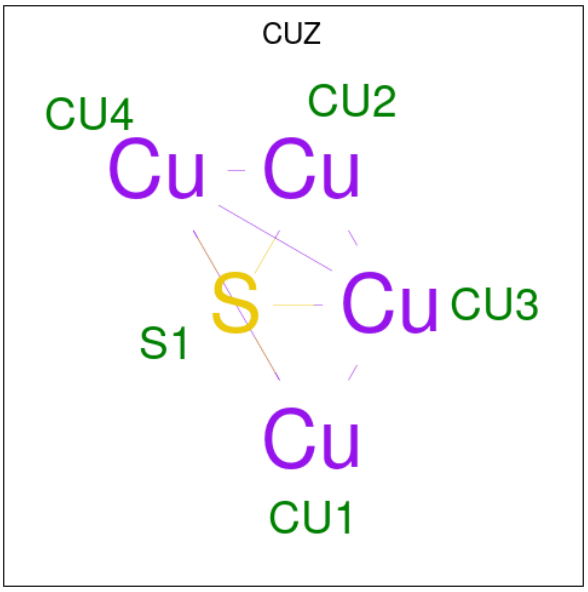
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Zn 2 2	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	8	4	1	3	0	0

- Molecule 11 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Cu	S		
11	B	1	5	4	1	0	0

- Molecule 12 is water.

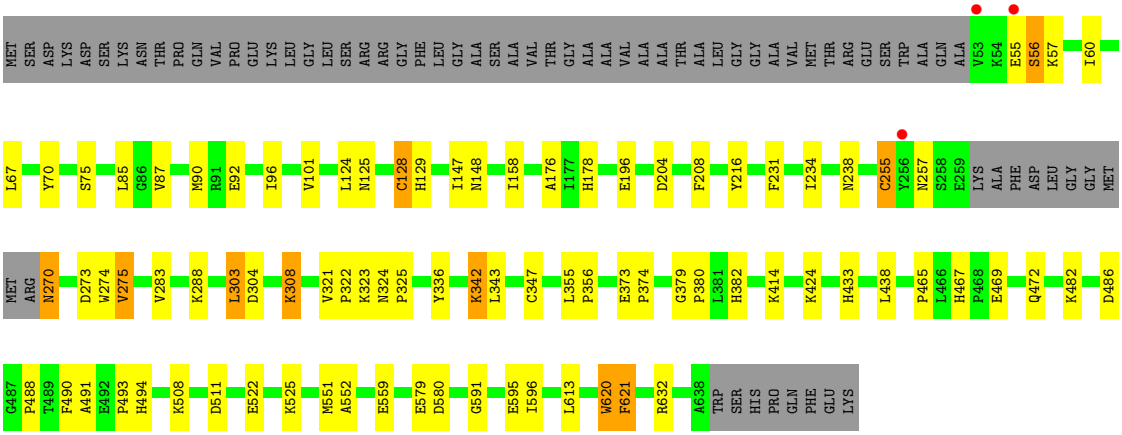
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	429	429	429	0	0
			Total	O		
12	B	327	327	327	0	0

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.

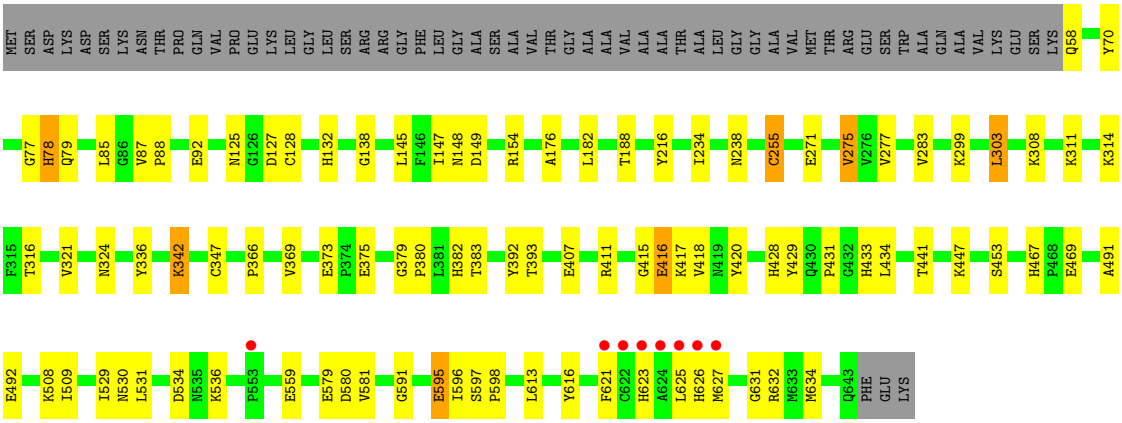
- Molecule 1: Nitrous-oxide reductase

Chain A:



- Molecule 1: Nitrous-oxide reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.55Å 76.67Å 109.06Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	69.43 – 1.79 69.43 – 1.79	Depositor EDS
% Data completeness (in resolution range)	69.4 (69.43-1.79) 69.6 (69.43-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.158 , 0.216 0.160 , 0.215	Depositor DCC
R_{free} test set	3703 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10021	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: CA, FMT, NA, B3P, CUZ, TRS, ZN, CL, CUA, K

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	0.46	0/4677	0.63	1/6334 (0.0%)
1	B	0.45	0/4736	0.62	1/6417 (0.0%)
All	All	0.46	0/9413	0.62	2/12751 (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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	613	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	303	LEU	CA-CB-CG	-5.29	103.13	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	TYR	Peptide
1	B	336	TYR	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	4552	0	4437	76	0
1	B	4617	0	4481	78	0
2	A	19	0	26	1	0
2	B	19	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	18	2	6	1	0
6	B	9	2	3	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	2	0	0	0	0
10	A	8	0	12	0	0
11	B	5	0	0	0	0
12	A	429	0	0	10	0
12	B	327	0	0	6	0
All	All	10017	4	8991	148	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 8.

