Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:15 PM EDT

PDB ID	:	7AQ6
Title	:	Pseudomonas stutzeri nitrous oxide reductase mutant, H583F
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Deposited on	:	2020-10-20
Resolution	:	1.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

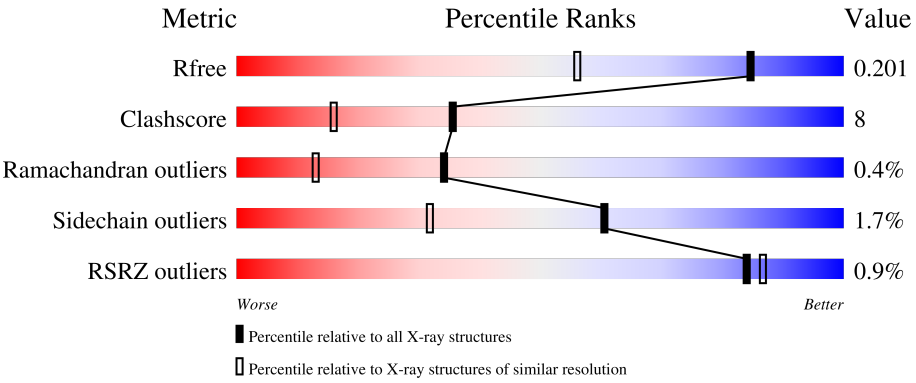
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	646	% 78% 12% • 9%
1	B	646	% 77% 13% • 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	A	716	-	-	X	-
6	FMT	B	2206	-	-	X	-
6	FMT	B	2211	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 10426 atoms, of which 6 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.

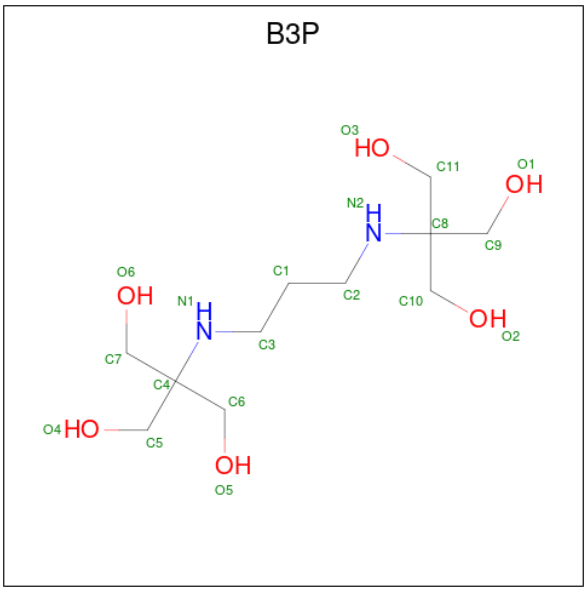
- Molecule 1 is a protein called Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	6	0
			4639	2936	794	877	32			
1	B	588	Total	C	N	O	S	0	2	0
			4650	2948	797	873	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	PHE	HIS	engineered mutation	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	583	PHE	HIS	engineered mutation	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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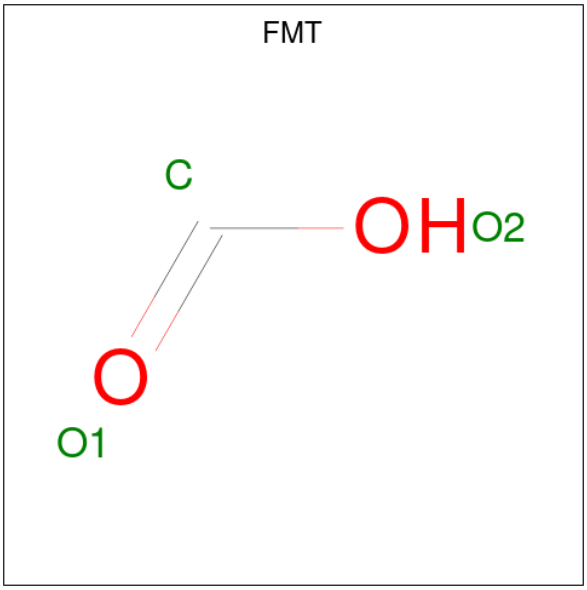
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

- 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 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	A	1	Total C H O 5 1 2 2	0	0

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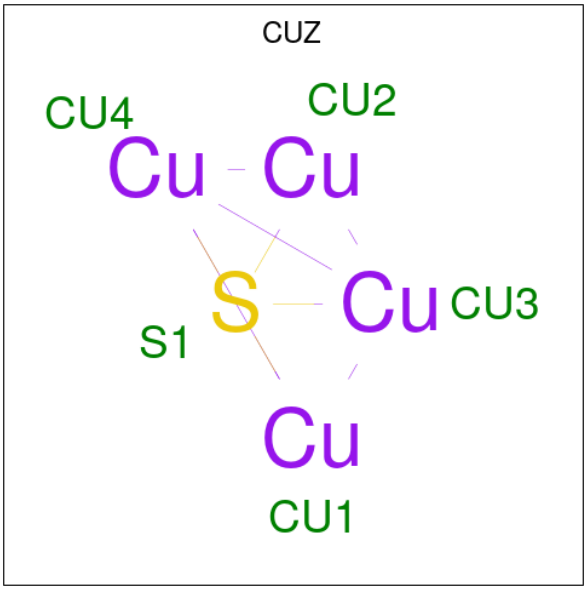
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H O 5 1 2 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0

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

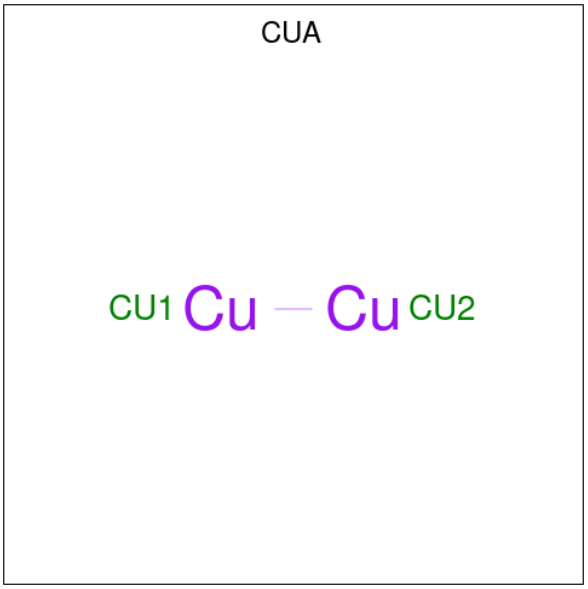
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu_4S) (labeled as "Ligand of Interest" by depositor).



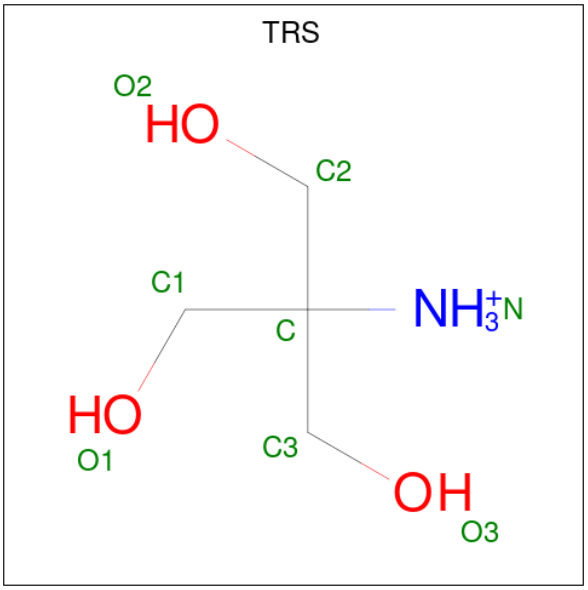
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cu S 5 4 1	0	0
8	B	1	Total Cu S 5 4 1	0	0

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cu 2 2	0	0
9	B	1	Total Cu 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
10	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 11 is water.

