



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2023 – 12:38 pm GMT

PDB ID : 7QW3  
Title : R396W mutant of the vanadium-dependent bromoperoxidase from *Corallina pilulifera* in complex with Br ion.  
Authors : Isupov, M.N.; Mitchell, D.; Littelchild, J.A.; Garcia-Rodriguez, E.  
Deposited on : 2022-01-24  
Resolution : 1.78 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
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) : 2.31.3

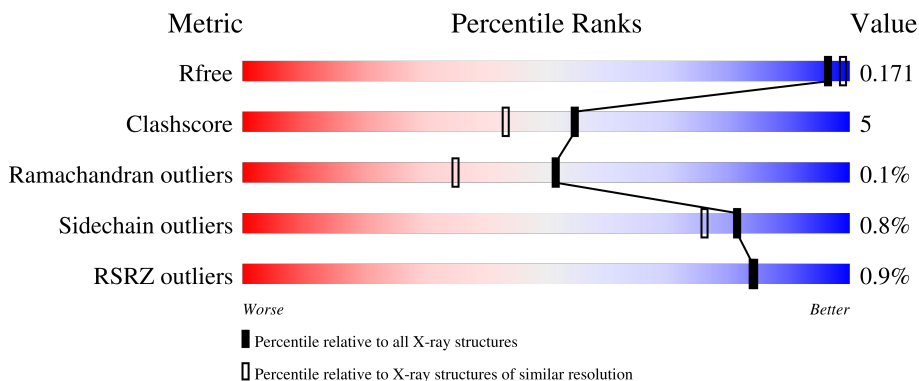
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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	AAA	598	
1	BBB	598	
1	CCC	598	
1	DDD	598	

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
4	BR	AAA	604	-	-	X	-
4	BR	AAA	617	-	-	X	-
4	BR	CCC	604	-	-	X	-
5	GOL	AAA	614	-	-	X	-
5	GOL	BBB	610	-	-	X	-
5	GOL	BBB	613	-	-	X	-
5	GOL	CCC	609	-	-	X	-
5	GOL	CCC	610	-	-	X	-
5	GOL	CCC	618	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23528 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.

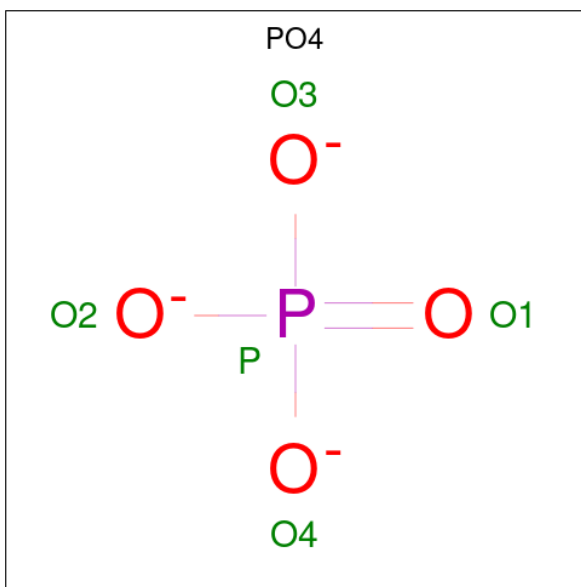
- Molecule 1 is a protein called Vanadium-dependent bromoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	S			
1	AAA	597	4876	2	3136	781	950	7	0	51	0
1	BBB	597	4831	2	3105	777	940	7	0	45	0
1	CCC	597	4903	2	3153	781	960	7	0	57	0
1	DDD	597	4917	2	3164	784	960	7	0	60	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	397	TRP	ARG	conflict	UNP O81959
AAA	423	ALA	PRO	conflict	UNP O81959
BBB	397	TRP	ARG	conflict	UNP O81959
BBB	423	ALA	PRO	conflict	UNP O81959
CCC	397	TRP	ARG	conflict	UNP O81959
CCC	423	ALA	PRO	conflict	UNP O81959
DDD	397	TRP	ARG	conflict	UNP O81959
DDD	423	ALA	PRO	conflict	UNP O81959

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O P 5 4 1	0	0
2	AAA	1	Total O P 5 4 1	0	0
2	AAA	1	Total O P 5 4 1	0	0
2	BBB	1	Total O P 5 4 1	0	0
2	BBB	1	Total O P 5 4 1	0	0
2	CCC	1	Total O P 5 4 1	0	0
2	CCC	1	Total O P 5 4 1	0	0
2	DDD	1	Total O P 5 4 1	0	0
2	DDD	1	Total O P 5 4 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0
3	BBB	1	Total Ca 1 1	0	0

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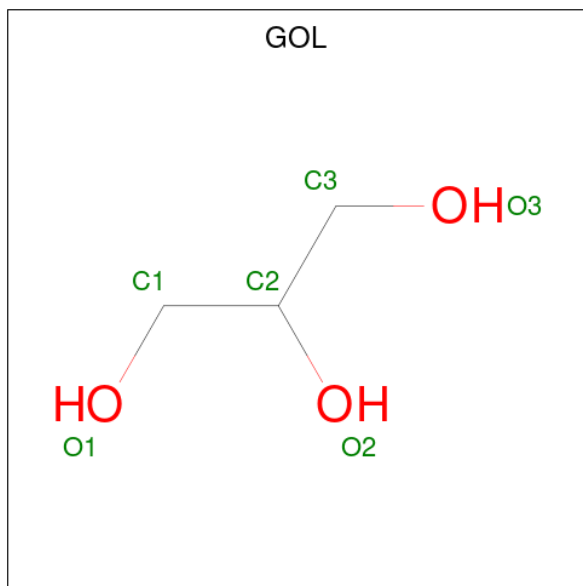
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total Ca 1 1	0	0
3	DDD	1	Total Ca 1 1	0	0

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	5	Total Br 5 5	0	0
4	BBB	4	Total Br 4 4	0	0
4	CCC	4	Total Br 4 4	0	0
4	DDD	3	Total Br 3 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 6 3 3	0	0
5	AAA	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	AAA	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	BBB	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0
5	CCC	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	CCC	1	Total	C	O	0	0
			6	3	3		
5	CCC	1	Total	C	O	0	0
			6	3	3		
5	CCC	1	Total	C	O	0	0
			6	3	3		
5	CCC	1	Total	C	O	0	0
			6	3	3		
5	CCC	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		
5	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	2	Total	Na	0	0
			2	2		
6	BBB	1	Total	Na	0	0
			1	1		
6	CCC	1	Total	Na	0	0
			1	1		
6	DDD	1	Total	Na	0	0
			1	1		



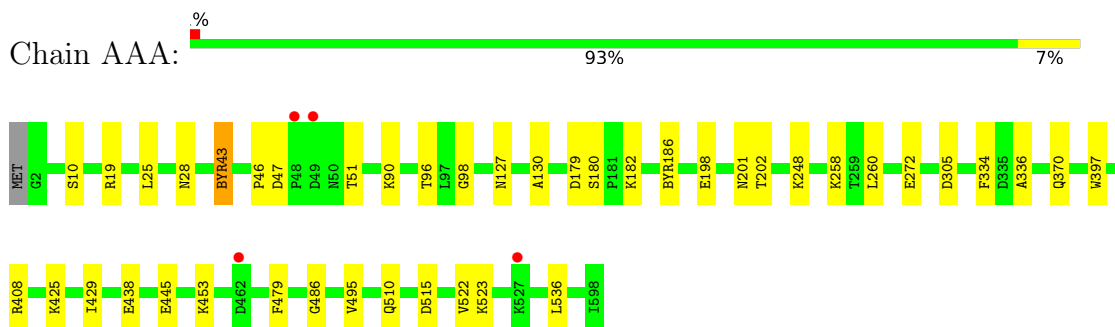
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	AAA	944	Total 944	O 944	0	0
7	BBB	910	Total 910	O 910	0	0
7	CCC	931	Total 931	O 931	0	0
7	DDD	912	Total 912	O 912	0	0

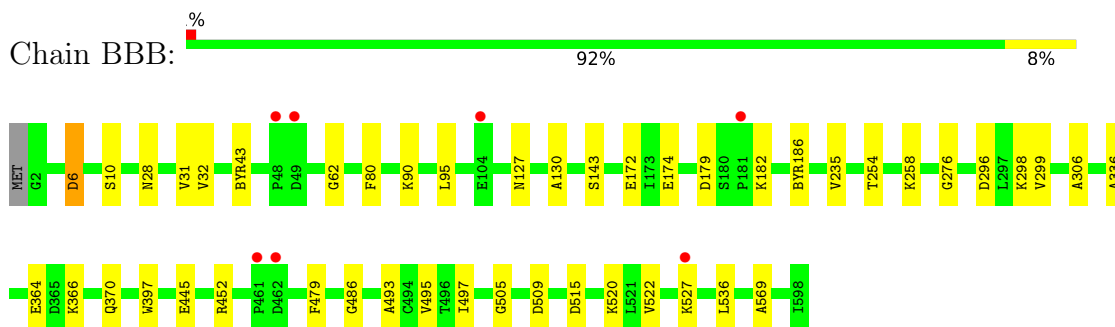
### 3 Residue-property plots [i](#)

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.