All (148) 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:B:559:GLU:OE2	1:B:632:ARG:NH2	2.00	0.93
1:B:632:ARG:NH1	12:B:801:HOH:O	2.01	0.92
1:A:511:ASP:HB2	12:A:1170:HOH:O	1.75	0.85
1:A:178:HIS:NE2	12:A:802:HOH:O	2.12	0.81
1:A:90:MET:HE2	12:A:998:HOH:O	1.81	0.81
1:B:78:HIS:ND1	12:B:802:HOH:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:HIS:CE1	1:B:508:LYS:HD2	2.19	0.78
1:B:283:VAL:HG13	1:B:303:LEU:HD13	1.65	0.77
1:B:508:LYS:C	1:B:509:ILE:HD12	2.05	0.77
1:B:58:GLN:N	12:B:803:HOH:O	2.18	0.76
1:B:469:GLU:HG3	1:B:492:GLU:HA	1.69	0.75
1:A:525:LYS:HD3	6:A:705:FMT:C	2.18	0.74
1:A:238:ASN:OD1	1:A:257:ASN:HB3	1.87	0.73
1:A:508:LYS:HD3	1:A:579:GLU:OE2	1.92	0.70
1:A:204:ASP:OD2	12:A:801:HOH:O	2.11	0.68
1:B:508:LYS:HG2	1:B:579:GLU:CG	2.24	0.68
1:B:308:LYS:O	1:B:311:LYS:HG2	1.94	0.67
1:A:595:GLU:HB2	1:A:620:TRP:CZ3	2.31	0.66
1:B:581:VAL:HG12	1:B:581:VAL:O	1.97	0.64
1:A:101:VAL:HG21	1:A:124:LEU:HD22	1.81	0.62
1:A:216:TYR:CD1	1:A:234:ILE:HG23	2.35	0.62
1:A:75:SER:OG	1:A:493:PRO:O	2.17	0.62
1:A:270:ASN:O	1:A:323:LYS:NZ	2.28	0.61
1:B:407:GLU:HB3	1:B:411:ARG:NH2	2.15	0.61
1:B:508:LYS:HG2	1:B:579:GLU:HG2	1.81	0.60
1:A:255[A]:CYS:HB3	1:A:274:TRP:CD1	2.37	0.59
1:B:314:LYS:HE2	12:B:1018:HOH:O	2.03	0.59
1:A:238:ASN:O	1:A:255[B]:CYS:HA	2.04	0.58
1:B:416:GLU:O	1:B:418:VAL:HG12	2.03	0.57
1:B:271:GLU:OE2	1:B:271:GLU:HA	2.04	0.57
1:B:623:HIS:CE1	1:B:625:LEU:HD23	2.40	0.57
1:A:347:CYS:O	1:A:373:GLU:HA	2.04	0.57
1:A:580:ASP:OD1	1:B:467:HIS:HB2	2.05	0.57
1:A:128:CYS:HB3	1:A:148:ASN:O	2.05	0.56
1:A:283:VAL:HG13	1:A:303:LEU:HD13	1.87	0.56
1:A:55:GLU:OE1	1:A:57:LYS:HD3	2.05	0.55
1:B:411:ARG:HB3	1:B:416:GLU:OE1	2.05	0.55
1:A:595:GLU:HG2	1:A:596:ILE:N	2.21	0.55
12:A:1155:HOH:O	1:B:627:MET:HE2	2.06	0.55
1:B:238:ASN:O	1:B:255:CYS:HB2	2.06	0.55
1:A:238:ASN:O	1:A:255[A]:CYS:HA	2.07	0.55
1:A:467:HIS:HB2	1:B:580:ASP:OD2	2.06	0.55
1:B:534:ASP:HB3	1:B:536:LYS:HD2	1.87	0.55
1:A:196:GLU:O	1:A:238:ASN:ND2	2.41	0.54
1:A:433:HIS:HB2	1:A:494:HIS:O	2.08	0.53
1:A:129:HIS:HB3	1:A:494:HIS:HD2	1.72	0.53
1:B:78:HIS:HA	1:B:127:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLY:O	1:B:417:LYS:N	2.41	0.53
1:A:613:LEU:HD11	1:A:632:ARG:HB3	1.91	0.53
1:B:85:LEU:HD22	1:B:92:GLU:HA	1.91	0.53
1:B:128:CYS:HB2	1:B:147:ILE:CD1	2.38	0.53
1:A:467:HIS:NE2	1:B:508:LYS:HD2	2.23	0.53
1:A:382:HIS:CE1	1:A:433:HIS:CE1	2.97	0.52
1:A:414:LYS:HE3	12:A:1113:HOH:O	2.08	0.52
1:B:580:ASP:OD2	12:B:804:HOH:O	2.19	0.52
1:A:178:HIS:HB3	12:A:919:HOH:O	2.09	0.52
1:A:56:SER:HB2	1:A:482:LYS:NZ	2.24	0.52
1:B:383:THR:HA	1:B:392:TYR:O	2.09	0.52
1:A:255[B]:CYS:HB2	1:A:274:TRP:CD1	2.44	0.51
1:B:58:GLN:OE1	1:B:447:LYS:HD2	2.10	0.51
1:A:55:GLU:HG2	1:A:56:SER:N	2.26	0.51
1:A:85:LEU:HD22	1:A:92:GLU:HA	1.92	0.51
1:A:70:TYR:HB2	1:A:87:VAL:HB	1.93	0.51
1:A:465:PRO:HD2	12:B:968:HOH:O	2.11	0.51
1:B:149:ASP:HB3	1:B:154:ARG:HB2	1.93	0.50
1:B:382:HIS:CE1	1:B:433:HIS:CE1	2.99	0.50
1:A:595:GLU:HB2	1:A:620:TRP:CH2	2.46	0.50
1:B:625:LEU:HD22	1:B:625:LEU:N	2.27	0.50
1:A:342:LYS:HG2	1:A:343:LEU:HD22	1.94	0.50
1:A:231:PHE:CE1	1:A:283:VAL:HG11	2.47	0.50
1:A:424:LYS:HE3	12:A:1134:HOH:O	2.13	0.49
1:B:508:LYS:O	1:B:509:ILE:HD12	2.11	0.49
1:A:591:GLY:HA2	1:B:125:ASN:OD1	2.13	0.49
1:A:125:ASN:OD1	1:B:591:GLY:HA2	2.13	0.48
1:A:613:LEU:HD11	1:A:632:ARG:HG2	1.95	0.48
1:A:493:PRO:O	1:A:494:HIS:CB	2.61	0.48
1:B:595:GLU:HG2	1:B:596:ILE:N	2.29	0.48
1:A:75:SER:HB2	1:A:147:ILE:HD11	1.95	0.48
1:A:490:PHE:O	1:A:491:ALA:HB3	2.13	0.48
1:A:255[B]:CYS:HG	1:A:274:TRP:HE1	1.62	0.47
2:A:701:B3P:H32	2:A:701:B3P:O6	2.14	0.47
1:B:85:LEU:HD23	1:B:85:LEU:N	2.28	0.47
1:B:379:GLY:N	1:B:380:PRO:HD3	2.29	0.47
2:B:701:B3P:N2	6:B:706:FMT:H	2.29	0.47
1:B:382:HIS:O	1:B:393:THR:HA	2.15	0.47
1:A:208:PHE:CD1	1:B:634:MET:HG2	2.50	0.47
1:B:77:GLY:HA2	1:B:128:CYS:O	2.16	0.46
1:B:275:VAL:HG13	1:B:321:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLU:O	1:B:416:GLU:HG2	2.15	0.46
1:B:407:GLU:HB3	1:B:411:ARG:HH22	1.78	0.46
1:A:469:GLU:O	1:A:488:PRO:HA	2.16	0.46
1:B:128:CYS:HB2	1:B:147:ILE:HD11	1.97	0.46
1:A:347:CYS:O	1:A:374:PRO:HD2	2.15	0.46
1:A:632:ARG:HD3	12:A:910:HOH:O	2.15	0.46
1:A:467:HIS:HE1	1:B:508:LYS:HD2	1.77	0.46
1:A:493:PRO:O	1:A:494:HIS:HB3	2.16	0.46
1:A:472:GLN:HG2	1:A:486:ASP:OD1	2.15	0.46
1:B:428:HIS:HA	1:B:429:TYR:CG	2.51	0.45
1:A:255[B]:CYS:SG	1:A:274:TRP:NE1	2.89	0.45
1:B:79:GLN:HB2	1:B:491:ALA:CB	2.47	0.45
1:B:299:LYS:HA	1:B:299:LYS:HD3	1.79	0.45
1:A:67:LEU:N	1:A:67:LEU:HD22	2.32	0.45
1:A:621:PHE:HB2	1:B:492:GLU:OE2	2.16	0.45
1:B:128:CYS:HB3	1:B:148:ASN:O	2.17	0.44
1:A:56:SER:HB2	1:A:482:LYS:HZ2	1.81	0.44
1:A:522:GLU:OE1	1:A:525:LYS:HE3	2.17	0.44
1:A:559:GLU:HA	1:A:632:ARG:O	2.17	0.44
1:A:438:LEU:HD23	1:A:438:LEU:N	2.33	0.44
1:B:508:LYS:HE3	1:B:579:GLU:OE2	2.18	0.44
1:B:623:HIS:HE1	1:B:625:LEU:HD23	1.81	0.44
1:B:347:CYS:O	1:B:373:GLU:HA	2.18	0.43
1:B:509:ILE:HD12	1:B:509:ILE:N	2.32	0.43
1:A:60:ILE:HG23	12:A:1126:HOH:O	2.18	0.43
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.99	0.43
1:B:87:VAL:HG13	1:B:88:PRO:HA	1.99	0.43
1:A:355:LEU:N	1:A:356:PRO:CD	2.81	0.43
1:B:132:HIS:O	1:B:145:LEU:HD12	2.18	0.43
1:B:277:VAL:O	1:B:316:THR:HA	2.19	0.43
1:A:304:ASP:OD2	1:A:308:LYS:NZ	2.43	0.43
1:B:366:PRO:O	1:B:369:VAL:HG22	2.20	0.42
1:B:431:PRO:HA	1:B:453:SER:HA	2.01	0.42
1:B:216:TYR:CD1	1:B:234:ILE:HG23	2.54	0.42
1:B:375:GLU:HG3	1:B:420:TYR:OH	2.20	0.42
1:A:273:ASP:HB2	1:A:325:PRO:HD2	2.02	0.42
1:B:616:TYR:CE1	1:B:631:GLY:HA3	2.54	0.42
2:B:701:B3P:HN2	6:B:706:FMT:H	1.83	0.42
1:A:551:MET:O	1:A:552:ALA:C	2.58	0.42
1:B:531:LEU:H	6:B:705:FMT:H	1.84	0.41
1:B:529:ILE:HD13	1:B:536:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASN:HA	6:B:705:FMT:H	2.02	0.41
1:A:238:ASN:CG	1:A:257:ASN:HB3	2.41	0.41
1:B:597:SER:HB3	1:B:598:PRO:HD2	2.02	0.41
1:A:379:GLY:N	1:A:380:PRO:HD3	2.36	0.41
1:B:508:LYS:HG2	1:B:579:GLU:CD	2.41	0.41
1:B:529:ILE:CD1	1:B:536:LYS:HD3	2.51	0.41
1:B:597:SER:HB3	1:B:598:PRO:CD	2.51	0.41
1:A:288:LYS:HA	1:A:288:LYS:HE2	2.03	0.41
1:B:138:GLY:O	1:B:441:THR:HB	2.21	0.41
1:B:375:GLU:HG3	1:B:375:GLU:H	1.75	0.41
1:A:255[A]:CYS:HB3	1:A:274:TRP:NE1	2.35	0.41
1:B:531:LEU:H	6:B:705:FMT:C	2.34	0.41
1:A:275:VAL:CG1	1:A:321:VAL:HG21	2.51	0.40
1:B:182:LEU:HB3	1:B:188:THR:HG23	2.04	0.40
1:A:322:PRO:HA	1:A:323:LYS:HA	1.92	0.40
1:A:324:ASN:HB3	1:A:342:LYS:HE2	2.04	0.40
1:A:96:ILE:HG21	1:A:158:ILE:HD13	2.03	0.40
1:B:324:ASN:O	1:B:342:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	577/646 (89%)	551 (96%)	24 (4%)	2 (0%)	41 27
1	B	585/646 (91%)	559 (96%)	23 (4%)	3 (0%)	29 15
All	All	1162/1292 (90%)	1110 (96%)	47 (4%)	5 (0%)	34 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	416	GLU
1	B	342	LYS
1	A	176	ALA
1	A	342	LYS
1	B	176	ALA