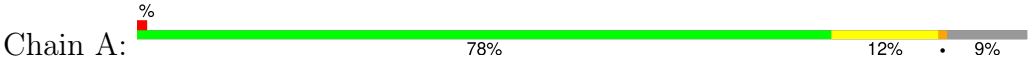
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	558	Total	O	0	0
			558	558		
11	B	463	Total	O	0	0
			463	463		

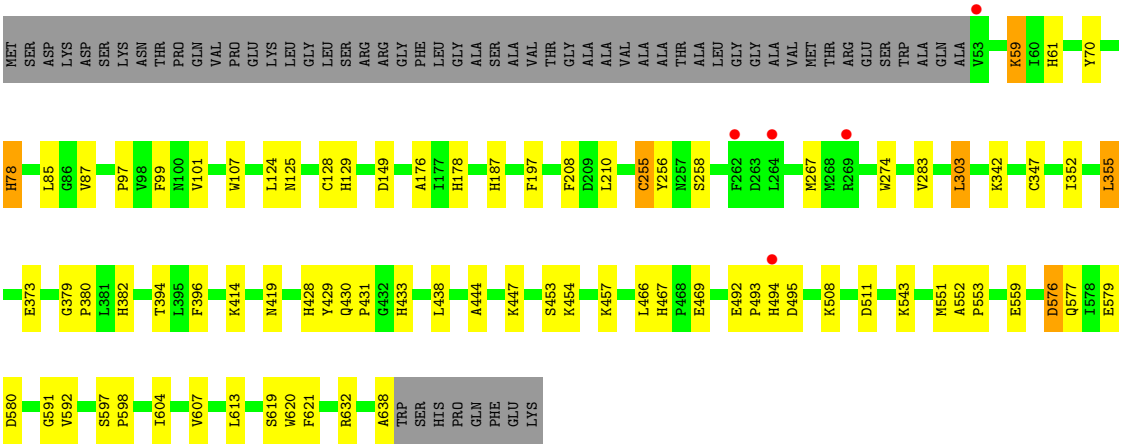
3 Residue-property plots (i)

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

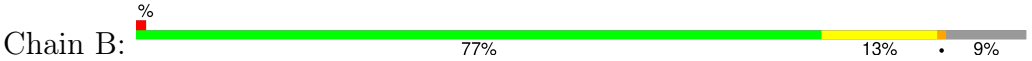
Chain A:

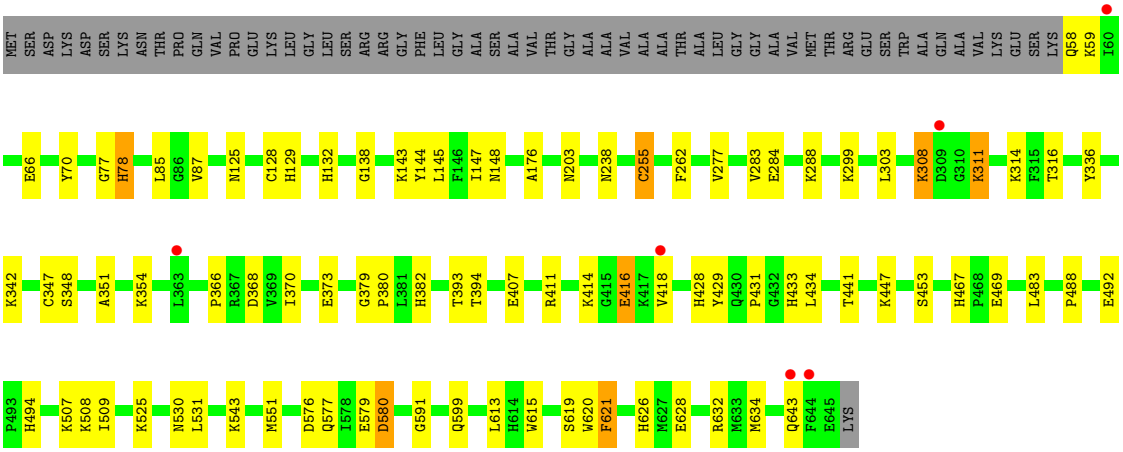




• Molecule 1: Nitrous-oxide reductase

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	69.05Å 76.59Å 108.63Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	108.44 – 1.51 108.44 – 1.51	Depositor EDS
% Data completeness (in resolution range)	64.7 (108.44-1.51) 64.9 (108.44-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.156 , 0.200 0.158 , 0.201	Depositor DCC
R_{free} test set	5773 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10426	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, B3P, CL, NA, CA, FMT, TRS, CUZ, CUA

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	0.50	1/4766 (0.0%)	0.66	3/6451 (0.0%)
1	B	0.46	0/4775	0.63	1/6470 (0.0%)
All	All	0.48	1/9541 (0.0%)	0.64	4/12921 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	CYS	CB-SG	-7.63	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	493	PRO	C-N-CA	-8.36	100.81	121.70
1	A	303	LEU	CA-CB-CG	-7.75	97.48	115.30
1	A	85	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	580	ASP	CB-CG-OD1	5.64	123.37	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4639	0	4521	72	0
1	B	4650	0	4505	88	1
2	A	19	0	26	1	0
2	B	19	0	26	1	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	30	4	10	4	0
6	B	12	2	4	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	8	0	12	0	1
11	A	558	0	0	17	5
11	B	463	0	0	20	2
All	All	10420	6	9104	149	7