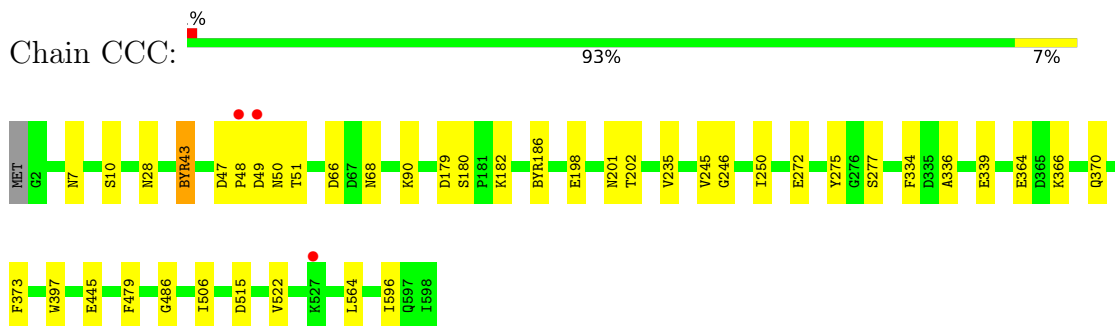
- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase

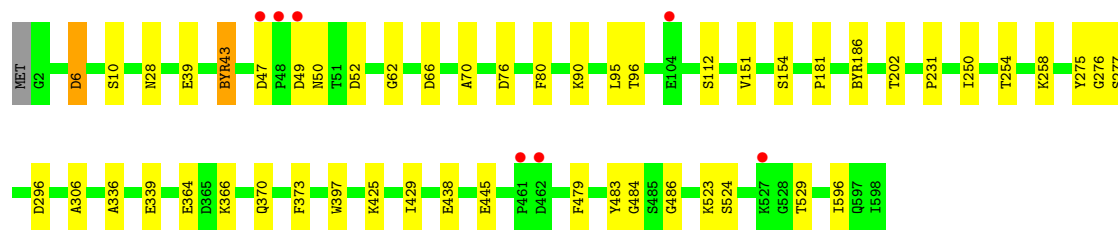


- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.48Å 182.48Å 177.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.78 29.98 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-1.78) 96.9 (29.98-1.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 1.78Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.143 , 0.171 0.143 , 0.171	Depositor DCC
$R_{free}$ test set	15613 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: CA, BR, PO4, NA, BYR, GOL

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	AAA	0.51	0/5092	0.73	1/6915 (0.0%)
1	BBB	0.50	0/5033	0.71	0/6834
1	CCC	0.53	0/5131	0.72	0/6970
1	DDD	0.50	0/5149	0.71	0/6997
All	All	0.51	0/20405	0.72	1/27716 (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	AAA	408	ARG	NE-CZ-NH1	5.41	123.00	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	AAA	4876	0	4900	47	0
1	BBB	4831	0	4842	50	0
1	CCC	4903	0	4924	53	0
1	DDD	4917	0	4949	51	0
2	AAA	15	0	0	1	0
2	BBB	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	10	0	0	1	0
2	DDD	10	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	5	0	0	6	0
4	BBB	4	0	0	3	0
4	CCC	4	0	0	5	0
4	DDD	3	0	0	3	0
5	AAA	60	0	79	7	0
5	BBB	48	0	62	12	0
5	CCC	66	0	87	19	0
5	DDD	60	0	79	7	0
6	AAA	2	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	944	0	0	17	0
7	BBB	910	0	0	14	1
7	CCC	931	0	0	19	0
7	DDD	912	0	0	21	0
All	All	23528	0	19922	205	1