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	498/544 (92%)	489 (98%)	9 (2%)	59	48
1	B	501/544 (92%)	493 (98%)	8 (2%)	62	54
All	All	999/1088 (92%)	982 (98%)	17 (2%)	62	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	128	CYS
1	A	255[A]	CYS
1	A	255[B]	CYS
1	A	270	ASN
1	A	275	VAL
1	A	308	LYS
1	A	620	TRP
1	A	621	PHE
1	B	78	HIS
1	B	255	CYS
1	B	275	VAL
1	B	303	LEU
1	B	434	LEU
1	B	595	GLU
1	B	621	PHE
1	B	626	HIS

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

Mol	Chain	Res	Type
1	A	513	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
2	B3P	A	701	-	18,18,18	0.92	1 (5%)	23,23,23	1.18	2 (8%)
6	FMT	A	706	-	2,2,2	0.58	0	1,1,1	0.00	0
6	FMT	A	713	-	2,2,2	0.61	0	1,1,1	0.06	0
6	FMT	B	706	-	2,2,2	0.72	0	1,1,1	0.24	0
2	B3P	B	701	-	18,18,18	0.84	0	23,23,23	1.18	4 (17%)
6	FMT	A	715	-	2,2,2	0.66	0	1,1,1	0.33	0
6	FMT	A	707	-	2,2,2	0.73	0	1,1,1	0.27	0
6	FMT	B	710	-	2,2,2	0.72	0	1,1,1	0.40	0
8	CUA	A	710	1	0,1,1	-	-	-		
6	FMT	B	705	-	2,2,2	0.68	0	1,1,1	0.19	0
10	TRS	A	714	-	7,7,7	0.26	0	9,9,9	0.58	0
6	FMT	A	708	-	2,2,2	0.71	0	1,1,1	0.15	0
11	CUZ	B	708	1,12	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FMT	A	705	-	2,2,2	0.67	0	1,1,1	0.25	0
8	CUA	B	709	1	0,1,1	-	-	-		