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 (149) 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:469[A]:GLU:HG3	1:A:492:GLU:HA	1.38	1.03
1:A:543:LYS:NZ	11:A:801:HOH:O	1.91	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:HB2	11:A:1242:HOH:O	1.64	0.96
1:A:577:GLN:HG2	11:A:1098:HOH:O	1.70	0.91
1:A:267:MET:HE2	1:B:628:GLU:HG3	1.52	0.91
1:A:267:MET:CE	1:B:628:GLU:HG3	2.07	0.85
1:B:469:GLU:HG3	1:B:492:GLU:HA	1.60	0.84
1:B:509:ILE:HD11	1:B:599:GLN:HG3	1.60	0.82
1:A:256:TYR:CE1	1:A:267:MET:HE3	2.16	0.81
1:B:314:LYS:NZ	11:B:2305:HOH:O	2.14	0.80
1:A:419:ASN:OD1	11:A:802:HOH:O	2.00	0.78
1:B:509:ILE:HD11	1:B:599:GLN:CG	2.15	0.77
1:A:467:HIS:CE1	1:B:508:LYS:HD2	2.20	0.77
1:A:638:ALA:HB2	11:A:1216:HOH:O	1.84	0.76
1:B:508:LYS:HG3	11:B:2401:HOH:O	1.86	0.74
1:B:508:LYS:HG2	1:B:579:GLU:CD	2.08	0.74
1:A:256:TYR:HE1	1:A:267:MET:HE3	1.52	0.73
1:B:283:VAL:HG13	1:B:303:LEU:HD13	1.71	0.73
1:B:543:LYS:HE3	11:B:2679:HOH:O	1.88	0.73
1:B:284:GLU:O	1:B:288:LYS:HD3	1.88	0.73
1:A:352:ILE:HA	1:A:355:LEU:HD22	1.71	0.72
1:B:407:GLU:HB3	11:B:2338:HOH:O	1.89	0.72
1:B:508:LYS:HG2	1:B:579:GLU:OE1	1.90	0.71
1:B:416:GLU:O	1:B:418:VAL:HG12	1.92	0.70
1:B:132:HIS:O	1:B:145:LEU:HD12	1.93	0.68
1:B:407:GLU:HG2	11:B:2474:HOH:O	1.95	0.67
1:A:267:MET:HE2	1:B:628:GLU:CG	2.23	0.67
1:B:576:ASP:OD2	11:B:2303:HOH:O	2.12	0.67
1:A:632:ARG:HD3	11:A:970:HOH:O	1.95	0.65
1:A:61:HIS:HB2	11:A:1225:HOH:O	1.96	0.65
1:A:283:VAL:HG13	1:A:303:LEU:HD13	1.79	0.65
2:A:701:B3P:H32	2:A:701:B3P:O6	1.98	0.64
1:B:507:LYS:O	11:B:2304:HOH:O	2.13	0.64
1:B:509:ILE:HD11	1:B:577:GLN:HG2	1.80	0.64
1:A:101:VAL:HG21	1:A:124:LEU:HD22	1.78	0.64
1:A:576:ASP:HB3	11:A:918:HOH:O	1.97	0.64
1:B:308:LYS:NZ	11:B:2310:HOH:O	2.31	0.63
1:B:509:ILE:CD1	1:B:577:GLN:HG2	2.30	0.62
1:A:469[A]:GLU:HG3	1:A:492:GLU:CA	2.24	0.60
1:B:632:ARG:HD3	11:B:2309:HOH:O	2.00	0.60
1:B:299:LYS:N	1:B:299:LYS:HD2	2.16	0.60
1:B:354:LYS:HE2	1:B:368:ASP:O	2.01	0.59
1:B:308:LYS:O	1:B:311:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:OD1	1:B:467:HIS:HB2	2.05	0.57
1:A:382:HIS:CE1	1:A:433:HIS:CE1	2.93	0.57
6:A:714:FMT:H	11:A:843:HOH:O	2.05	0.56
1:B:59:LYS:NZ	1:B:66:GLU:OE1	2.25	0.56
1:A:78:HIS:NE2	1:B:619:SER:O	2.39	0.56
1:A:467:HIS:HB2	1:B:580:ASP:OD1	2.05	0.56
1:B:308:LYS:HG3	11:B:2310:HOH:O	2.05	0.56
1:B:366:PRO:HG3	11:B:2551:HOH:O	2.06	0.56
1:A:508:LYS:HD3	1:A:579:GLU:OE2	2.05	0.56
1:A:379:GLY:N	1:A:380:PRO:HD3	2.21	0.55
1:B:411:ARG:HH11	1:B:411:ARG:HG3	1.71	0.55
1:A:256:TYR:CE1	1:A:267:MET:CE	2.89	0.53
1:B:203:ASN:HD22	6:B:2211:FMT:C	2.22	0.52
1:A:178:HIS:HB3	11:A:832:HOH:O	2.10	0.52
1:A:267:MET:HE1	1:B:628:GLU:HG3	1.90	0.51
1:B:379:GLY:N	1:B:380:PRO:HD3	2.25	0.51
1:B:411:ARG:HD2	1:B:416:GLU:OE1	2.10	0.51
1:B:411:ARG:HG3	1:B:411:ARG:NH1	2.26	0.51
1:A:347:CYS:O	1:A:373:GLU:HA	2.11	0.51
1:A:613:LEU:HD11	1:A:632:ARG:HB3	1.91	0.51
1:B:308:LYS:HB2	1:B:311:LYS:HE3	1.93	0.50
1:A:592:VAL:HG13	1:A:604:ILE:HD13	1.94	0.50
1:A:59:LYS:HG3	11:A:904:HOH:O	2.12	0.50
1:A:467:HIS:HE1	1:B:508:LYS:HD2	1.69	0.50
1:B:508:LYS:NZ	11:B:2317:HOH:O	2.44	0.50
1:B:509:ILE:CD1	1:B:599:GLN:HG3	2.37	0.50
1:B:351:ALA:HB3	1:B:354:LYS:HD3	1.92	0.49
1:B:132:HIS:C	1:B:145:LEU:HD12	2.31	0.49
1:B:347:CYS:O	1:B:373:GLU:HA	2.12	0.49
11:A:847:HOH:O	1:B:494:HIS:HE1	1.96	0.49
1:B:78:HIS:N	1:B:78:HIS:CD2	2.81	0.49
1:B:382:HIS:CE1	1:B:433:HIS:CE1	3.01	0.49
1:A:70:TYR:HB2	1:A:87:VAL:HB	1.95	0.48
1:A:255:CYS:HB2	11:A:835:HOH:O	2.12	0.48
1:A:466:LEU:HD11	1:B:620[B]:TRP:CZ2	2.48	0.48
1:B:58:GLN:OE1	1:B:447:LYS:HD2	2.13	0.48
1:A:619:SER:O	1:B:78:HIS:NE2	2.47	0.48
1:B:78:HIS:CD2	1:B:78:HIS:H	2.27	0.48
1:B:348:SER:HB3	1:B:370:ILE:HD12	1.95	0.48
1:B:382:HIS:NE2	1:B:433:HIS:CD2	2.82	0.48
1:B:579:GLU:HG3	11:B:2576:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:LEU:CD1	1:A:632:ARG:HB3	2.44	0.47
1:B:530:ASN:HA	6:B:2206:FMT:H	1.94	0.47
1:B:431:PRO:HA	1:B:453:SER:HA	1.97	0.47
1:A:256:TYR:HE1	1:A:267:MET:CE	2.24	0.47
1:B:143:LYS:HE2	1:B:144:TYR:CZ	2.50	0.47
1:A:632:ARG:HD2	1:B:262:PHE:HB2	1.96	0.47
1:B:128:CYS:HB2	1:B:147:ILE:CD1	2.45	0.46
1:A:551:MET:HG2	1:A:576:ASP:OD1	2.15	0.46
1:B:128:CYS:HB3	1:B:148:ASN:O	2.15	0.46
1:B:509:ILE:HD11	1:B:599:GLN:HG2	1.94	0.46
1:A:429:TYR:CD2	1:A:457:LYS:HD2	2.51	0.46
1:A:255:CYS:HB3	1:A:274:TRP:CD1	2.51	0.46
1:A:438:LEU:HB2	1:A:444:ALA:HA	1.97	0.46
1:A:208:PHE:CD1	1:B:634:MET:HG2	2.51	0.46
1:A:210:LEU:HG	11:B:2596:HOH:O	2.15	0.46
1:A:494:HIS:HB3	11:A:839:HOH:O	2.16	0.45
1:B:238:ASN:O	1:B:255:CYS:HB2	2.16	0.45
6:A:716:FMT:H	11:B:2640:HOH:O	2.16	0.45
1:A:433:HIS:ND1	1:A:495:ASP:OD2	2.50	0.45
1:B:643:GLN:OE1	1:B:643:GLN:N	2.48	0.45
1:B:428:HIS:HA	1:B:429:TYR:CG	2.52	0.45
1:B:129:HIS:CE1	1:B:494:HIS:CE1	3.05	0.45
1:B:77:GLY:HA2	1:B:128:CYS:O	2.16	0.45
1:B:621:PHE:CD2	1:B:626:HIS:CD2	3.05	0.44
2:B:2202:B3P:HN2	6:B:2207:FMT:C	2.30	0.44
1:A:97:PRO:HB2	1:A:107:TRP:CG	2.53	0.44
1:A:125:ASN:OD1	1:B:591:GLY:HA2	2.17	0.44
1:A:70:TYR:OH	1:A:447[B]:LYS:HE3	2.18	0.44
1:B:380:PRO:HA	1:B:394:THR:O	2.18	0.44
1:B:382:HIS:O	1:B:393:THR:HA	2.18	0.44
1:B:414:LYS:HE3	11:B:2415:HOH:O	2.16	0.44
6:A:716:FMT:C	11:B:2640:HOH:O	2.65	0.44
1:A:431:PRO:HA	1:A:453:SER:HA	2.00	0.44
1:B:525:LYS:NZ	11:B:2311:HOH:O	2.35	0.44
1:A:382:HIS:NE2	1:A:433:HIS:NE2	2.65	0.44
1:A:559:GLU:HA	1:A:632:ARG:O	2.18	0.43
1:A:78:HIS:HE1	1:A:492:GLU:OE2	2.01	0.43
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.99	0.43
1:A:187:HIS:ND1	6:A:706:FMT:H	2.33	0.43
1:A:396:PHE:CE1	1:A:430:GLN:HB3	2.54	0.43
1:B:314:LYS:NZ	11:B:2302:HOH:O	2.04	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:HE3	11:A:1174:HOH:O	2.18	0.43
1:B:613:LEU:HD21	1:B:632:ARG:HB3	2.01	0.43
1:A:99:PHE:CE2	1:A:149:ASP:HB2	2.54	0.43
1:A:258:SER:HB2	1:A:274:TRP:CH2	2.54	0.42
1:A:187:HIS:HE1	11:A:1241:HOH:O	2.01	0.42
1:A:97:PRO:HB2	1:A:107:TRP:CD1	2.53	0.42
1:B:128:CYS:HB2	1:B:147:ILE:HD11	2.00	0.42
1:A:129:HIS:CD2	1:A:494:HIS:CE1	3.08	0.42
1:A:197:PHE:HB3	1:B:615:TRP:CD1	2.55	0.42
1:A:256:TYR:CD1	1:A:267:MET:HE3	2.53	0.42
1:A:258:SER:HB2	1:A:274:TRP:CZ3	2.55	0.42
1:B:203:ASN:HB3	6:B:2211:FMT:H	2.02	0.42
1:B:579:GLU:HB3	11:B:2401:HOH:O	2.19	0.42
1:A:454:LYS:HE2	11:A:1041:HOH:O	2.19	0.42
1:B:138:GLY:O	1:B:441:THR:HB	2.20	0.42
1:B:277:VAL:O	1:B:316:THR:HA	2.20	0.41
1:A:380:PRO:HA	1:A:394:THR:O	2.21	0.41
1:B:531:LEU:H	6:B:2206:FMT:C	2.32	0.41
1:A:428:HIS:HA	1:A:429:TYR:CG	2.56	0.41
1:B:433:HIS:HB2	1:B:494:HIS:O	2.21	0.41
1:A:552:ALA:HA	1:A:553:PRO:HA	1.87	0.41
1:A:597:SER:HB3	1:A:598:PRO:CD	2.50	0.40
1:A:591:GLY:HA2	1:B:125:ASN:OD1	2.21	0.40
1:B:469:GLU:O	1:B:488:PRO:HA	2.21	0.40

All (7) 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:1329:HOH:O	11:A:1356:HOH:O[2_546]	1.80	0.40
11:B:2663:HOH:O	11:B:2711:HOH:O[2_645]	1.87	0.33
11:B:2637:HOH:O	11:B:2683:HOH:O[2_645]	2.09	0.11
11:A:1327:HOH:O	11:A:1329:HOH:O[2_556]	2.11	0.09
10:A:711:TRS:O3	11:A:1354:HOH:O[2_546]	2.16	0.04
11:A:864:HOH:O	11:A:1337:HOH:O[2_646]	2.18	0.02
1:B:643:GLN:OE1	11:A:1279:HOH:O[1_655]	2.19	0.01

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	590/646 (91%)	567 (96%)	21 (4%)	2 (0%)	41 18
1	B	588/646 (91%)	564 (96%)	21 (4%)	3 (0%)	29 9
All	All	1178/1292 (91%)	1131 (96%)	42 (4%)	5 (0%)	34 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	LYS
1	A	342	LYS
1	B	416	GLU
1	A	176	ALA
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	507/545 (93%)	499 (98%)	8 (2%)	62 35
1	B	505/545 (93%)	496 (98%)	9 (2%)	59 29
All	All	1012/1090 (93%)	995 (98%)	17 (2%)	60 32

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

Mol	Chain	Res	Type
1	A	59	LYS

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Mol	Chain	Res	Type
1	A	78	HIS
1	A	255	CYS
1	A	355	LEU
1	A	576	ASP
1	A	607	VAL
1	A	620	TRP
1	A	621	PHE
1	B	78	HIS
1	B	85	LEU
1	B	255	CYS
1	B	308	LYS
1	B	311	LYS
1	B	434	LEU
1	B	483	LEU
1	B	551	MET
1	B	621	PHE