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 (205) 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:BBB:364[A]:GLU:OE2	1:BBB:366[A]:LYS:HE2	1.26	1.24
1:CCC:47[A]:ASP:OD2	7:CCC:701:HOH:O	1.61	1.17
1:CCC:51[A]:THR:HG21	7:CCC:791:HOH:O	0.97	1.15
1:CCC:51[A]:THR:O	7:CCC:702:HOH:O	1.65	1.13
1:DDD:47[B]:ASP:OD1	1:DDD:49[B]:ASP:OD1	1.69	1.11
1:BBB:179[A]:ASP:OD1	7:BBB:701:HOH:O	1.66	1.10
1:AAA:510[B]:GLN:NE2	1:AAA:523[B]:LYS:HG2	1.67	1.08
1:BBB:493:ALA:O	1:BBB:497[B]:ILE:HD13	1.55	1.07
1:DDD:47[B]:ASP:CG	1:DDD:49[B]:ASP:OD1	1.95	1.04
1:BBB:509[B]:ASP:OD1	7:BBB:702:HOH:O	1.74	1.03
1:BBB:445[A]:GLU:HG2	7:BBB:714:HOH:O	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:179[A]:ASP:OD1	7:CCC:703:HOH:O	1.81	0.98
1:CCC:47[B]:ASP:OD1	1:CCC:49[B]:ASP:OD1	1.80	0.98
1:AAA:445[A]:GLU:HG2	7:AAA:703:HOH:O	1.64	0.98
1:BBB:31[B]:VAL:HG23	1:BBB:143:SER:HA	1.46	0.96
1:CCC:50[B]:ASN:O	7:CCC:704:HOH:O	1.83	0.94
1:BBB:364[A]:GLU:OE2	1:BBB:366[A]:LYS:CE	2.16	0.93
1:AAA:510[B]:GLN:NE2	1:AAA:523[B]:LYS:CG	2.30	0.93
1:AAA:179[A]:ASP:OD1	7:AAA:701:HOH:O	1.87	0.91
1:CCC:66:ASP:OD2	5:CCC:610:GOL:H12	1.73	0.88
1:BBB:493:ALA:O	1:BBB:497[B]:ILE:CD1	2.21	0.87
1:DDD:90[B]:LYS:HG3	7:DDD:725:HOH:O	1.75	0.86
1:DDD:254[B]:THR:CG2	7:DDD:843:HOH:O	2.24	0.84
1:CCC:47[B]:ASP:OD2	7:CCC:705:HOH:O	1.95	0.84
1:BBB:254[B]:THR:HG22	7:BBB:727:HOH:O	1.79	0.83
1:BBB:258[B]:LYS:NZ	7:BBB:704:HOH:O	2.12	0.81
1:DDD:90[B]:LYS:HE2	7:DDD:1380:HOH:O	1.81	0.80
1:CCC:43:BYR:BR	7:CCC:1618:HOH:O	2.56	0.78
1:CCC:47[B]:ASP:CG	1:CCC:49[B]:ASP:OD1	2.21	0.78
1:CCC:336:ALA:HB2	5:CCC:613:GOL:H31	1.64	0.78
1:AAA:272[B]:GLU:OE2	5:AAA:610:GOL:O2	2.03	0.77
1:AAA:445[B]:GLU:HG3	7:AAA:1372:HOH:O	1.83	0.76
1:DDD:202[B]:THR:HG21	7:DDD:995:HOH:O	1.86	0.76
1:CCC:90[B]:LYS:HG3	7:CCC:921:HOH:O	1.87	0.75
1:CCC:68:ASN:HD22	5:CCC:610:GOL:H11	1.50	0.75
1:BBB:31[B]:VAL:HG21	7:BBB:1026:HOH:O	1.87	0.74
1:BBB:296[B]:ASP:OD2	5:BBB:610:GOL:O2	2.04	0.74
1:CCC:336:ALA:HA	5:CCC:613:GOL:H11	1.69	0.74
1:DDD:366[B]:LYS:HE3	7:DDD:1289:HOH:O	1.88	0.73
1:DDD:429[A]:ILE:HD12	7:DDD:858:HOH:O	1.88	0.72
1:DDD:6[A]:ASP:OD2	7:DDD:701:HOH:O	2.08	0.72
1:CCC:272[B]:GLU:OE2	5:CCC:609:GOL:O2	2.06	0.72
1:DDD:43:BYR:BR	7:DDD:1488:HOH:O	2.63	0.71
1:CCC:445[A]:GLU:HG2	7:CCC:784:HOH:O	1.90	0.71
1:CCC:202[B]:THR:HG21	7:CCC:1248:HOH:O	1.90	0.71
1:CCC:272[B]:GLU:OE1	5:CCC:609:GOL:O2	2.05	0.71
1:BBB:336:ALA:HB2	5:BBB:612:GOL:H12	1.70	0.71
1:BBB:90[A]:LYS:HG3	7:BBB:886:HOH:O	1.91	0.71
1:CCC:272[B]:GLU:CD	5:CCC:609:GOL:HO2	1.93	0.70
1:BBB:364[A]:GLU:OE1	7:BBB:703:HOH:O	2.09	0.70
5:CCC:618:GOL:H11	7:CCC:1331:HOH:O	1.93	0.69
1:CCC:47[A]:ASP:CG	7:CCC:701:HOH:O	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:68:ASN:HB2	5:CCC:610:GOL:H11	1.75	0.68
1:AAA:202[B]:THR:HG21	7:AAA:1256:HOH:O	1.92	0.68
1:DDD:80:PHE:HA	1:DDD:95[B]:LEU:HD21	1.75	0.68
1:AAA:336:ALA:HA	5:AAA:614:GOL:H11	1.77	0.67
1:DDD:254[B]:THR:HG22	7:DDD:843:HOH:O	1.87	0.67
1:CCC:445[A]:GLU:OE1	7:CCC:706:HOH:O	2.12	0.67
1:BBB:31[B]:VAL:CG2	7:BBB:1026:HOH:O	2.42	0.67
1:DDD:445[A]:GLU:HG2	7:DDD:739:HOH:O	1.93	0.67
1:CCC:364[A]:GLU:OE2	1:CCC:366[A]:LYS:HE2	1.95	0.67
1:AAA:51:THR:HG21	7:AAA:742:HOH:O	1.95	0.66
5:CCC:618:GOL:H31	1:DDD:336:ALA:HB2	1.77	0.66
1:BBB:336:ALA:HA	5:BBB:612:GOL:H32	1.76	0.66
1:BBB:31[B]:VAL:HG23	1:BBB:143:SER:CA	2.24	0.66
1:CCC:272[B]:GLU:CD	5:CCC:609:GOL:O2	2.33	0.66
1:AAA:336:ALA:HB2	5:AAA:614:GOL:H31	1.78	0.65
1:DDD:523[B]:LYS:HD3	1:DDD:524:SER:O	1.96	0.65
1:AAA:486:GLY:HA3	4:AAA:604:BR:BR	2.52	0.65
1:BBB:299:VAL:HG23	5:BBB:610:GOL:H31	1.79	0.64
4:CCC:617:BR:BR	1:DDD:486:GLY:HA3	2.53	0.64
4:BBB:615:BR:BR	1:CCC:28:ASN:ND2	2.82	0.64
1:BBB:174:GLU:HG3	5:BBB:613:GOL:H11	1.81	0.63
1:DDD:47[B]:ASP:OD2	1:DDD:49[B]:ASP:OD1	2.15	0.63
1:CCC:515[B]:ASP:OD2	1:CCC:522[B]:VAL:HG11	1.99	0.63
1:DDD:254[B]:THR:HG21	7:DDD:843:HOH:O	1.93	0.62
1:DDD:429[A]:ILE:CD1	7:DDD:858:HOH:O	2.47	0.62
1:AAA:429[A]:ILE:HD12	7:AAA:848:HOH:O	2.00	0.62
1:DDD:70:ALA:HB3	5:DDD:609:GOL:H32	1.83	0.61
1:CCC:68:ASN:HD22	5:CCC:610:GOL:C1	2.13	0.61
1:BBB:28:ASN:ND2	4:BBB:606:BR:BR	2.83	0.60
1:DDD:43:BYR:BR	7:DDD:1598:HOH:O	2.72	0.60
1:DDD:296[B]:ASP:OD2	5:DDD:611:GOL:O2	2.19	0.60
4:AAA:617:BR:BR	1:BBB:486:GLY:HA3	2.57	0.59
1:AAA:258[B]:LYS:NZ	1:AAA:260[B]:LEU:HD21	2.17	0.59
1:BBB:31[B]:VAL:CG2	1:BBB:143:SER:HA	2.27	0.58
1:CCC:515[B]:ASP:OD2	1:CCC:522[B]:VAL:CG1	2.52	0.58
1:AAA:510[B]:GLN:HE22	1:AAA:523[B]:LYS:HG2	1.67	0.58
1:BBB:445[B]:GLU:HG3	7:BBB:1395:HOH:O	2.03	0.57
1:AAA:336:ALA:HB2	5:AAA:614:GOL:C3	2.35	0.57
1:BBB:497[B]:ILE:HD12	1:BBB:497[B]:ILE:H	1.69	0.57
5:CCC:618:GOL:C3	1:DDD:336:ALA:HB2	2.35	0.57
1:BBB:497[B]:ILE:CD1	1:BBB:497[B]:ILE:H	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:96[B]:THR:HG23	7:AAA:810:HOH:O	2.04	0.56
1:AAA:258[B]:LYS:NZ	7:AAA:705:HOH:O	2.36	0.56
1:CCC:486:GLY:HA3	4:CCC:604:BR:BR	2.59	0.56
1:BBB:336:ALA:HB2	5:BBB:612:GOL:C1	2.36	0.56
1:AAA:510[B]:GLN:HE22	1:AAA:523[B]:LYS:CD	2.19	0.56
1:AAA:272[B]:GLU:OE1	5:AAA:610:GOL:H12	2.04	0.56
1:AAA:198:GLU:O	1:AAA:202[B]:THR:OG1	2.21	0.55
1:BBB:364[A]:GLU:CD	1:BBB:366[A]:LYS:HE2	2.21	0.55
1:AAA:510[B]:GLN:NE2	1:AAA:523[B]:LYS:CD	2.69	0.55
1:AAA:510[B]:GLN:HE22	1:AAA:523[B]:LYS:CE	2.19	0.55
1:DDD:76:ASP:CG	1:DDD:96[B]:THR:HG21	2.27	0.55
1:AAA:495[B]:VAL:HG13	1:AAA:536:LEU:HB3	1.88	0.55
1:AAA:90[A]:LYS:HG3	7:AAA:835:HOH:O	2.06	0.54
1:CCC:336:ALA:HB2	5:CCC:613:GOL:C3	2.37	0.54
1:AAA:90[A]:LYS:HE2	7:DDD:1380:HOH:O	2.08	0.54
1:AAA:429[A]:ILE:HD11	7:AAA:795:HOH:O	2.07	0.54
1:CCC:90[B]:LYS:NZ	7:CCC:707:HOH:O	2.20	0.53
1:CCC:201:ASN:OD1	1:CCC:202[B]:THR:HG23	2.09	0.53
1:CCC:250[B]:ILE:CD1	1:CCC:277:SER:HA	2.39	0.53
1:AAA:515:ASP:OD1	1:AAA:522[B]:VAL:HG11	2.09	0.53
1:AAA:28:ASN:ND2	4:AAA:606:BR:BR	2.89	0.53
1:AAA:425:LYS:HE2	7:AAA:1406:HOH:O	2.09	0.53
1:CCC:180[A]:SER:OG	1:CCC:182:LYS:HG2	2.09	0.52
1:CCC:43:BYR:BR	7:CCC:1529:HOH:O	2.74	0.52
1:BBB:497[B]:ILE:CD1	1:BBB:569:ALA:HB1	2.40	0.51
1:BBB:298:LYS:NZ	7:BBB:713:HOH:O	2.44	0.51
1:BBB:497[B]:ILE:HD11	1:BBB:569:ALA:HB1	1.91	0.51
1:DDD:231:PRO:HD3	5:DDD:616:GOL:H12	1.92	0.51
1:DDD:529[B]:THR:HG22	7:DDD:1328:HOH:O	2.10	0.51
1:AAA:510[B]:GLN:HE22	1:AAA:523[B]:LYS:CG	2.21	0.50
1:AAA:510[B]:GLN:HE21	1:AAA:523[B]:LYS:HG2	1.66	0.50
1:BBB:6[B]:ASP:OD1	1:CCC:7:ASN:O	2.30	0.50
1:DDD:6[A]:ASP:CG	7:DDD:701:HOH:O	2.49	0.50
5:CCC:616:GOL:H2	7:CCC:1058:HOH:O	2.13	0.49
4:AAA:617:BR:BR	2:BBB:601:PO4:O3	2.87	0.48
1:BBB:80:PHE:HA	1:BBB:95[A]:LEU:HD21	1.95	0.48
1:BBB:31[B]:VAL:HG22	1:BBB:32:VAL:N	2.29	0.47
1:CCC:522[B]:VAL:HG12	7:CCC:1130:HOH:O	2.14	0.47
1:DDD:151[B]:VAL:HG12	1:DDD:154:SER:HB3	1.95	0.47
1:DDD:596[A]:ILE:HD12	4:DDD:604:BR:BR	2.68	0.47
1:CCC:235[B]:VAL:HG21	5:CCC:615:GOL:H2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:180[B]:SER:OG	1:AAA:182:LYS:HG2	2.14	0.47
1:CCC:10:SER:HB2	4:CCC:606:BR:BR	2.70	0.47
1:DDD:28:ASN:ND2	4:DDD:605:BR:BR	2.91	0.47
1:AAA:51:THR:HB	1:CCC:506:ILE:CD1	2.45	0.47
1:CCC:51[A]:THR:CG2	7:CCC:791:HOH:O	1.87	0.46
1:DDD:364[A]:GLU:OE1	1:DDD:366[A]:LYS:HE2	2.15	0.46
1:BBB:497[B]:ILE:HD11	1:BBB:569:ALA:CB	2.44	0.46
1:CCC:596[B]:ILE:HD12	4:CCC:605:BR:BR	2.70	0.46
1:DDD:66:ASP:OD2	5:DDD:609:GOL:C3	2.63	0.46
2:CCC:601:PO4:O3	4:CCC:604:BR:BR	2.89	0.46
1:BBB:182:LYS:NZ	5:BBB:613:GOL:H12	2.30	0.45
1:DDD:258[B]:LYS:NZ	7:DDD:715:HOH:O	2.49	0.45
1:BBB:299:VAL:CG2	5:BBB:610:GOL:H31	2.45	0.45
1:AAA:429[A]:ILE:CD1	7:AAA:848:HOH:O	2.61	0.45
1:CCC:66:ASP:OD2	5:CCC:610:GOL:C1	2.56	0.45
5:CCC:618:GOL:H2	7:CCC:1372:HOH:O	2.17	0.45
1:DDD:39:GLU:CG	1:DDD:151[B]:VAL:HG23	2.46	0.45
1:DDD:95[B]:LEU:HD12	1:DDD:95[B]:LEU:HA	1.85	0.45
1:DDD:250[B]:ILE:CD1	1:DDD:277:SER:HA	2.47	0.45
1:AAA:248:LYS:NZ	7:AAA:719:HOH:O	2.50	0.45
1:BBB:515:ASP:CG	1:BBB:520[B]:LYS:NZ	2.71	0.45
1:BBB:495[B]:VAL:HG13	1:BBB:536:LEU:HB3	1.99	0.44
1:AAA:201:ASN:OD1	1:AAA:202[B]:THR:HG23	2.17	0.44
1:BBB:527[B]:LYS:O	1:BBB:527[B]:LYS:HD2	2.18	0.44
1:AAA:43:BYR:BR	7:AAA:1517:HOH:O	2.77	0.44
1:BBB:452:ARG:NH1	7:BBB:709:HOH:O	2.42	0.44
1:CCC:250[B]:ILE:HD11	1:CCC:277:SER:HA	2.00	0.44
1:DDD:250[B]:ILE:HD11	1:DDD:277:SER:HA	2.00	0.44
1:CCC:339:GLU:HG3	1:DDD:275:TYR:CZ	2.53	0.44
1:AAA:46:PRO:HG3	5:AAA:611:GOL:H31	2.00	0.44
5:BBB:613:GOL:H32	7:BBB:906:HOH:O	2.18	0.43
1:BBB:505:GLY:HA2	5:BBB:608:GOL:H12	1.99	0.43
5:AAA:614:GOL:H2	7:AAA:1231:HOH:O	2.19	0.43
1:DDD:425:LYS:HE2	7:DDD:1386:HOH:O	2.17	0.43
1:DDD:70:ALA:CB	5:DDD:609:GOL:H32	2.47	0.43
1:AAA:334:PHE:O	1:BBB:276:GLY:HA2	2.19	0.43
1:DDD:112:SER:HB2	5:DDD:611:GOL:H2	2.00	0.43
1:CCC:275:TYR:CZ	1:DDD:339:GLU:HG3	2.54	0.42
1:AAA:127:ASN:HB3	1:AAA:130:ALA:HB2	2.02	0.42
1:AAA:453[A]:LYS:HG3	7:AAA:931:HOH:O	2.19	0.42
1:AAA:98:GLY:HA2	1:AAA:305:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:47[B]:ASP:OD2	1:CCC:49[B]:ASP:OD1	2.36	0.42
1:CCC:334:PHE:O	1:DDD:276:GLY:HA2	2.19	0.42
1:CCC:245[B]:VAL:HG12	1:CCC:246:GLY:O	2.19	0.42
1:DDD:62:GLY:HA2	1:DDD:306:ALA:HB2	2.02	0.42
1:AAA:47[A]:ASP:OD1	1:AAA:47[A]:ASP:C	2.58	0.41
1:BBB:62:GLY:HA2	1:BBB:306:ALA:HB2	2.02	0.41
1:BBB:127:ASN:HB3	1:BBB:130:ALA:HB2	2.02	0.41
1:AAA:10:SER:HB2	4:AAA:605:BR:BR	2.75	0.41
1:BBB:172:GLU:O	5:BBB:613:GOL:H2	2.20	0.41
1:CCC:68:ASN:ND2	5:CCC:610:GOL:H11	2.26	0.41
1:DDD:181[B]:PRO:HG2	7:DDD:1105:HOH:O	2.20	0.41
1:AAA:19:ARG:HG3	7:AAA:1130:HOH:O	2.19	0.41
1:DDD:76:ASP:CG	1:DDD:96[B]:THR:CG2	2.88	0.41
1:DDD:438[B]:GLU:OE1	7:DDD:702:HOH:O	2.22	0.41
5:BBB:610:GOL:H32	7:BBB:1250:HOH:O	2.19	0.41
1:DDD:50[B]:ASN:OD1	1:DDD:52[B]:ASP:HB2	2.20	0.41
1:CCC:47[A]:ASP:HA	1:CCC:48:PRO:HD3	1.94	0.40
1:AAA:258[B]:LYS:HZ2	1:AAA:260[B]:LEU:HD21	1.84	0.40
1:BBB:515:ASP:OD1	1:BBB:522:VAL:HG11	2.21	0.40
1:CCC:198:GLU:O	1:CCC:202[B]:THR:OG1	2.31	0.40
1:DDD:10:SER:HB2	4:DDD:606:BR:BR	2.76	0.40
1:DDD:483:TYR:HA	1:DDD:484:GLY:HA2	1.90	0.40
2:AAA:601:PO4:O1	4:AAA:604:BR:BR	2.94	0.40
1:BBB:10:SER:HB2	4:BBB:605:BR:BR	2.77	0.40
5:DDD:611:GOL:H31	7:DDD:1259:HOH:O	2.21	0.40