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
2	B3P	A	701	-	-	1/28/28/28	-
2	B3P	B	701	-	-	3/28/28/28	-
10	TRS	A	714	-	-	9/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	B3P	C3-N1	2.01	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	B3P	C2-N2-C8	-2.52	112.47	116.17
2	B	701	B3P	O3-C11-C8	-2.52	106.57	111.68
2	A	701	B3P	O5-C6-C4	-2.21	107.19	111.68
2	B	701	B3P	O1-C9-C8	-2.20	107.20	111.68
2	B	701	B3P	O2-C10-C8	-2.14	107.33	111.68
2	B	701	B3P	C1-C3-N1	-2.02	106.09	110.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	B3P	C10-C8-N2-C2
2	B	701	B3P	C11-C8-N2-C2
10	A	714	TRS	N-C-C1-O1
10	A	714	TRS	N-C-C3-O3
10	A	714	TRS	C2-C-C1-O1
2	A	701	B3P	C5-C4-N1-C3
2	B	701	B3P	C9-C8-N2-C2
10	A	714	TRS	C3-C-C2-O2
10	A	714	TRS	C2-C-C3-O3

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Mol	Chain	Res	Type	Atoms
10	A	714	TRS	C1-C-C2-O2
10	A	714	TRS	C3-C-C1-O1
10	A	714	TRS	N-C-C2-O2
10	A	714	TRS	C1-C-C3-O3

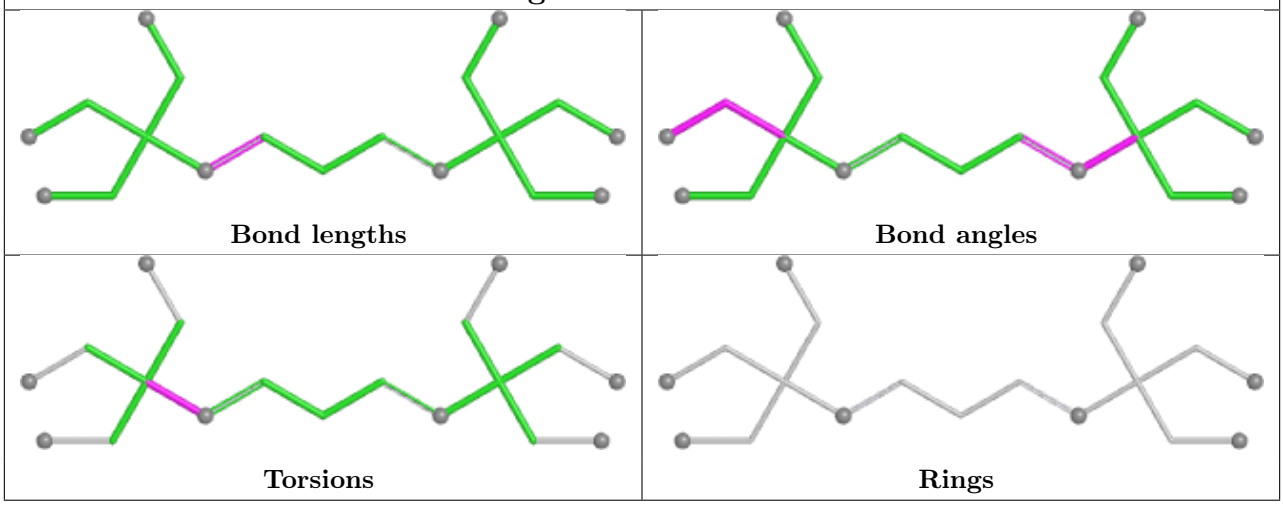
There are no ring outliers.

5 monomers are involved in 7 short contacts:

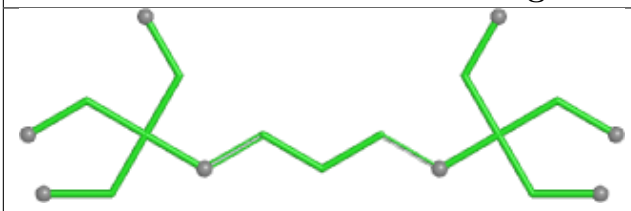
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	B3P	1	0
6	B	706	FMT	2	0
2	B	701	B3P	2	0
6	B	705	FMT	3	0
6	A	705	FMT	1	0

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.