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

Mol	Chain	Res	Type
1	A	78	HIS
1	B	494	HIS

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 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
6	FMT	A	713	-	2,2,2	0.65	0	1,1,1	0.07	0
9	CUA	A	710	1	0,1,1	-	-	-		
6	FMT	A	718	-	2,2,2	0.66	0	1,1,1	0.38	0
6	FMT	A	717	-	2,2,2	0.73	0	1,1,1	0.42	0
2	B3P	B	2202	-	18,18,18	0.85	0	23,23,23	1.21	3 (13%)
6	FMT	A	707	-	2,2,2	0.69	0	1,1,1	0.12	0
6	FMT	A	716	-	2,2,2	0.71	0	1,1,1	0.08	0
6	FMT	B	2207	-	2,2,2	0.65	0	1,1,1	0.12	0
6	FMT	A	712	-	2,2,2	0.64	0	1,1,1	0.12	0
10	TRS	A	711	-	7,7,7	0.29	0	9,9,9	0.57	0
9	CUA	B	2210	1	0,1,1	-	-	-		
6	FMT	A	706	-	2,2,2	0.65	0	1,1,1	0.05	0
6	FMT	A	715	-	2,2,2	0.73	0	1,1,1	0.24	0
6	FMT	A	714	-	2,2,2	0.69	0	1,1,1	0.17	0
2	B3P	A	701	-	18,18,18	0.88	1 (5%)	23,23,23	1.07	2 (8%)
6	FMT	B	2211	-	2,2,2	0.55	0	1,1,1	0.11	0
6	FMT	A	705	-	2,2,2	0.69	0	1,1,1	0.19	0
6	FMT	B	2206	-	2,2,2	0.65	0	1,1,1	0.19	0
6	FMT	B	2201	-	2,2,2	0.67	0	1,1,1	0.37	0
8	CUZ	A	709	11,1	0,9,9	-	-	-		
8	CUZ	B	2209	11,1	0,9,9	-	-	-		

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	B	2202	-	-	1/28/28/28	-
10	TRS	A	711	-	-	1/9/9/9	-
2	B3P	A	701	-	-	0/28/28/28	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	B3P	C3-N1	2.40	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	B3P	C2-N2-C8	-2.38	112.69	116.17
2	A	701	B3P	O4-C5-C4	-2.28	107.05	111.68
2	B	2202	B3P	O3-C11-C8	-2.27	107.07	111.68
2	B	2202	B3P	C1-C3-N1	-2.23	105.58	110.98
2	B	2202	B3P	C9-C8-N2	2.13	115.36	109.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2202	B3P	C11-C8-C9-O1
10	A	711	TRS	N-C-C2-O2

There are no ring outliers.

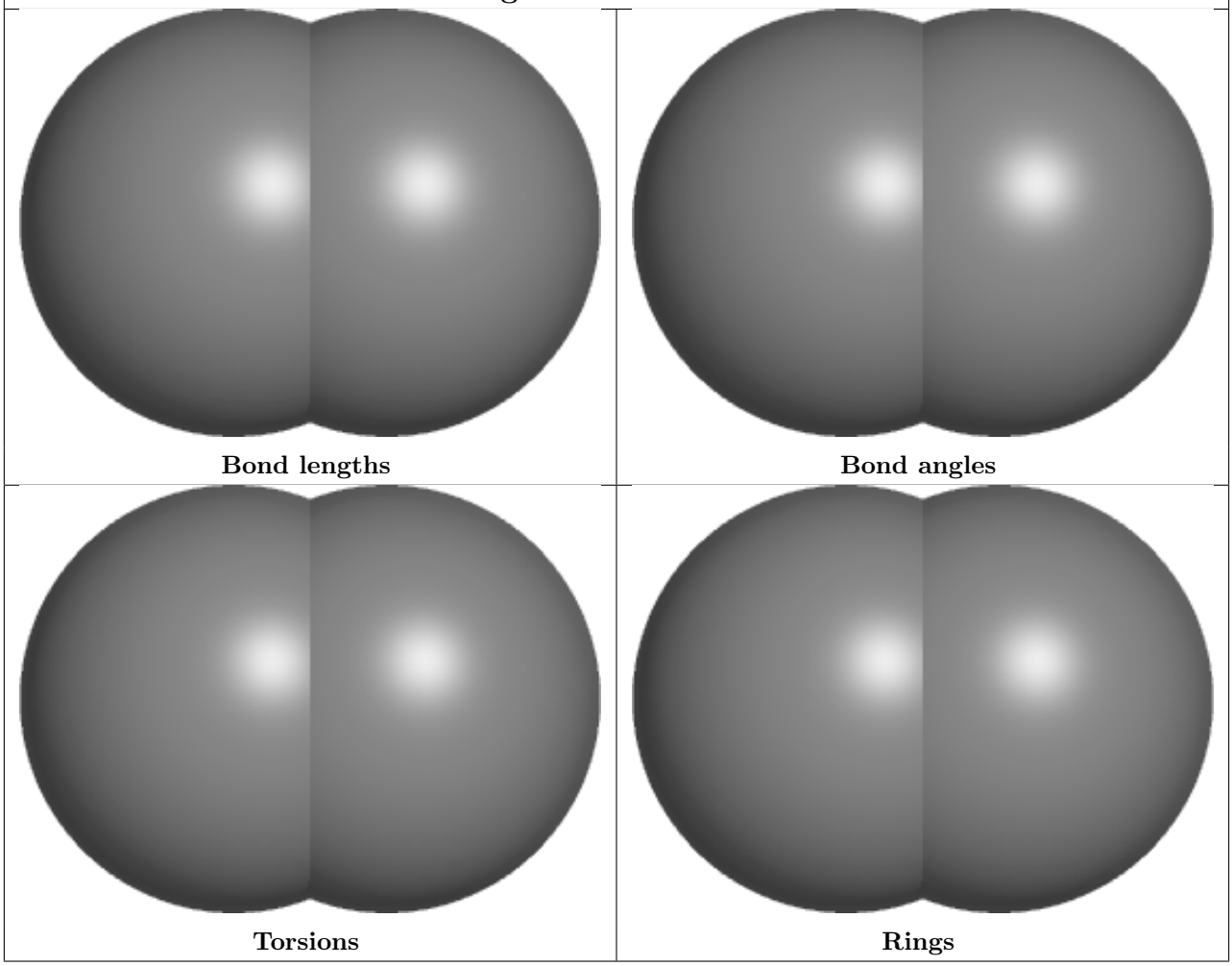
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2202	B3P	1	0
6	A	716	FMT	2	0
6	B	2207	FMT	1	0
10	A	711	TRS	0	1
6	A	706	FMT	1	0
6	A	714	FMT	1	0
2	A	701	B3P	1	0
6	B	2211	FMT	2	0
6	B	2206	FMT	2	0

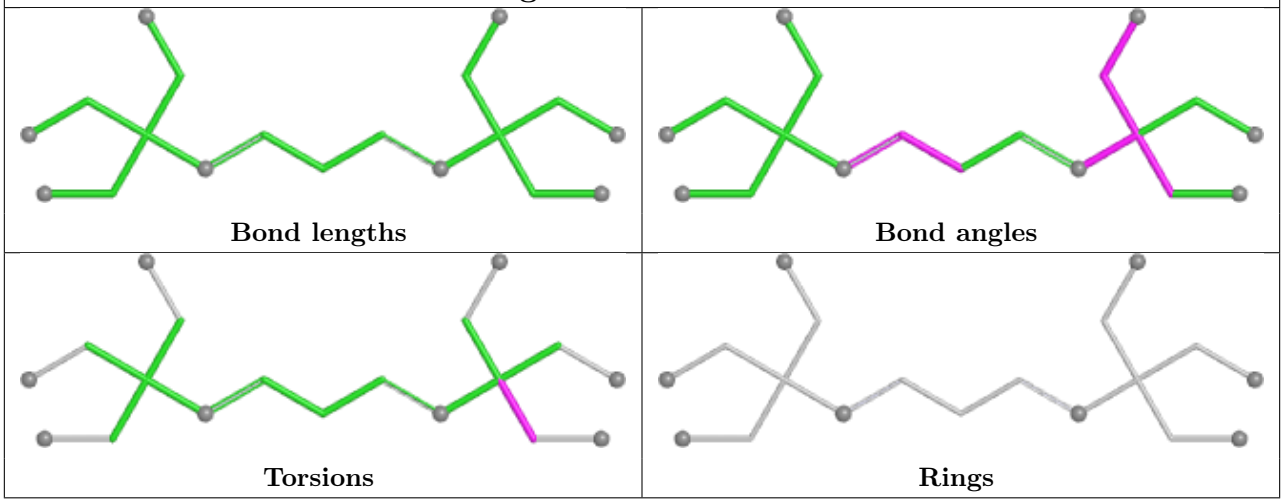
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