All (1) 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)
7:BBB:1217:HOH:O	7:BBB:1278:HOH:O[3_565]	2.17	0.03

## 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	AAA	645/598 (108%)	637 (99%)	8 (1%)	0	100	100
1	BBB	638/598 (107%)	630 (99%)	8 (1%)	0	100	100
1	CCC	650/598 (109%)	639 (98%)	10 (2%)	1 (0%)	47	32
1	DDD	653/598 (109%)	644 (99%)	8 (1%)	1 (0%)	47	32
All	All	2586/2392 (108%)	2550 (99%)	34 (1%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	373	PHE
1	DDD	373	PHE

### 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	AAA	539/489 (110%)	534 (99%)	5 (1%)	78	72
1	BBB	532/489 (109%)	525 (99%)	7 (1%)	69	59
1	CCC	544/489 (111%)	541 (99%)	3 (1%)	86	82
1	DDD	547/489 (112%)	542 (99%)	5 (1%)	78	72
All	All	2162/1956 (110%)	2142 (99%)	20 (1%)	81	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	370	GLN
1	AAA	397	TRP
1	AAA	438[A]	GLU
1	AAA	438[B]	GLU
1	AAA	479	PHE
1	BBB	6[A]	ASP

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Mol	Chain	Res	Type
1	BBB	6[B]	ASP
1	BBB	235[A]	VAL
1	BBB	235[B]	VAL
1	BBB	370	GLN
1	BBB	397	TRP
1	BBB	479	PHE
1	CCC	370	GLN
1	CCC	397	TRP
1	CCC	479	PHE
1	DDD	6[A]	ASP
1	DDD	6[B]	ASP
1	DDD	370	GLN
1	DDD	397	TRP
1	DDD	479	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	BYR	DDD	186	1	12,13,14	0.93	0	14,17,19	1.84	3 (21%)
1	BYR	CCC	43	1	12,13,14	1.00	0	14,17,19	1.09	1 (7%)
1	BYR	DDD	43	1	12,13,14	0.89	0	14,17,19	1.34	2 (14%)
1	BYR	AAA	186	1	12,13,14	0.96	0	14,17,19	1.99	3 (21%)
1	BYR	AAA	43	1	12,13,14	0.81	0	14,17,19	1.02	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	BYR	BBB	43	1	12,13,14	1.06	0	14,17,19	1.47	4 (28%)
1	BYR	BBB	186	1	12,13,14	0.89	0	14,17,19	1.92	2 (14%)
1	BYR	CCC	186	1	12,13,14	1.10	0	14,17,19	1.89	3 (21%)

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
1	BYR	DDD	186	1	-	0/5/6/8	0/1/1/1
1	BYR	CCC	43	1	-	0/5/6/8	0/1/1/1
1	BYR	DDD	43	1	-	1/5/6/8	0/1/1/1
1	BYR	AAA	186	1	-	0/5/6/8	0/1/1/1
1	BYR	AAA	43	1	-	0/5/6/8	0/1/1/1
1	BYR	BBB	43	1	-	2/5/6/8	0/1/1/1
1	BYR	BBB	186	1	-	0/5/6/8	0/1/1/1
1	BYR	CCC	186	1	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	186	BYR	CG-CB-CA	-4.73	104.52	114.10
1	CCC	186	BYR	CG-CB-CA	-4.63	104.73	114.10
1	AAA	186	BYR	BR-CE2-CZ	4.62	123.10	119.31
1	DDD	186	BYR	CG-CB-CA	-4.54	104.91	114.10
1	BBB	186	BYR	CG-CB-CA	-4.52	104.94	114.10
1	BBB	186	BYR	BR-CE2-CZ	4.38	122.91	119.31
1	DDD	186	BYR	BR-CE2-CZ	4.10	122.67	119.31
1	CCC	186	BYR	BR-CE2-CZ	3.95	122.55	119.31
1	DDD	43	BYR	CD2-CE2-CZ	3.21	123.64	121.00
1	BBB	43	BYR	CE1-CZ-CE2	2.34	119.90	118.00
1	AAA	43	BYR	CD2-CE2-CZ	2.33	122.92	121.00
1	DDD	43	BYR	CG-CD2-CE2	-2.26	117.07	120.28
1	CCC	43	BYR	CD2-CE2-CZ	2.20	122.81	121.00
1	DDD	186	BYR	BR-CE2-CD2	-2.15	114.73	118.39
1	BBB	43	BYR	CG-CB-CA	-2.10	109.85	114.10
1	AAA	186	BYR	BR-CE2-CD2	-2.06	114.88	118.39
1	CCC	186	BYR	BR-CE2-CD2	-2.04	114.91	118.39
1	BBB	43	BYR	CD2-CE2-CZ	2.03	122.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	43	BYR	CG-CD2-CE2	-2.03	117.40	120.28