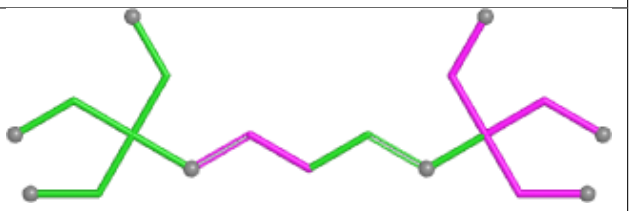
Ligand B3P A 701



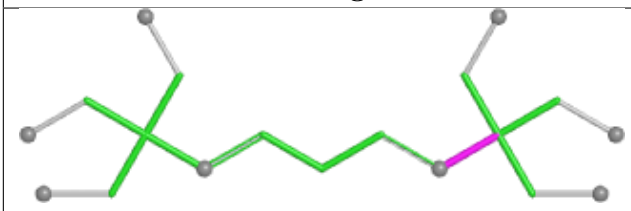
Ligand B3P B 701



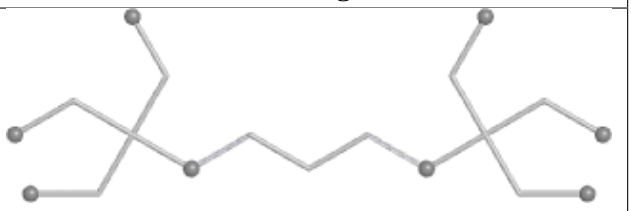
Bond lengths



Bond angles

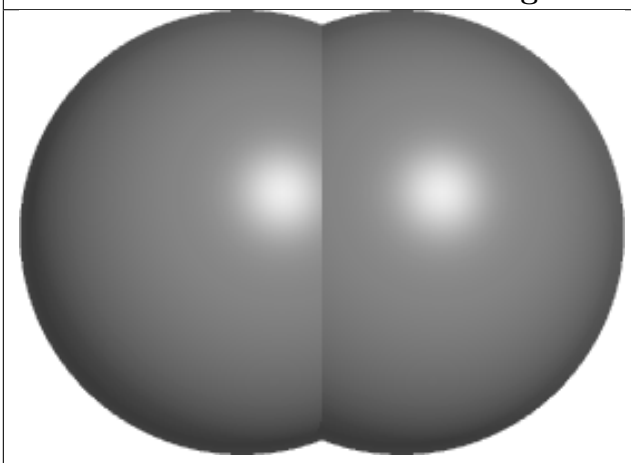


Torsions

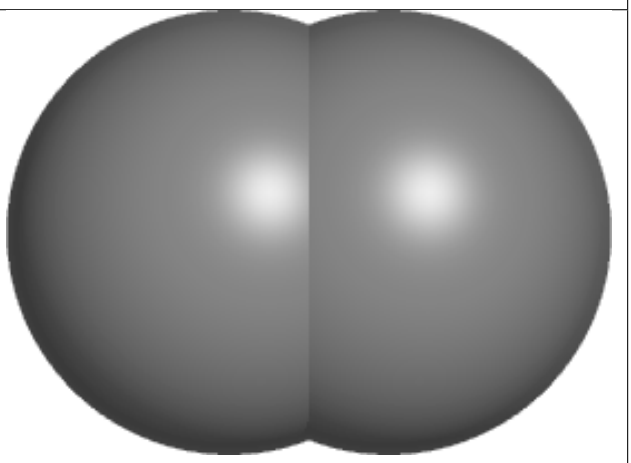


Rings

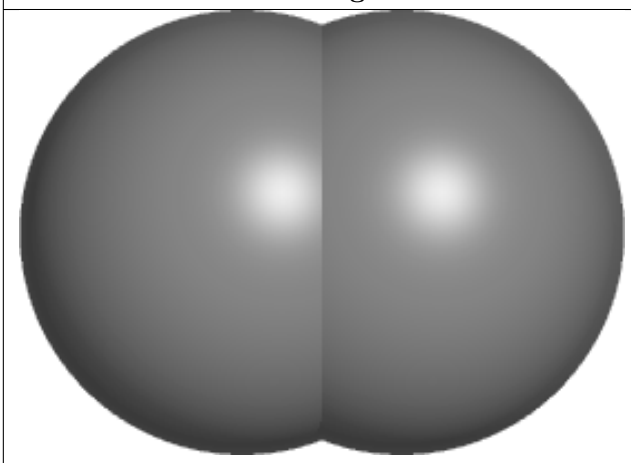
Ligand CUA A 710



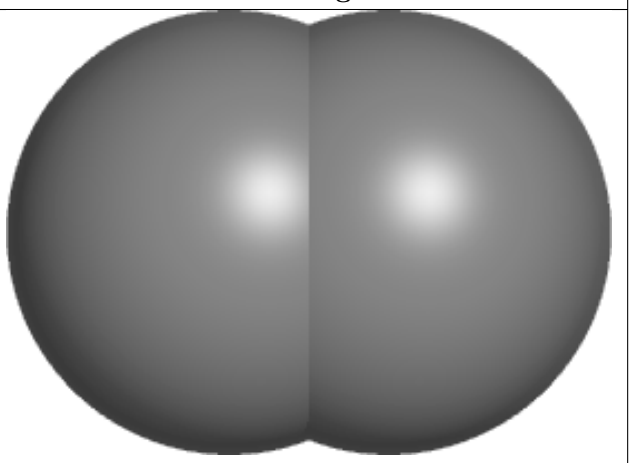
Bond lengths



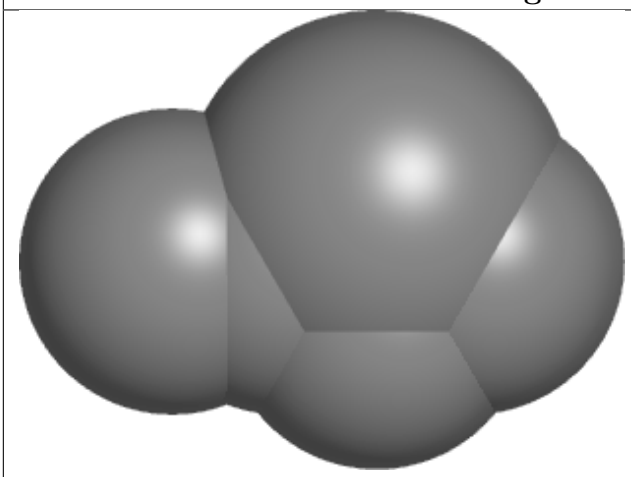
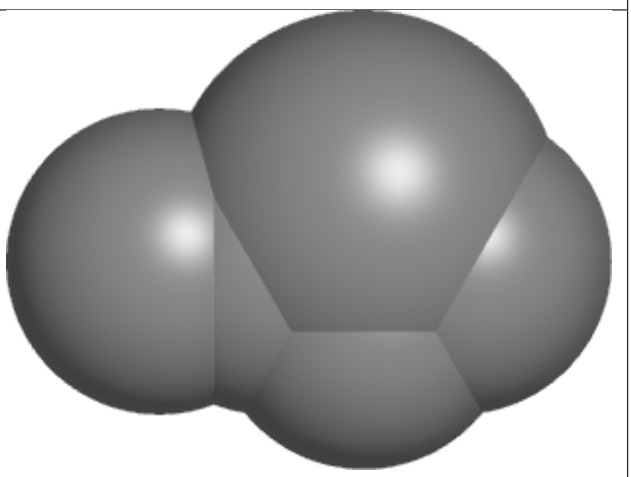
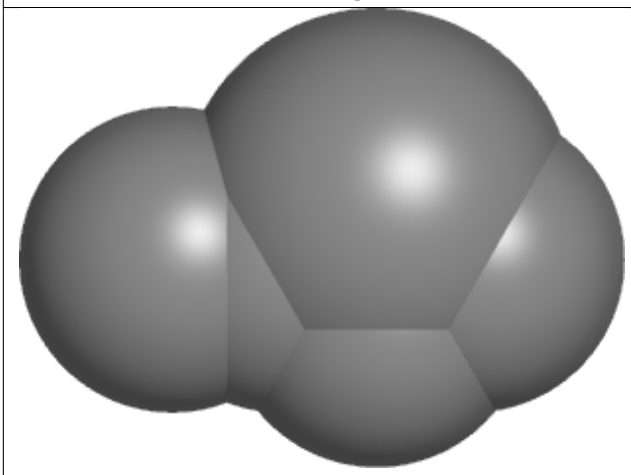
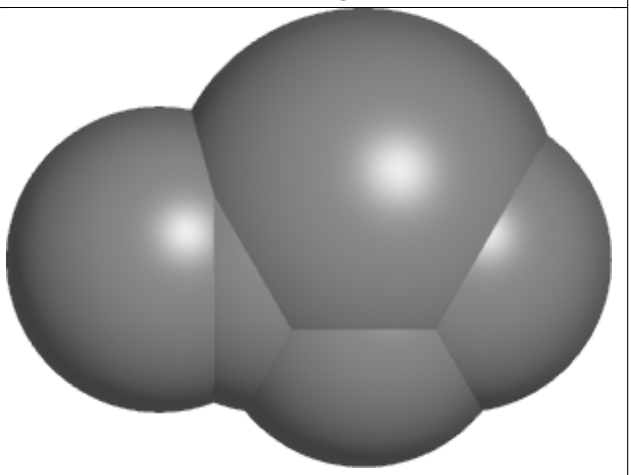
Bond angles