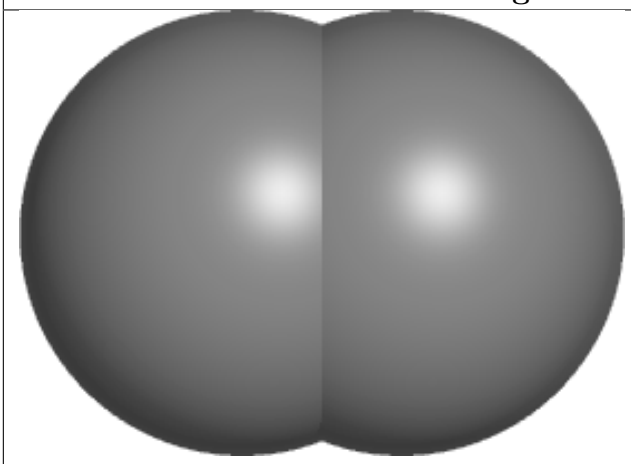
Ligand CUA A 710



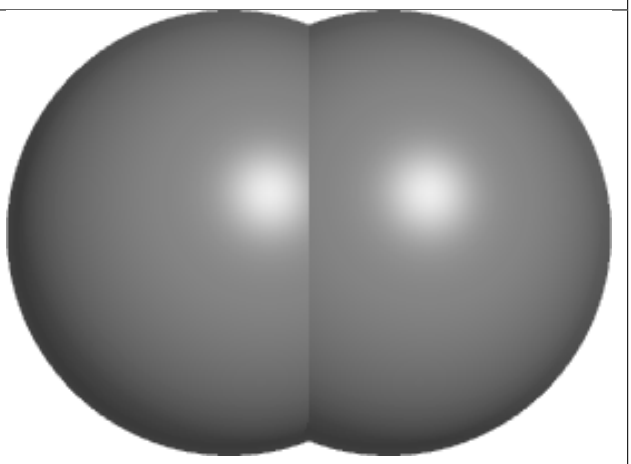
Ligand B3P B 2202



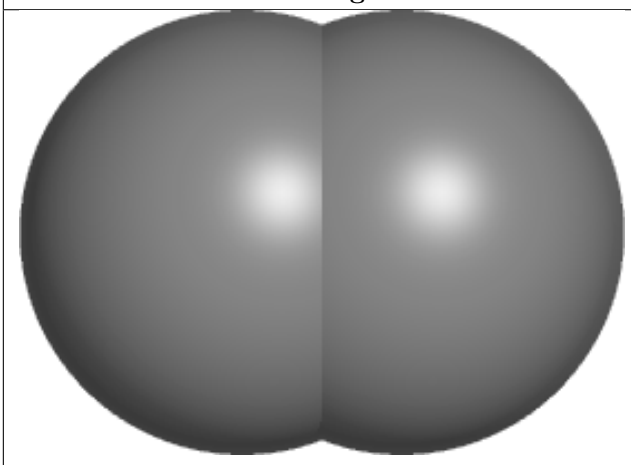
Ligand CUA B 2210



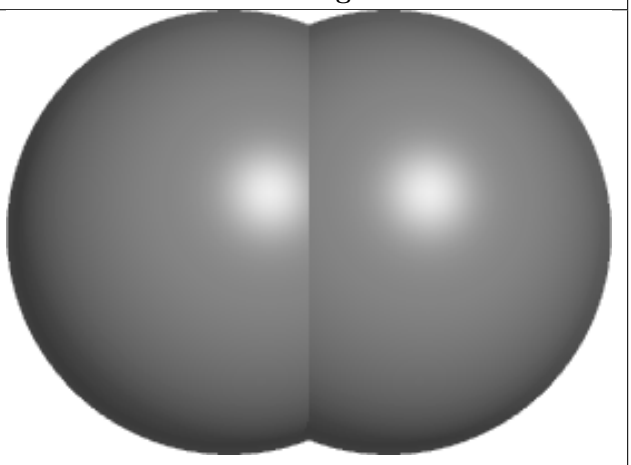
Bond lengths



Bond angles

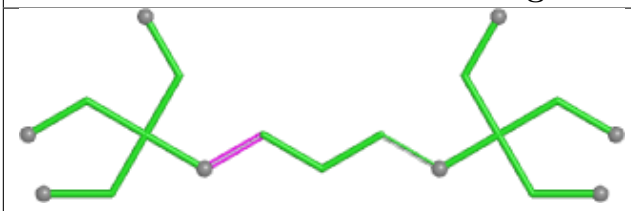


Torsions

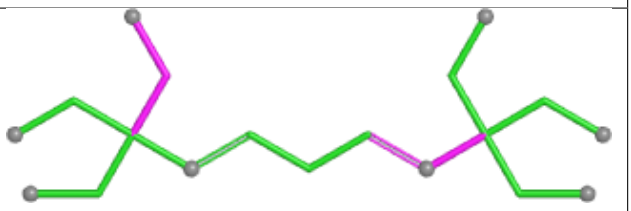


Rings

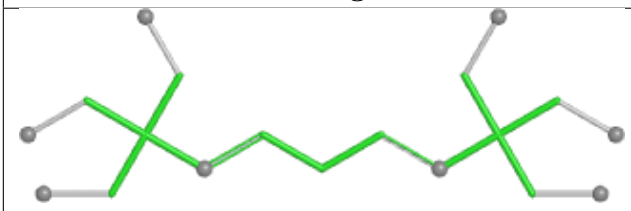
Ligand B3P A 701



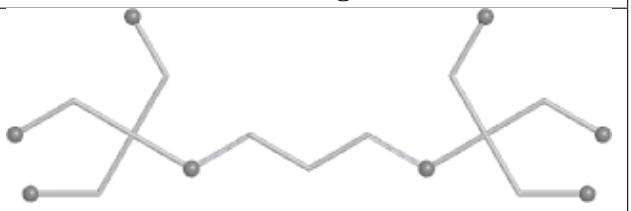
Bond lengths



Bond angles

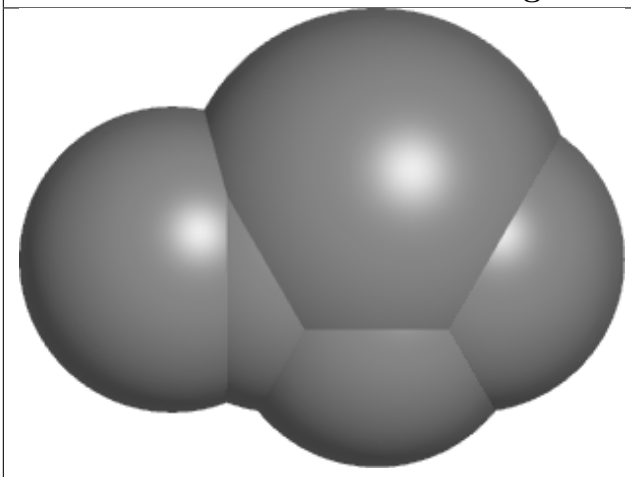


Torsions

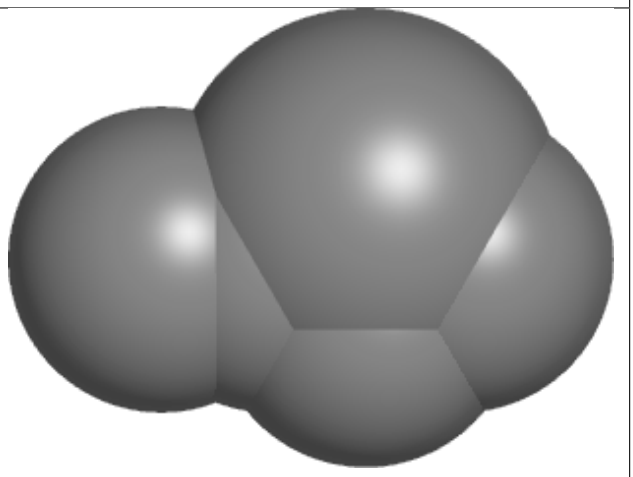


Rings

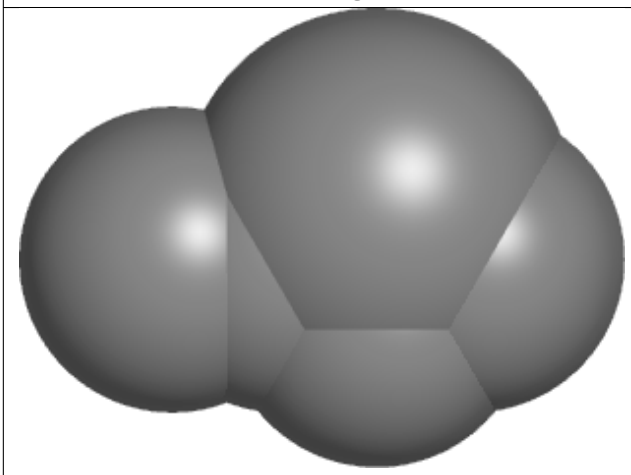
Ligand CUZ A 709



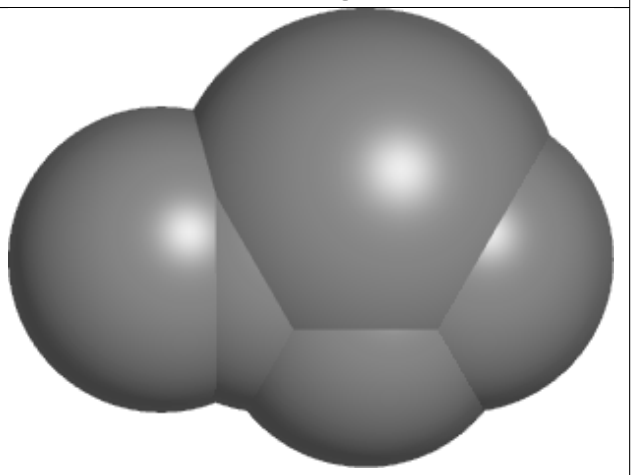
Bond lengths



Bond angles

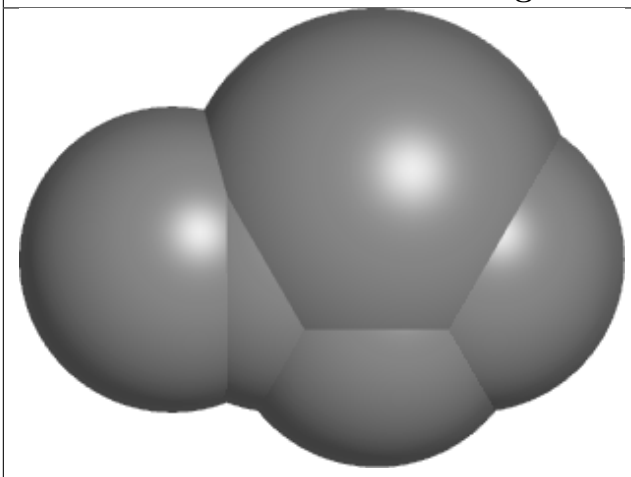


Torsions

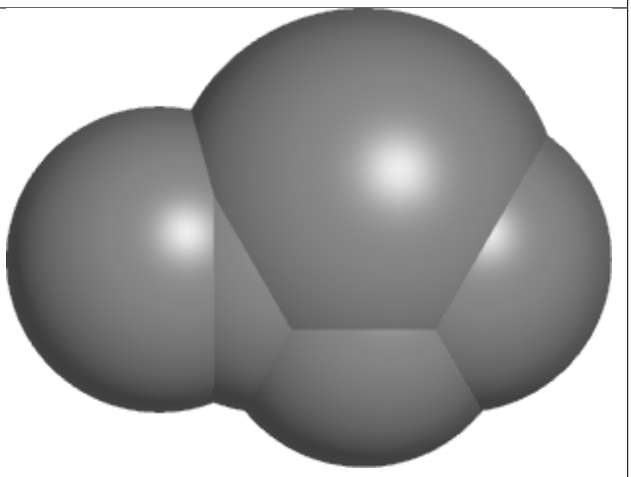


Rings

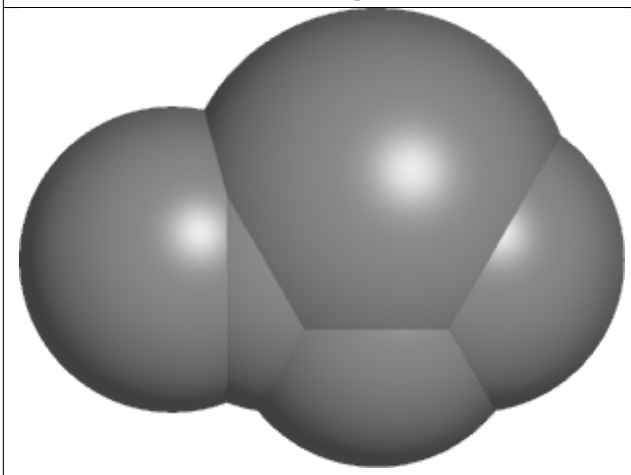
Ligand CUZ B 2209



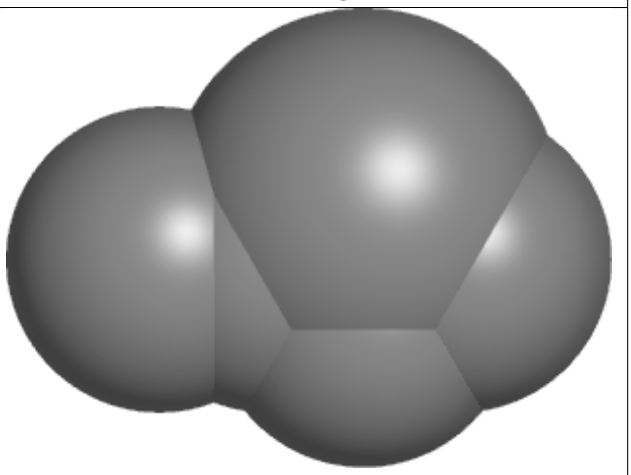
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	586/646 (90%)	-0.57	5 (0%)	84	87	12, 23, 46, 75	0
1	B	588/646 (91%)	-0.49	6 (1%)	82	85	14, 28, 51, 83	0
All	All	1174/1292 (90%)	-0.53	11 (0%)	84	87	12, 26, 48, 83	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	644	PHE	3.4
1	B	643	GLN	3.2
1	B	60	ILE	3.2
1	A	269	ARG	2.9
1	A	262	PHE	2.6
1	B	363	LEU	2.5
1	B	309	ASP	2.5
1	A	53	VAL	2.3
1	A	494	HIS	2.2
1	B	418	VAL	2.1