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	43	BYR	CA-CB-CG-CD1
1	BBB	43	BYR	CA-CB-CG-CD2
1	DDD	43	BYR	CA-CB-CG-CD1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	CCC	43	BYR	2	0
1	DDD	43	BYR	2	0
1	AAA	43	BYR	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 25 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GOL	AAA	610	-	5,5,5	0.16	0	5,5,5	0.42	0
5	GOL	BBB	607	-	5,5,5	0.23	0	5,5,5	0.30	0
5	GOL	BBB	614	-	5,5,5	0.20	0	5,5,5	0.47	0
5	GOL	DDD	611	-	5,5,5	0.14	0	5,5,5	0.39	0
2	PO4	CCC	601	-	4,4,4	1.33	1 (25%)	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	AAA	615	-	5,5,5	0.19	0	5,5,5	0.47	0
5	GOL	CCC	610	-	5,5,5	0.24	0	5,5,5	0.27	0
2	PO4	CCC	603	-	4,4,4	0.68	0	6,6,6	0.65	0
5	GOL	DDD	610	-	5,5,5	0.15	0	5,5,5	0.58	0
2	PO4	DDD	603	-	4,4,4	0.93	0	6,6,6	0.78	0
5	GOL	AAA	609	6	5,5,5	0.36	0	5,5,5	0.57	0
5	GOL	DDD	607	-	5,5,5	0.21	0	5,5,5	0.41	0
5	GOL	BBB	609	-	5,5,5	0.11	0	5,5,5	0.50	0
2	PO4	DDD	601	-	4,4,4	1.03	0	6,6,6	0.62	0
5	GOL	CCC	615	-	5,5,5	0.13	0	5,5,5	0.37	0
5	GOL	BBB	608	6	5,5,5	0.32	0	5,5,5	0.42	0
5	GOL	CCC	609	-	5,5,5	0.19	0	5,5,5	0.70	0
5	GOL	AAA	612	-	5,5,5	0.19	0	5,5,5	0.47	0
5	GOL	DDD	609	-	5,5,5	0.32	0	5,5,5	0.67	0
5	GOL	CCC	608	6	5,5,5	0.47	0	5,5,5	0.49	0
5	GOL	CCC	613	-	5,5,5	0.14	0	5,5,5	0.60	0
5	GOL	DDD	608	6	5,5,5	0.36	0	5,5,5	0.39	0
5	GOL	CCC	616	-	5,5,5	0.26	0	5,5,5	0.50	0
5	GOL	DDD	613	-	5,5,5	0.17	0	5,5,5	0.23	0
5	GOL	CCC	611	-	5,5,5	0.11	0	5,5,5	0.29	0
5	GOL	DDD	616	-	5,5,5	0.15	0	5,5,5	0.63	0
5	GOL	AAA	611	-	5,5,5	0.26	0	5,5,5	0.57	0
2	PO4	AAA	603	-	4,4,4	1.72	1 (25%)	6,6,6	0.66	0
5	GOL	BBB	612	6	5,5,5	0.14	0	5,5,5	0.37	0
2	PO4	AAA	619	-	4,4,4	2.13	1 (25%)	6,6,6	0.57	0
5	GOL	CCC	612	-	5,5,5	0.23	0	5,5,5	0.29	0
2	PO4	AAA	601	-	4,4,4	1.07	0	6,6,6	0.96	0
5	GOL	BBB	613	-	5,5,5	0.19	0	5,5,5	0.66	0
5	GOL	CCC	618	-	5,5,5	0.12	0	5,5,5	0.48	0
5	GOL	CCC	607	-	5,5,5	0.31	0	5,5,5	0.45	0
5	GOL	AAA	613	-	5,5,5	0.15	0	5,5,5	0.47	0
5	GOL	CCC	614	-	5,5,5	0.21	0	5,5,5	0.38	0
5	GOL	AAA	616	-	5,5,5	0.14	0	5,5,5	0.37	0
5	GOL	DDD	612	-	5,5,5	0.14	0	5,5,5	0.34	0
5	GOL	DDD	615	-	5,5,5	0.14	0	5,5,5	0.38	0
5	GOL	AAA	614	-	5,5,5	0.14	0	5,5,5	0.42	0
5	GOL	BBB	611	-	5,5,5	0.19	0	5,5,5	0.10	0
5	GOL	AAA	608	-	5,5,5	0.42	0	5,5,5	0.47	0
2	PO4	BBB	601	-	4,4,4	0.38	0	6,6,6	0.84	0
5	GOL	DDD	614	-	5,5,5	0.16	0	5,5,5	0.40	0
5	GOL	BBB	610	-	5,5,5	0.13	0	5,5,5	0.48	0
2	PO4	BBB	603	-	4,4,4	0.40	0	6,6,6	0.62	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	AAA	618	-	5,5,5	0.17	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	AAA	610	-	-	2/4/4/4	-
5	GOL	BBB	607	-	-	0/4/4/4	-
5	GOL	BBB	614	-	-	0/4/4/4	-
5	GOL	DDD	611	-	-	4/4/4/4	-
5	GOL	AAA	615	-	-	0/4/4/4	-
5	GOL	CCC	610	-	-	2/4/4/4	-
5	GOL	DDD	610	-	-	1/4/4/4	-
5	GOL	AAA	609	6	-	0/4/4/4	-
5	GOL	DDD	607	-	-	0/4/4/4	-
5	GOL	BBB	609	-	-	1/4/4/4	-
5	GOL	CCC	615	-	-	2/4/4/4	-
5	GOL	BBB	608	6	-	0/4/4/4	-
5	GOL	CCC	609	-	-	4/4/4/4	-
5	GOL	AAA	612	-	-	0/4/4/4	-
5	GOL	DDD	609	-	-	2/4/4/4	-
5	GOL	CCC	608	6	-	0/4/4/4	-
5	GOL	CCC	613	-	-	2/4/4/4	-
5	GOL	DDD	608	6	-	0/4/4/4	-
5	GOL	CCC	616	-	-	3/4/4/4	-
5	GOL	DDD	613	-	-	0/4/4/4	-
5	GOL	CCC	611	-	-	0/4/4/4	-
5	GOL	DDD	616	-	-	2/4/4/4	-
5	GOL	AAA	611	-	-	2/4/4/4	-
5	GOL	BBB	612	6	-	2/4/4/4	-
5	GOL	CCC	612	-	-	0/4/4/4	-
5	GOL	BBB	613	-	-	0/4/4/4	-
5	GOL	CCC	618	-	-	4/4/4/4	-
5	GOL	CCC	607	-	-	0/4/4/4	-
5	GOL	AAA	613	-	-	0/4/4/4	-
5	GOL	CCC	614	-	-	0/4/4/4	-
5	GOL	AAA	616	-	-	4/4/4/4	-
5	GOL	DDD	612	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	DDD	615	-	-	1/4/4/4	-
5	GOL	AAA	614	-	-	2/4/4/4	-
5	GOL	BBB	611	-	-	0/4/4/4	-
5	GOL	AAA	608	-	-	0/4/4/4	-
5	GOL	DDD	614	-	-	3/4/4/4	-
5	GOL	BBB	610	-	-	4/4/4/4	-
5	GOL	AAA	618	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	619	PO4	P-O1	3.83	1.59	1.50
2	AAA	603	PO4	P-O1	2.90	1.57	1.50
2	CCC	601	PO4	P-O1	2.23	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	614	GOL	O1-C1-C2-C3
5	AAA	616	GOL	C1-C2-C3-O3
5	AAA	618	GOL	C1-C2-C3-O3
5	BBB	610	GOL	O1-C1-C2-O2
5	BBB	610	GOL	O1-C1-C2-C3
5	BBB	610	GOL	O2-C2-C3-O3
5	BBB	612	GOL	C1-C2-C3-O3
5	BBB	612	GOL	O2-C2-C3-O3
5	CCC	610	GOL	O1-C1-C2-C3
5	CCC	613	GOL	O1-C1-C2-C3
5	CCC	618	GOL	C1-C2-C3-O3
5	DDD	609	GOL	O1-C1-C2-C3
5	DDD	611	GOL	O1-C1-C2-C3
5	DDD	614	GOL	O1-C1-C2-C3
5	DDD	616	GOL	O1-C1-C2-O2
5	DDD	616	GOL	O1-C1-C2-C3
5	AAA	614	GOL	O1-C1-C2-O2
5	CCC	613	GOL	O1-C1-C2-O2
5	CCC	618	GOL	O2-C2-C3-O3
5	AAA	610	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	AAA	611	GOL	O1-C1-C2-C3
5	AAA	616	GOL	O1-C1-C2-C3
5	AAA	618	GOL	O1-C1-C2-C3
5	BBB	609	GOL	C1-C2-C3-O3
5	BBB	610	GOL	C1-C2-C3-O3
5	CCC	609	GOL	O1-C1-C2-C3
5	CCC	609	GOL	C1-C2-C3-O3
5	CCC	616	GOL	C1-C2-C3-O3
5	CCC	618	GOL	O1-C1-C2-C3
5	DDD	610	GOL	C1-C2-C3-O3
5	DDD	611	GOL	C1-C2-C3-O3
5	DDD	614	GOL	C1-C2-C3-O3
5	AAA	610	GOL	O1-C1-C2-O2
5	CCC	609	GOL	O1-C1-C2-O2
5	CCC	610	GOL	O1-C1-C2-O2
5	CCC	616	GOL	O2-C2-C3-O3
5	DDD	609	GOL	O1-C1-C2-O2
5	DDD	611	GOL	O1-C1-C2-O2
5	AAA	616	GOL	O1-C1-C2-O2
5	AAA	618	GOL	O2-C2-C3-O3
5	CCC	609	GOL	O2-C2-C3-O3
5	CCC	618	GOL	O1-C1-C2-O2
5	DDD	611	GOL	O2-C2-C3-O3
5	AAA	616	GOL	O2-C2-C3-O3
5	CCC	616	GOL	O1-C1-C2-O2
5	DDD	615	GOL	O2-C2-C3-O3
5	AAA	611	GOL	O1-C1-C2-O2
5	DDD	614	GOL	O1-C1-C2-O2
5	CCC	615	GOL	C1-C2-C3-O3
5	CCC	615	GOL	O2-C2-C3-O3

There are no ring outliers.

19 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	610	GOL	2	0
5	DDD	611	GOL	3	0
2	CCC	601	PO4	1	0
5	CCC	610	GOL	6	0
5	CCC	615	GOL	1	0
5	BBB	608	GOL	1	0
5	CCC	609	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	DDD	609	GOL	3	0
5	CCC	613	GOL	3	0
5	CCC	616	GOL	1	0
5	DDD	616	GOL	1	0
5	AAA	611	GOL	1	0
5	BBB	612	GOL	3	0
2	AAA	601	PO4	1	0
5	BBB	613	GOL	4	0
5	CCC	618	GOL	4	0
5	AAA	614	GOL	4	0
2	BBB	601	PO4	1	0
5	BBB	610	GOL	4	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 [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, 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	AAA	595/598 (99%)	-0.68	4 (0%) 87 88	10, 15, 29, 67	0
1	BBB	595/598 (99%)	-0.67	7 (1%) 79 79	11, 16, 30, 85	0
1	CCC	595/598 (99%)	-0.71	3 (0%) 91 91	9, 14, 26, 68	0
1	DDD	595/598 (99%)	-0.67	7 (1%) 79 79	10, 15, 29, 68	0
All	All	2380/2392 (99%)	-0.68	21 (0%) 84 84	9, 15, 29, 85	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	48	PRO	4.4
1	CCC	48	PRO	4.1
1	AAA	48	PRO	4.1
1	AAA	49[A]	ASP	3.3
1	DDD	104[A]	GLU	3.3
1	DDD	49[A]	ASP	3.2
1	BBB	48	PRO	3.1
1	CCC	49[A]	ASP	3.1
1	AAA	527[A]	LYS	3.1
1	BBB	104[A]	GLU	3.0
1	CCC	527[A]	LYS	2.7
1	BBB	462	ASP	2.4
1	BBB	461	PRO	2.2
1	BBB	49	ASP	2.2
1	DDD	461	PRO	2.2
1	DDD	527[A]	LYS	2.1
1	AAA	462[A]	ASP	2.1
1	BBB	527[A]	LYS	2.1
1	DDD	462	ASP	2.1
1	BBB	181	PRO	2.0
1	DDD	47[A]	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	BYR	CCC	186	13/14	0.94	0.08	18,21,28,29	1
1	BYR	BBB	186	13/14	0.96	0.07	19,22,28,31	1
1	BYR	AAA	43	13/14	0.97	0.06	11,14,18,26	1
1	BYR	AAA	186	13/14	0.97	0.06	18,22,26,30	1
1	BYR	DDD	186	13/14	0.97	0.06	18,23,29,34	1
1	BYR	BBB	43	13/14	0.98	0.05	13,15,16,21	1
1	BYR	DDD	43	13/14	0.98	0.05	12,15,18,27	1
1	BYR	CCC	43	13/14	0.98	0.05	11,12,16,25	1