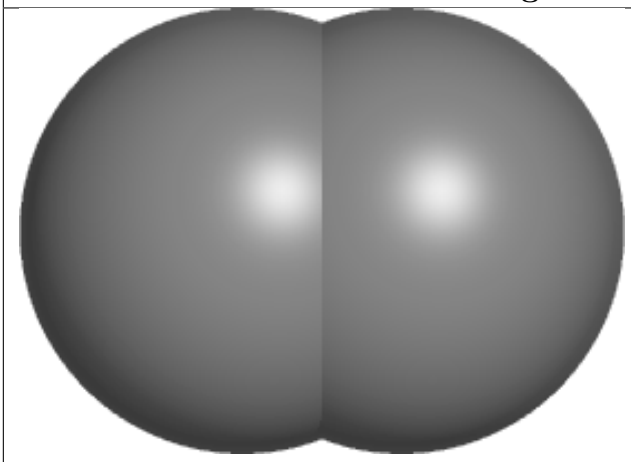
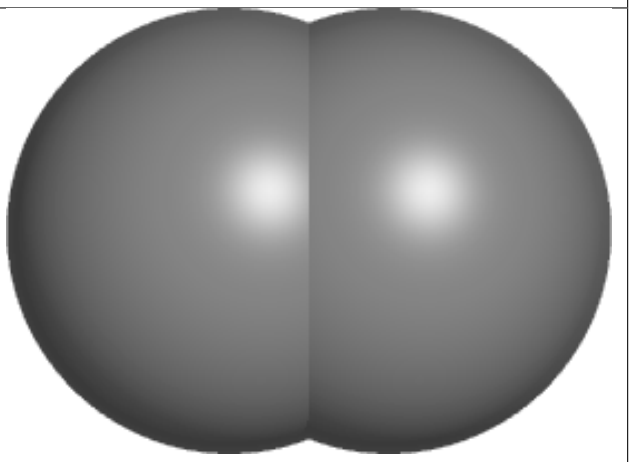
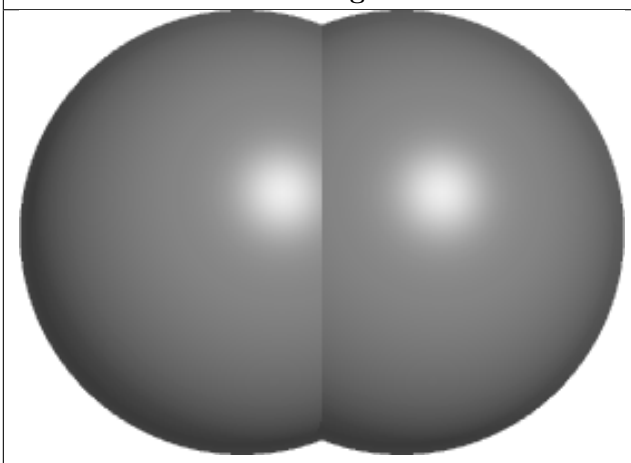
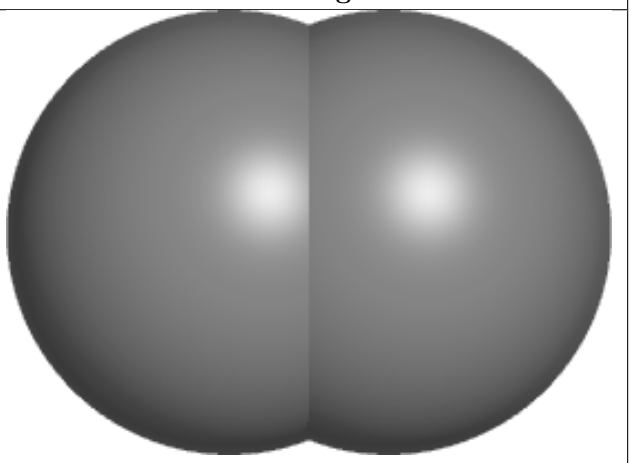


Torsions



Rings

Ligand CUZ B 708	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CUA B 709	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	576/646 (89%)	-0.38	3 (0%)	91	89	18, 31, 57, 100	0
1	B	586/646 (90%)	-0.31	8 (1%)	75	72	21, 37, 65, 93	0
All	All	1162/1292 (89%)	-0.35	11 (0%)	84	82	18, 34, 62, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	621	PHE	4.0
1	A	53	VAL	3.7
1	B	623	HIS	3.1
1	B	622	CYS	2.8
1	B	626	HIS	2.6
1	B	625	LEU	2.4
1	B	627	MET	2.4
1	B	624	ALA	2.3
1	A	55	GLU	2.3
1	B	553	PRO	2.2
1	A	256	TYR	2.1

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)