1	A	264	LEU	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

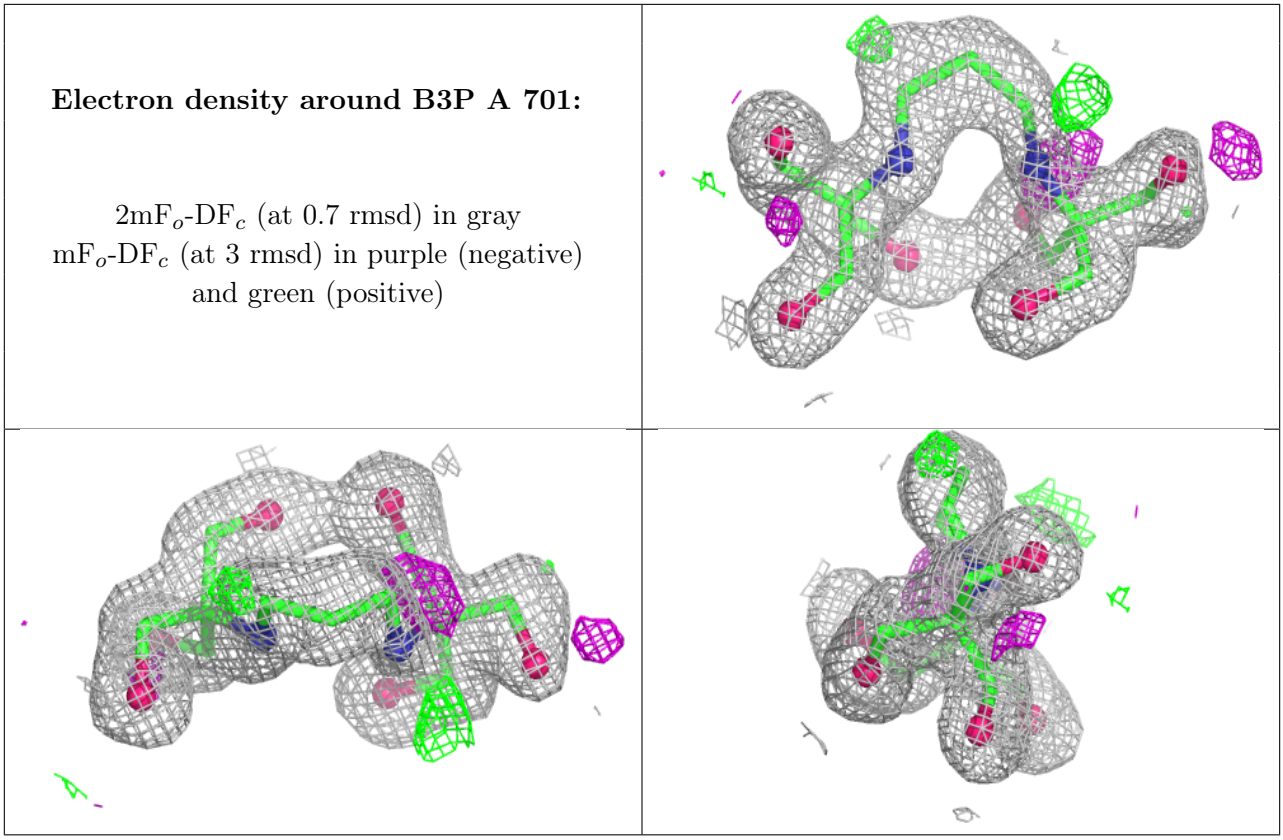
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	FMT	A	712	3/3	0.59	0.25	55,55,63,64	0
6	FMT	B	2201	3/3	0.62	0.26	64,65,78,79	0
6	FMT	A	707	3/3	0.64	0.15	64,64,67,68	0
6	FMT	A	714	3/3	0.66	0.24	59,59,63,64	0
6	FMT	A	705	3/3	0.68	0.14	58,58,61,63	0
6	FMT	A	715	3/3	0.75	0.13	57,57,59,59	0
6	FMT	A	718	3/3	0.83	0.22	47,49,59,65	0
6	FMT	A	717	3/3	0.84	0.14	64,67,80,81	0
2	B3P	A	701	19/19	0.87	0.12	25,33,42,43	0
6	FMT	A	716	3/3	0.88	0.25	54,54,55,56	0
2	B3P	B	2202	19/19	0.91	0.09	25,29,35,35	0
6	FMT	A	706	3/3	0.91	0.14	29,29,51,57	0
6	FMT	B	2206	3/3	0.92	0.19	45,45,46,54	0
10	TRS	A	711	8/8	0.92	0.14	35,39,45,48	0
5	K	A	704	1/1	0.93	0.08	23,23,23,23	1
6	FMT	A	713	3/3	0.94	0.14	24,24,44,53	0
8	CUZ	B	2209	5/5	0.95	0.07	24,25,31,34	5
9	CUA	A	710	2/2	0.95	0.08	22,22,22,35	2
6	FMT	B	2211	3/3	0.95	0.14	22,22,32,43	0
9	CUA	B	2210	2/2	0.96	0.07	25,25,25,52	2
8	CUZ	A	709	5/5	0.96	0.10	10,24,37,50	5
6	FMT	B	2207	3/3	0.97	0.12	21,21,42,43	0
3	NA	B	2203	1/1	0.99	0.05	24,24,24,24	1
5	K	B	2205	1/1	0.99	0.09	15,15,15,15	1
4	CA	A	703	1/1	0.99	0.07	16,16,16,16	1
4	CA	B	2204	1/1	0.99	0.07	25,25,25,25	1
7	CL	A	708	1/1	0.99	0.08	19,19,19,19	1
7	CL	B	2208	1/1	1.00	0.07	27,27,27,27	1
3	NA	A	702	1/1	1.00	0.06	16,16,16,16	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.