## 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
5	GOL	AAA	616	6/6	0.82	0.16	30,50,63,84	0
5	GOL	CCC	609	6/6	0.84	0.17	20,25,41,47	6
2	PO4	AAA	619	5/5	0.86	0.17	30,38,50,67	0
5	GOL	CCC	616	6/6	0.89	0.15	21,36,60,61	0
5	GOL	AAA	611	6/6	0.90	0.15	20,33,56,57	0
5	GOL	DDD	609	6/6	0.90	0.14	26,32,53,55	0
5	GOL	AAA	618	6/6	0.92	0.13	24,37,71,76	0
5	GOL	AAA	610	6/6	0.92	0.12	26,51,67,68	0
5	GOL	DDD	613	6/6	0.92	0.10	21,34,39,41	0
5	GOL	DDD	614	6/6	0.92	0.12	27,39,69,71	0
5	GOL	BBB	610	6/6	0.93	0.21	23,30,67,92	0
5	GOL	BBB	613	6/6	0.93	0.19	18,49,75,85	0
5	GOL	AAA	615	6/6	0.93	0.10	23,35,43,46	0
5	GOL	CCC	613	6/6	0.93	0.10	31,36,40,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	CCC	614	6/6	0.94	0.10	21,32,46,57	0
5	GOL	AAA	609	6/6	0.94	0.08	20,22,25,26	0
5	GOL	AAA	614	6/6	0.94	0.13	33,51,56,69	0
5	GOL	CCC	612	6/6	0.94	0.07	16,23,23,26	0
5	GOL	AAA	608	6/6	0.94	0.09	15,19,21,25	0
5	GOL	DDD	616	6/6	0.94	0.17	25,39,54,73	0
6	NA	BBB	616	1/1	0.94	0.08	33,33,33,33	0
5	GOL	BBB	612	6/6	0.95	0.09	32,45,50,50	0
5	GOL	CCC	618	6/6	0.95	0.13	28,40,65,68	0
5	GOL	DDD	608	6/6	0.95	0.09	18,20,21,22	0
5	GOL	CCC	610	6/6	0.95	0.12	14,23,37,81	0
5	GOL	DDD	611	6/6	0.95	0.12	28,31,42,48	0
5	GOL	AAA	612	6/6	0.95	0.08	24,34,40,43	0
5	GOL	BBB	614	6/6	0.95	0.13	25,35,55,70	0
5	GOL	CCC	608	6/6	0.95	0.10	19,20,22,23	0
6	NA	AAA	621	1/1	0.95	0.07	34,34,34,34	0
5	GOL	CCC	615	6/6	0.95	0.12	17,49,59,64	0
5	GOL	DDD	612	6/6	0.96	0.08	23,26,29,34	0
5	GOL	BBB	609	6/6	0.96	0.08	24,35,45,54	0
5	GOL	BBB	608	6/6	0.96	0.09	21,23,25,26	0
5	GOL	DDD	615	6/6	0.96	0.13	16,41,63,65	0
5	GOL	BBB	611	6/6	0.96	0.08	21,26,33,35	0
5	GOL	DDD	610	6/6	0.96	0.08	22,30,41,42	0
5	GOL	CCC	607	6/6	0.96	0.07	13,20,22,26	0
6	NA	CCC	619	1/1	0.96	0.09	33,33,33,33	0
6	NA	DDD	617	1/1	0.96	0.09	32,32,32,32	0
2	PO4	AAA	603	5/5	0.97	0.07	26,27,31,36	5
6	NA	AAA	620	1/1	0.97	0.09	37,37,37,37	0
5	GOL	DDD	607	6/6	0.97	0.07	14,24,28,29	0
5	GOL	AAA	613	6/6	0.97	0.08	19,22,29,30	0
5	GOL	CCC	611	6/6	0.97	0.07	20,33,40,50	0
5	GOL	BBB	607	6/6	0.97	0.06	14,21,26,27	0
2	PO4	DDD	603	5/5	0.98	0.12	32,34,46,55	0
2	PO4	BBB	603	5/5	0.98	0.11	30,36,38,41	0
2	PO4	CCC	603	5/5	0.98	0.16	31,39,47,49	0
4	BR	AAA	617	1/1	0.99	0.03	23,23,23,23	1
4	BR	BBB	605	1/1	0.99	0.03	24,24,24,24	1
4	BR	BBB	615	1/1	0.99	0.04	22,22,22,22	1
4	BR	CCC	605	1/1	0.99	0.02	20,20,20,20	1
4	BR	CCC	617	1/1	0.99	0.03	21,21,21,21	1
4	BR	DDD	605	1/1	0.99	0.02	19,19,19,19	1
4	BR	DDD	606	1/1	0.99	0.03	24,24,24,24	1

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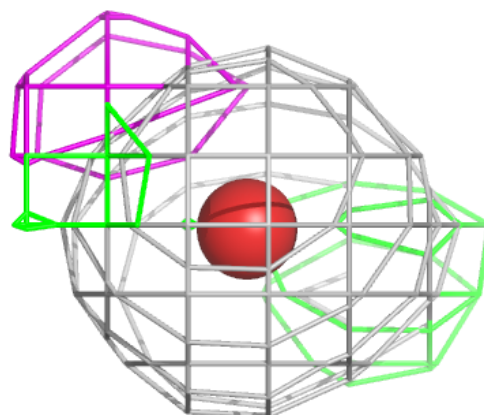
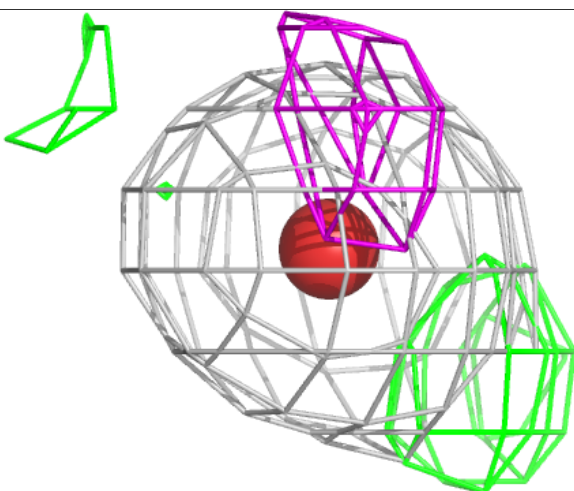
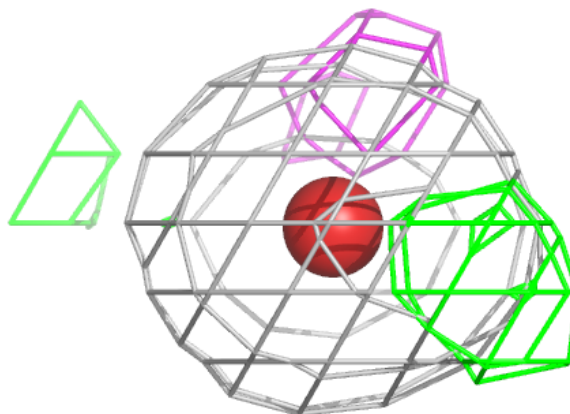
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	CCC	601	5/5	0.99	0.04	13,14,17,18	0
2	PO4	BBB	601	5/5	0.99	0.05	15,17,18,23	0
2	PO4	DDD	601	5/5	0.99	0.04	16,16,17,19	0
2	PO4	AAA	601	5/5	0.99	0.04	14,16,17,22	0
3	CA	BBB	602	1/1	0.99	0.03	15,15,15,15	0
3	CA	DDD	602	1/1	0.99	0.02	13,13,13,13	0
4	BR	AAA	604	1/1	0.99	0.04	21,21,21,21	1
4	BR	AAA	605	1/1	0.99	0.02	22,22,22,22	1
4	BR	AAA	606	1/1	0.99	0.03	23,23,23,23	1
4	BR	AAA	607	1/1	0.99	0.02	22,22,22,22	1
4	BR	CCC	606	1/1	1.00	0.02	22,22,22,22	1
3	CA	AAA	602	1/1	1.00	0.03	16,16,16,16	0
4	BR	DDD	604	1/1	1.00	0.02	22,22,22,22	1
4	BR	BBB	606	1/1	1.00	0.03	23,23,23,23	1
3	CA	CCC	602	1/1	1.00	0.02	15,15,15,15	0
4	BR	CCC	604	1/1	1.00	0.03	20,20,20,20	1
4	BR	BBB	604	1/1	1.00	0.02	22,22,22,22	1