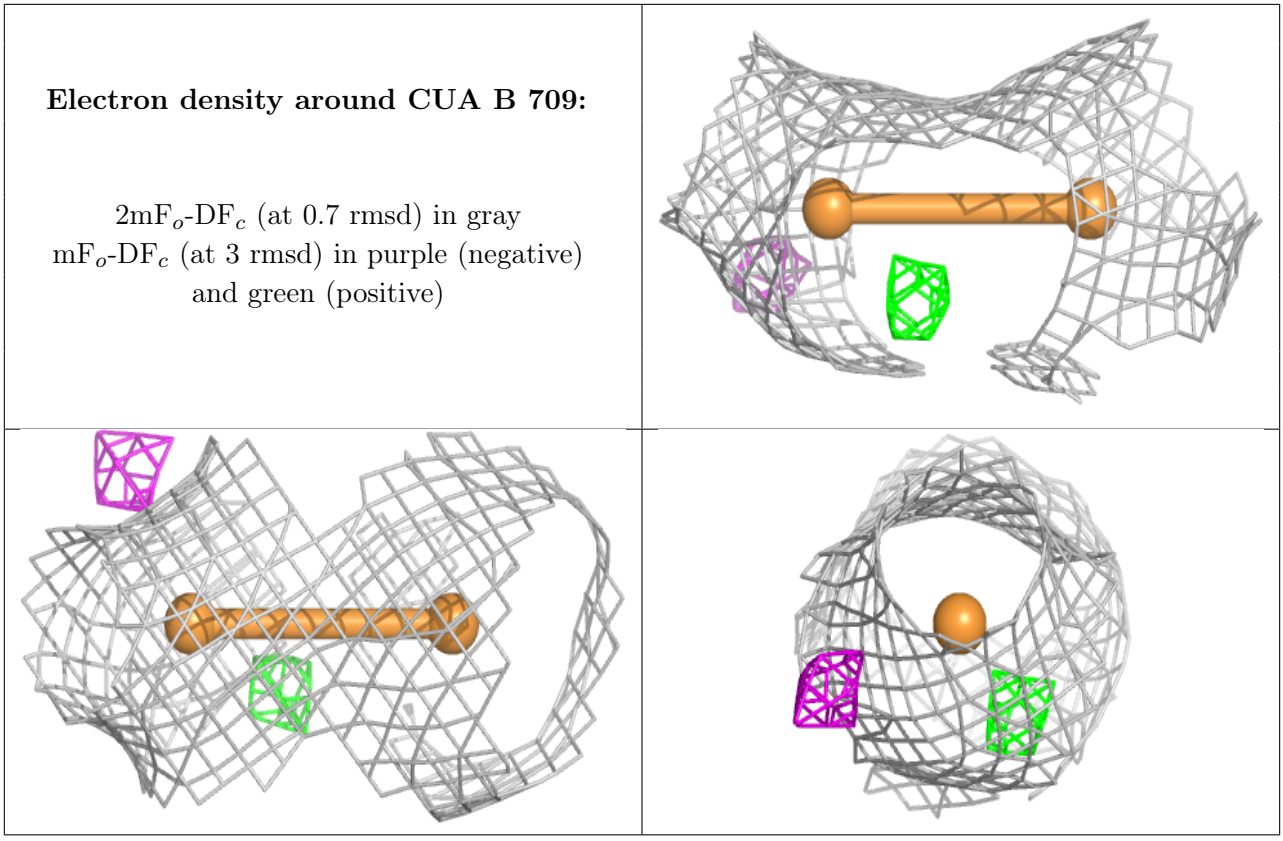
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FMT	A	715	3/3	0.60	0.17	68,71,85,88	0
5	K	A	704	1/1	0.62	0.11	94,94,94,94	0
6	FMT	B	710	3/3	0.67	0.29	76,78,94,95	0
6	FMT	A	705	3/3	0.80	0.16	62,62,67,69	0
6	FMT	A	708	3/3	0.81	0.13	62,62,63,66	0
6	FMT	A	707	3/3	0.82	0.11	66,66,73,78	0
6	FMT	B	705	3/3	0.84	0.26	75,75,77,77	0
6	FMT	A	713	3/3	0.86	0.14	35,35,53,55	0
10	TRS	A	714	8/8	0.88	0.14	45,56,57,63	0
4	CA	A	703	1/1	0.89	0.10	44,44,44,44	1
8	CUA	B	709	2/2	0.90	0.05	47,47,47,77	1
6	FMT	A	706	3/3	0.90	0.18	36,36,60,70	0
2	B3P	A	701	19/19	0.95	0.07	27,32,37,45	0
2	B3P	B	701	19/19	0.95	0.07	22,29,36,36	0
3	NA	B	702	1/1	0.96	0.06	38,38,38,38	1
11	CUZ	B	708	5/5	0.96	0.06	34,42,50,54	4
6	FMT	B	706	3/3	0.97	0.14	40,40,46,57	0
5	K	B	704	1/1	0.97	0.05	35,35,35,35	1
8	CUA	A	710	2/2	0.97	0.06	37,37,37,55	2
3	NA	A	702	1/1	0.98	0.05	32,32,32,32	0
9	ZN	A	711	1/1	0.98	0.03	46,46,46,46	1
7	CL	B	707	1/1	0.99	0.10	35,35,35,35	1
4	CA	B	703	1/1	0.99	0.07	28,28,28,28	1
7	CL	A	709	1/1	0.99	0.09	27,27,27,27	1
9	ZN	A	712	1/1	1.00	0.07	34,34,34,34	1

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.

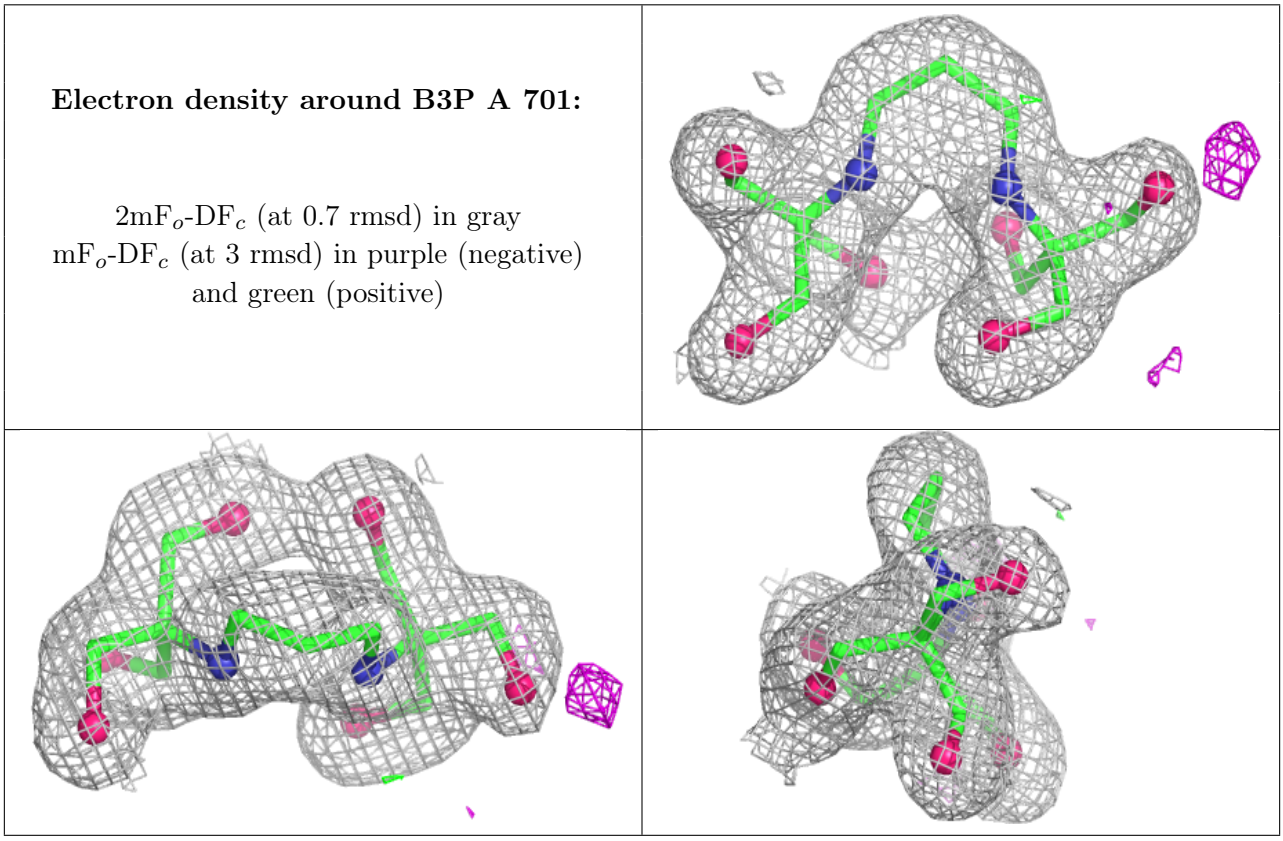
Electron density around CUA B 709:

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



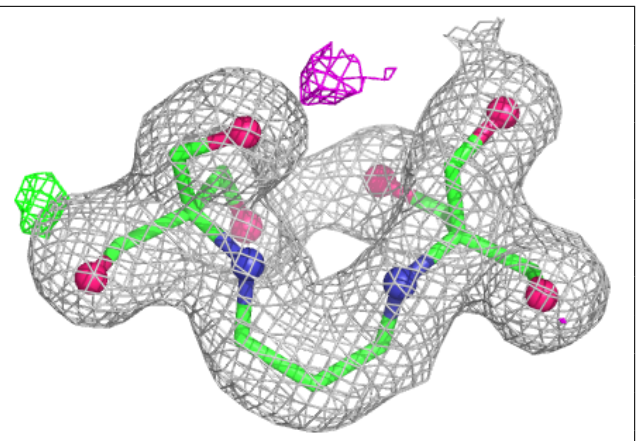
Electron density around B3P A 701:

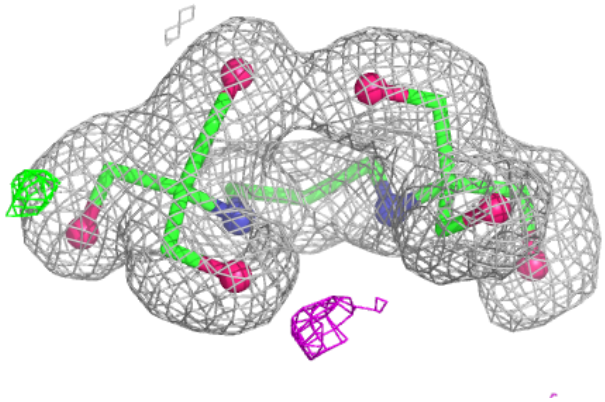
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

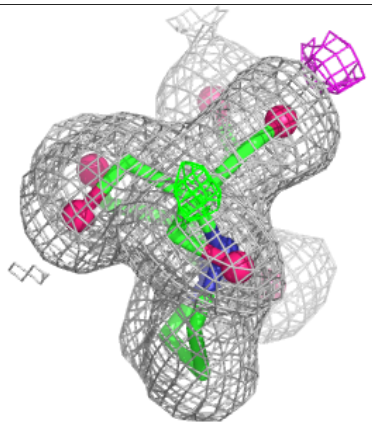


Electron density around B3P B 701:

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

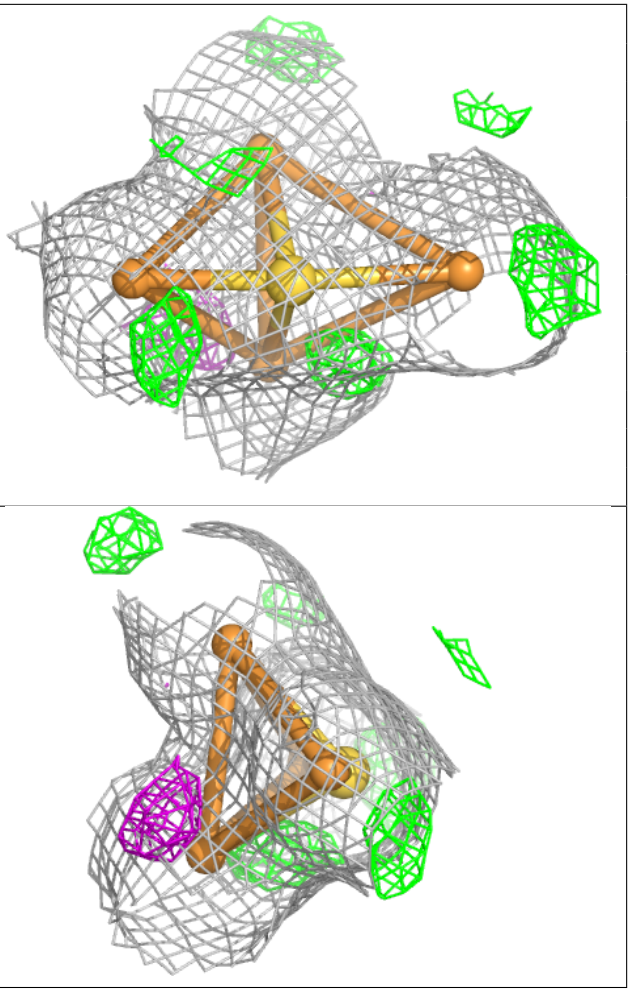






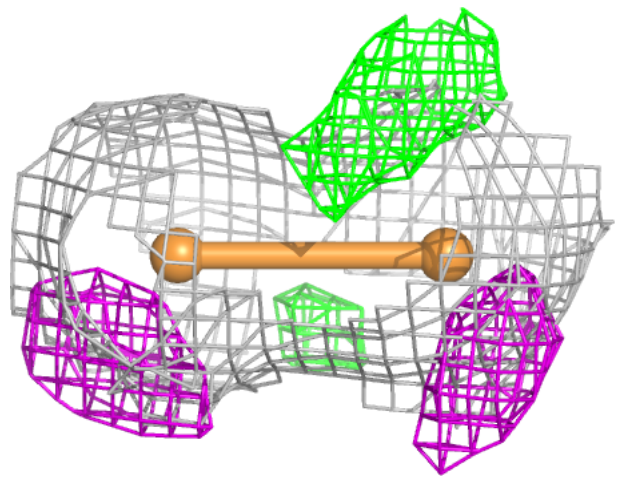
Electron density around CUZ B 708:

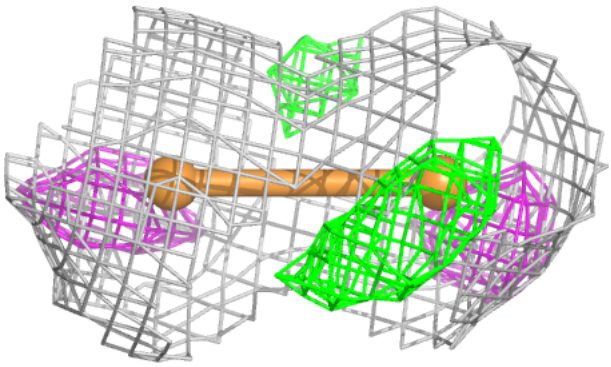
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

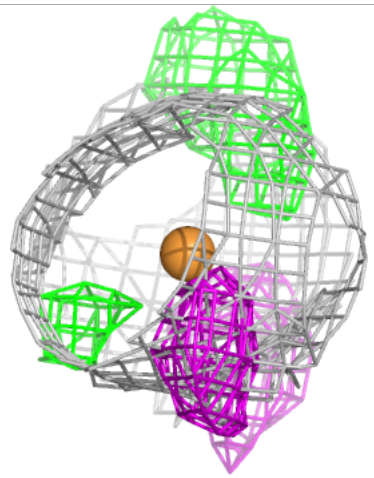


Electron density around CUA A 710:

$2mF_o$-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.