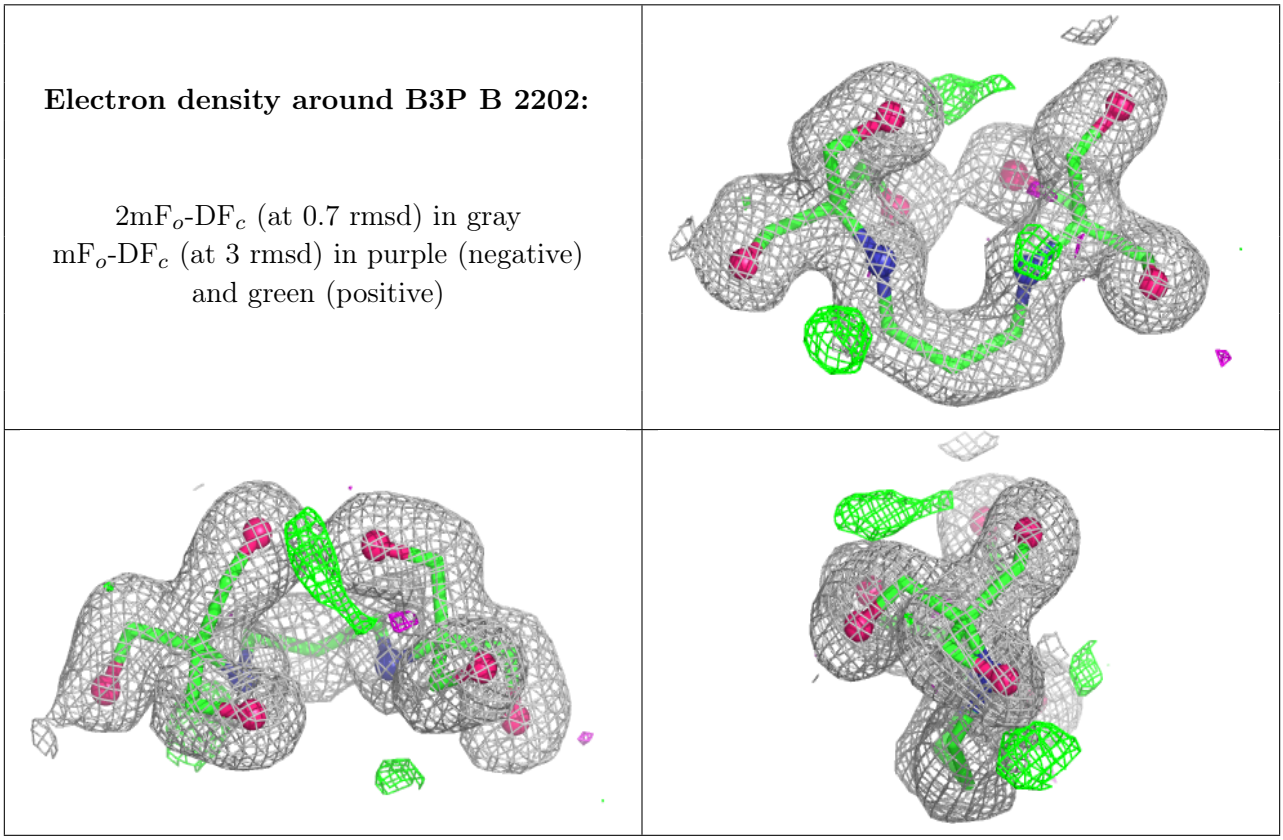
Electron density around B3P A 701:

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



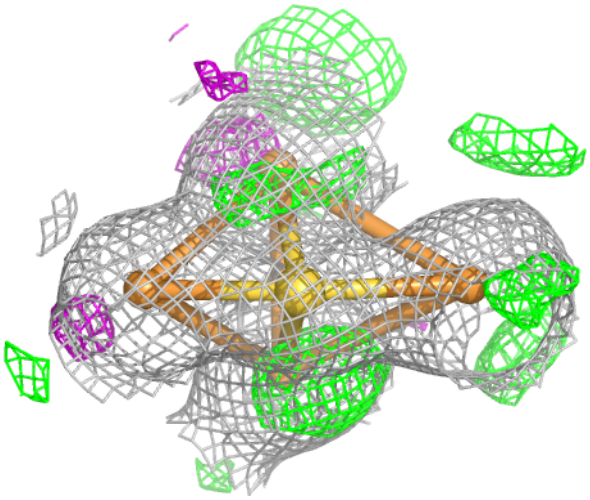
Electron density around B3P B 2202:

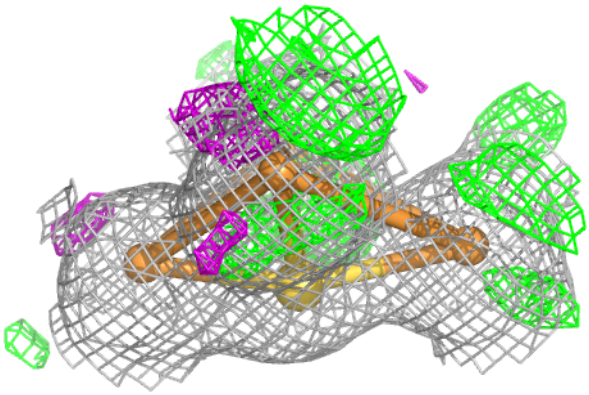
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

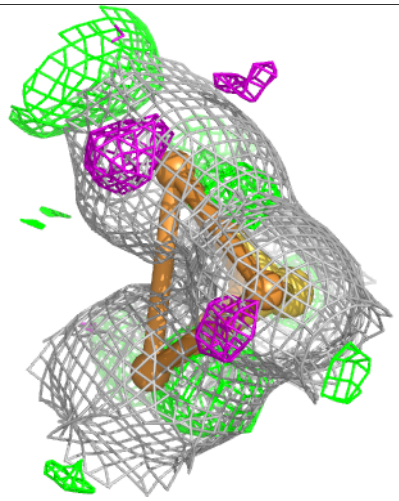


Electron density around CUZ B 2209:

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

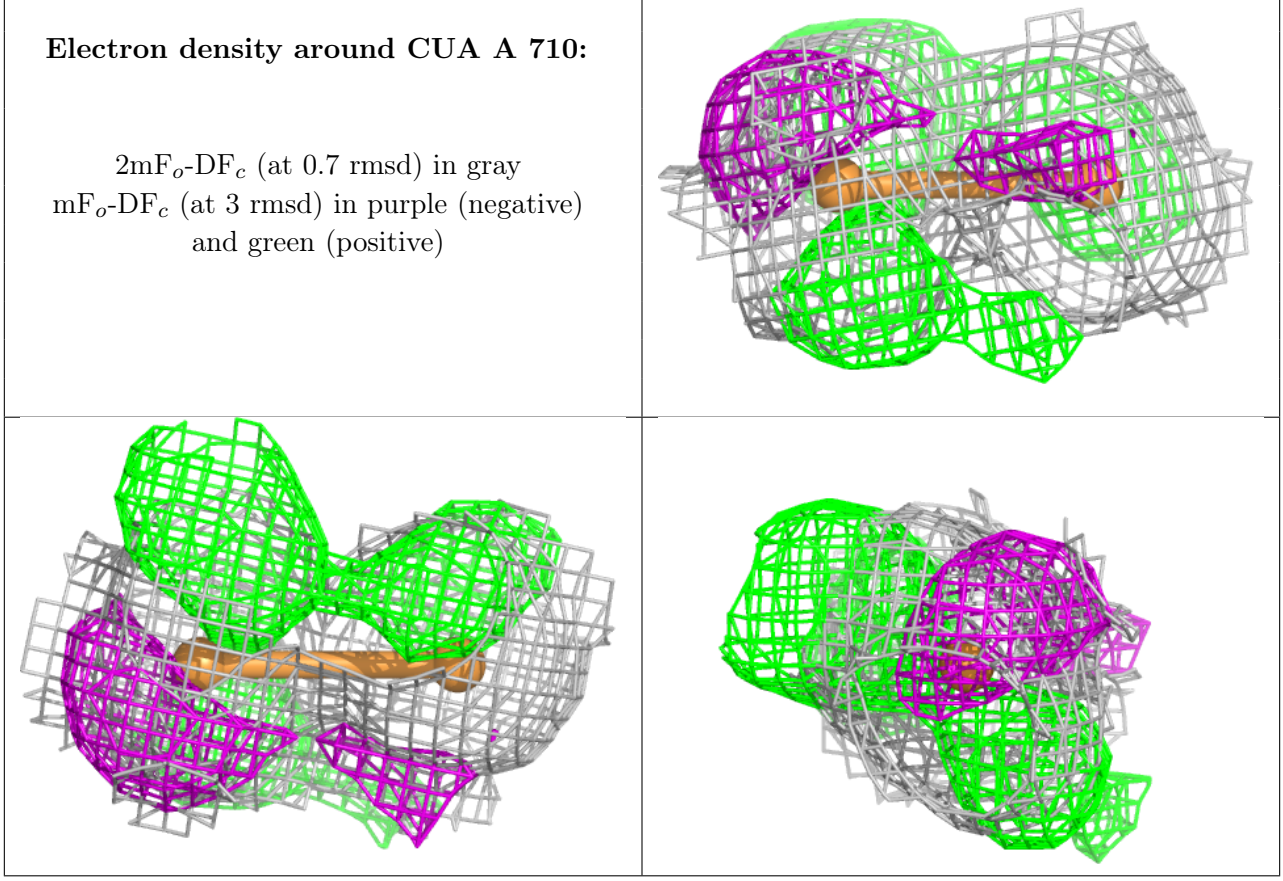






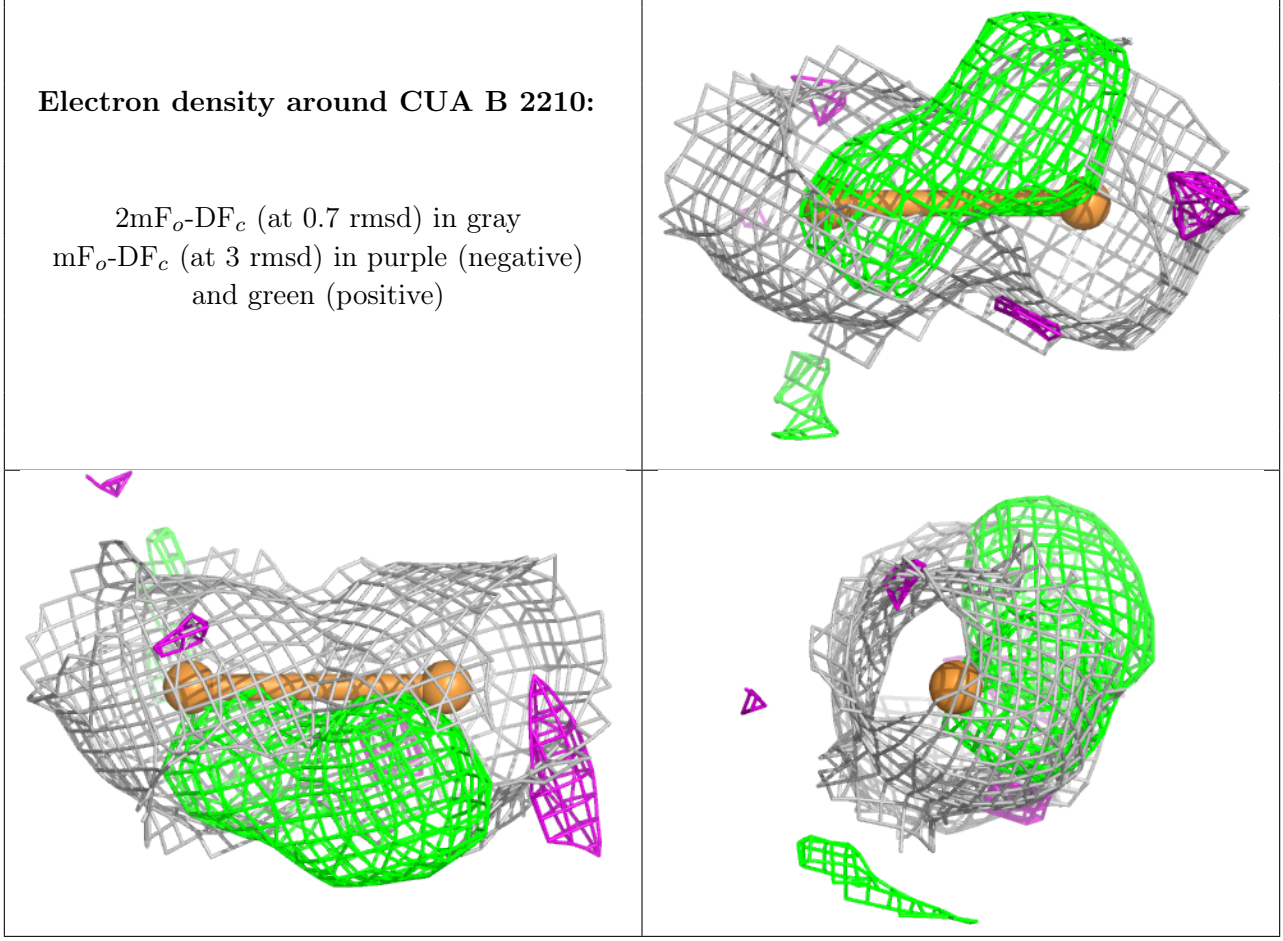
Electron density around CUA A 710:

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



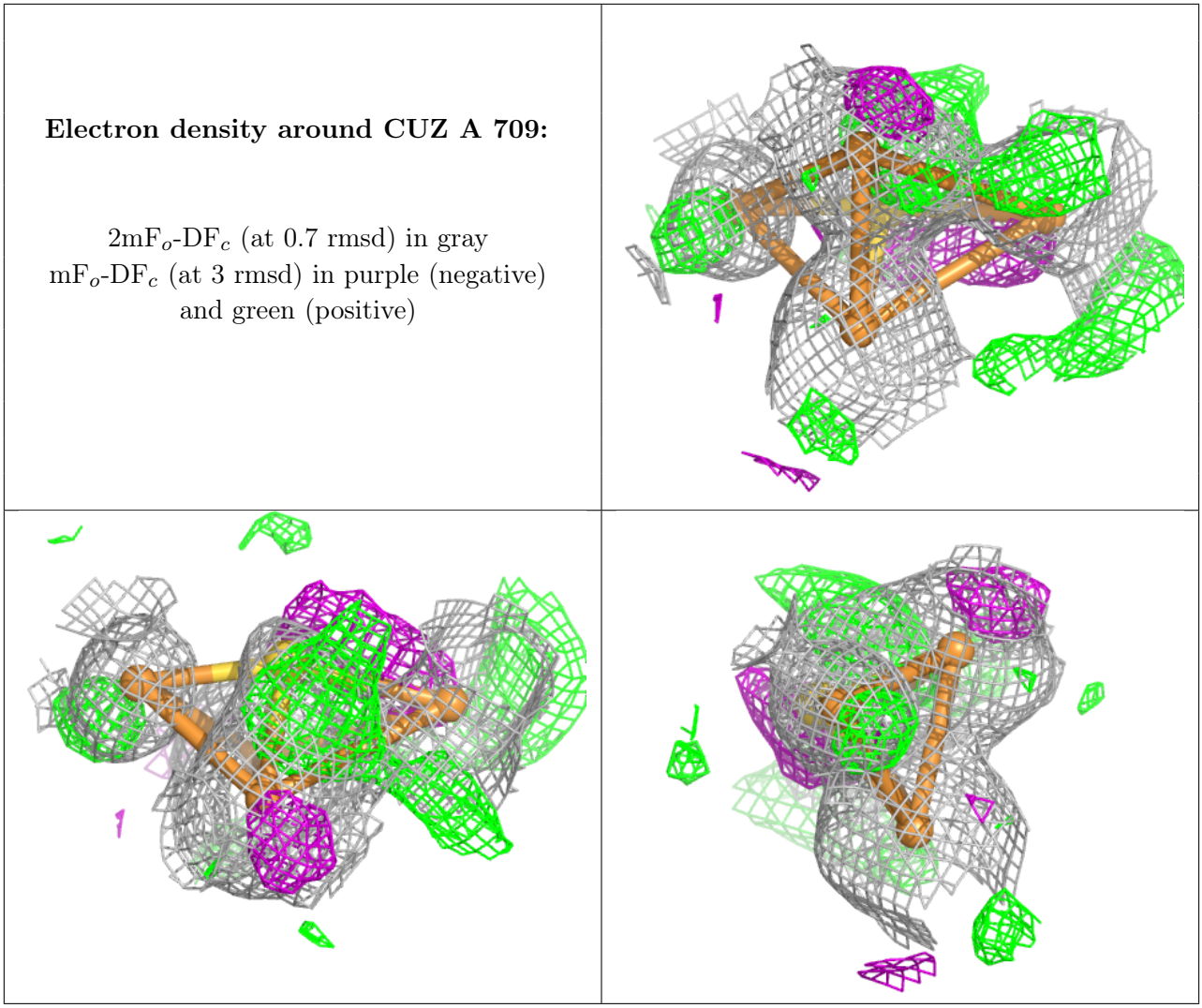
Electron density around CUA B 2210:

$2mF_o$-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 A 709:

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



6.5 Other polymers

There are no such residues in this entry.