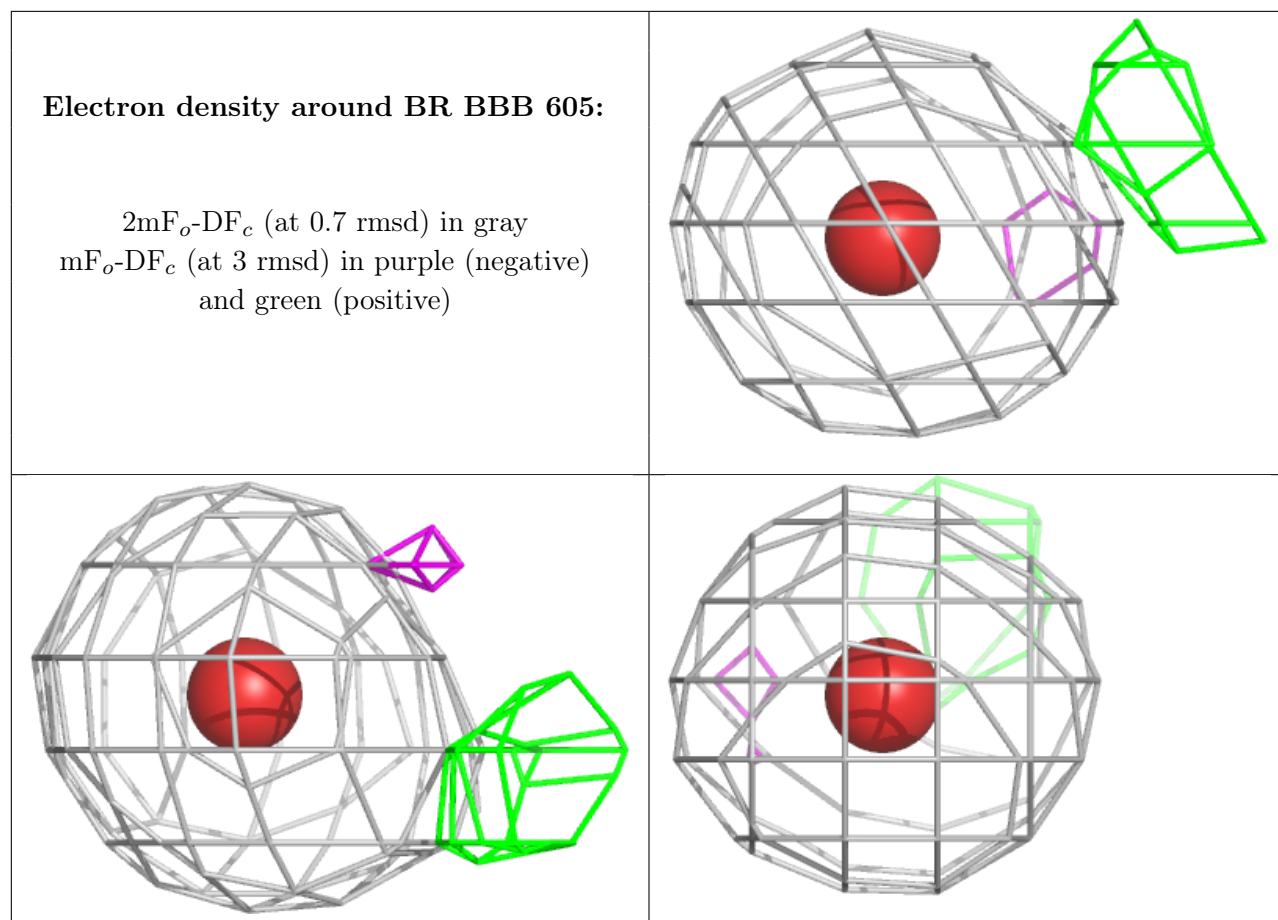
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around BR AAA 617:**

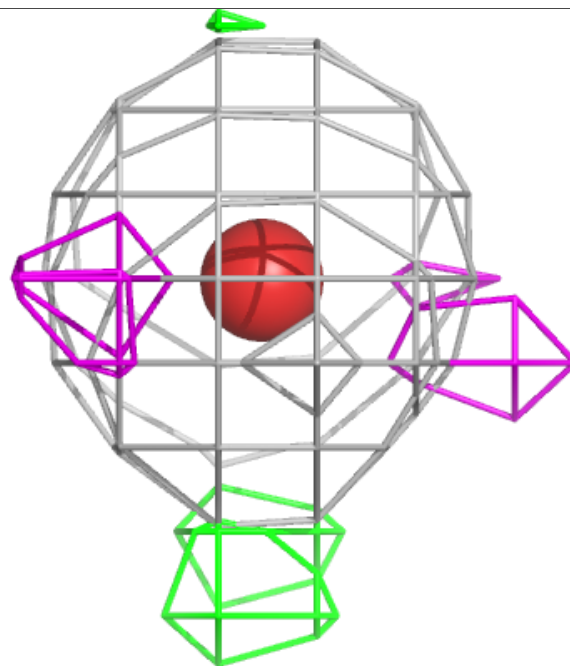
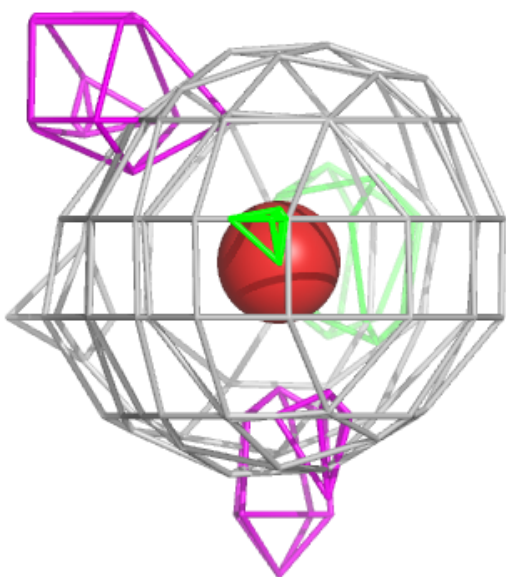
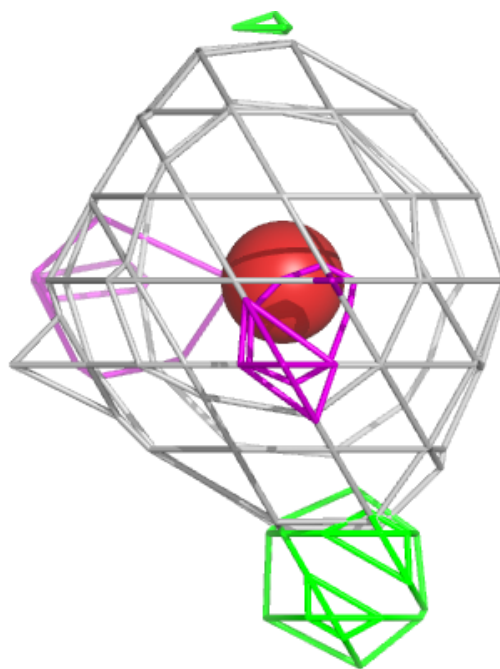
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





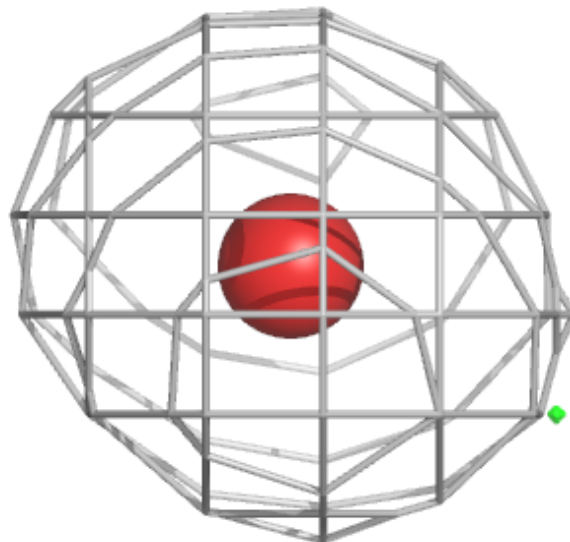
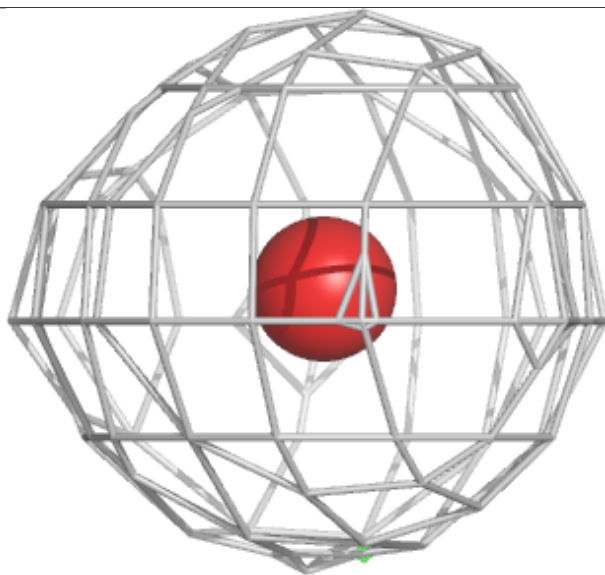
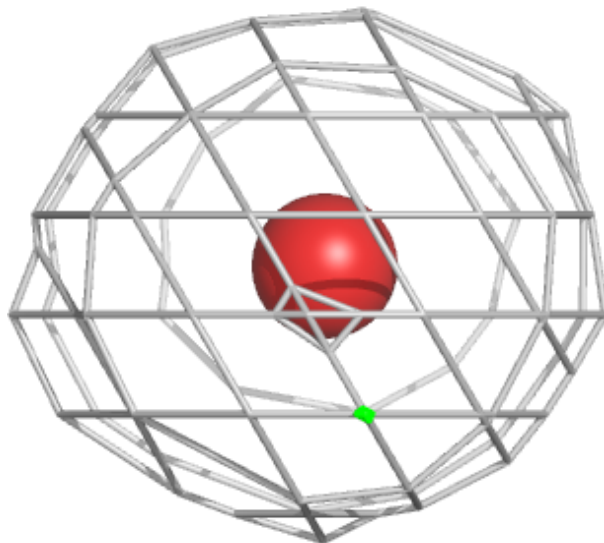
**Electron density around BR BBB 615:**

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



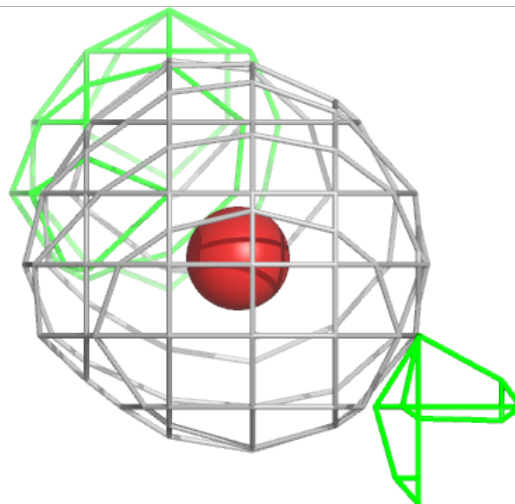
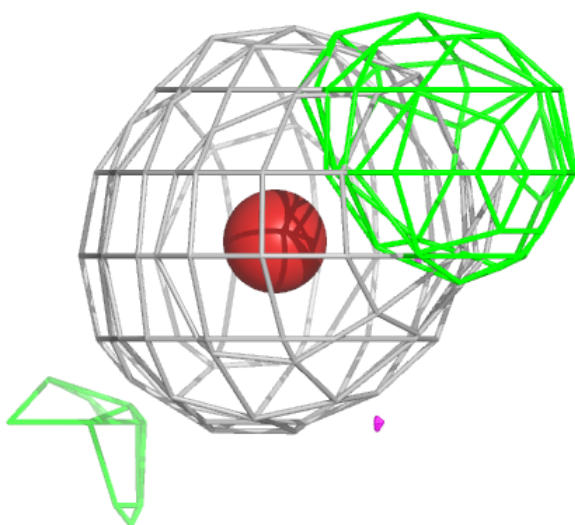
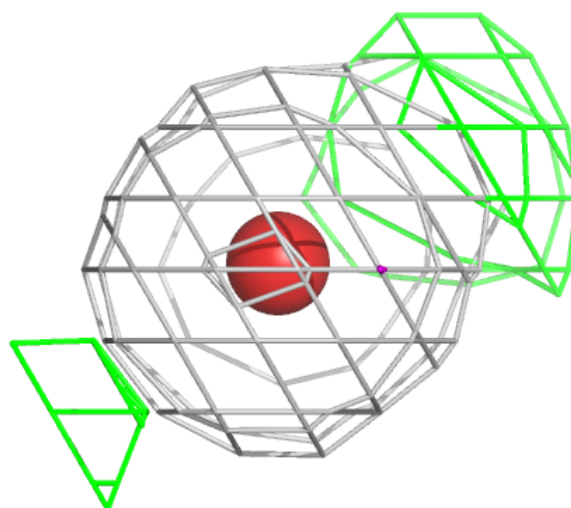
**Electron density around BR CCC 605:**

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



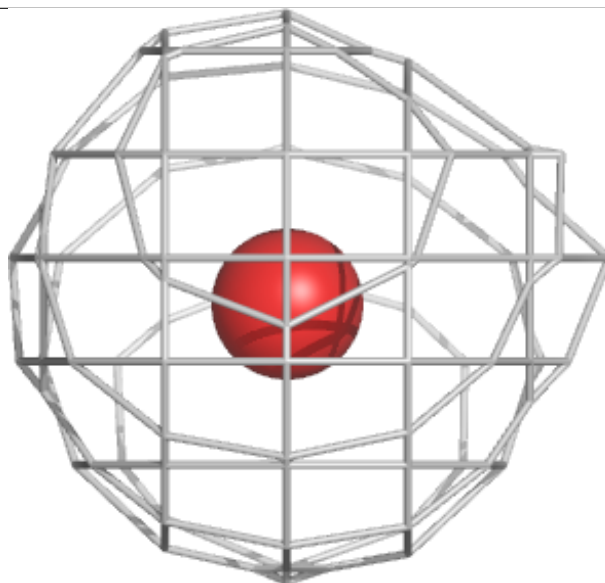
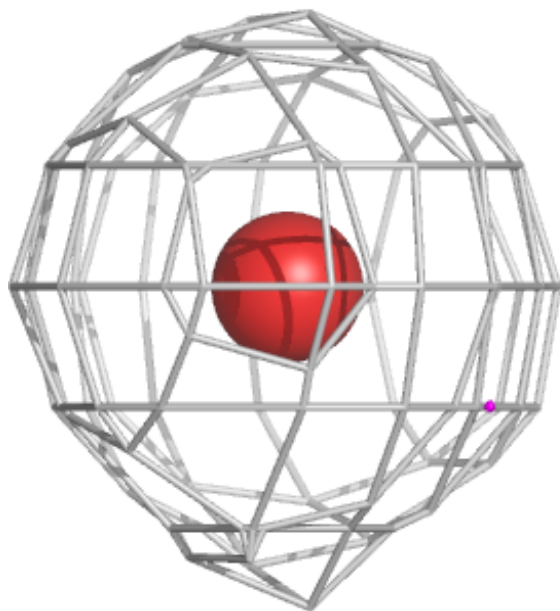
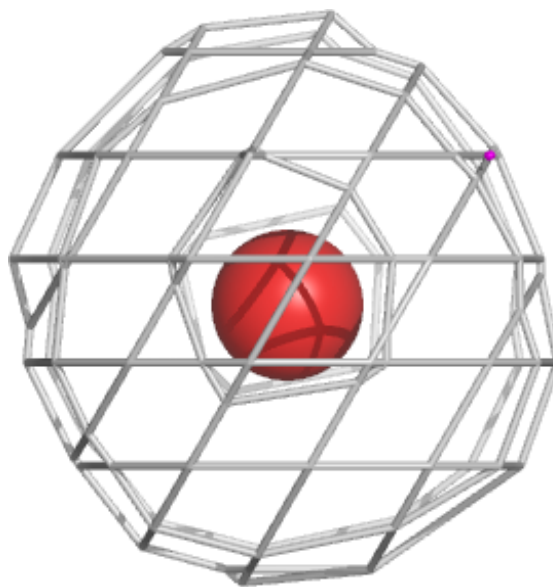
**Electron density around BR CCC 617:**

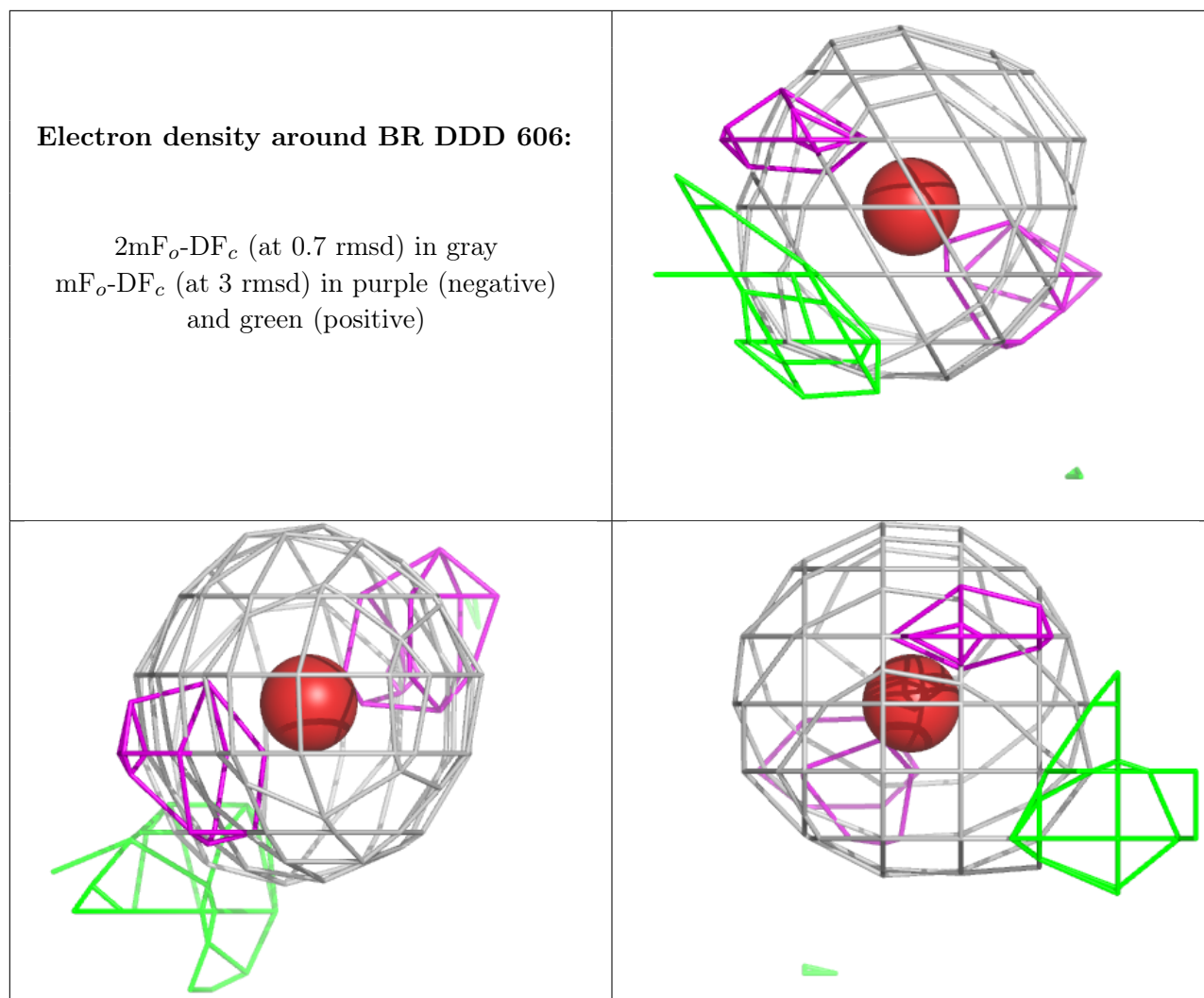
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

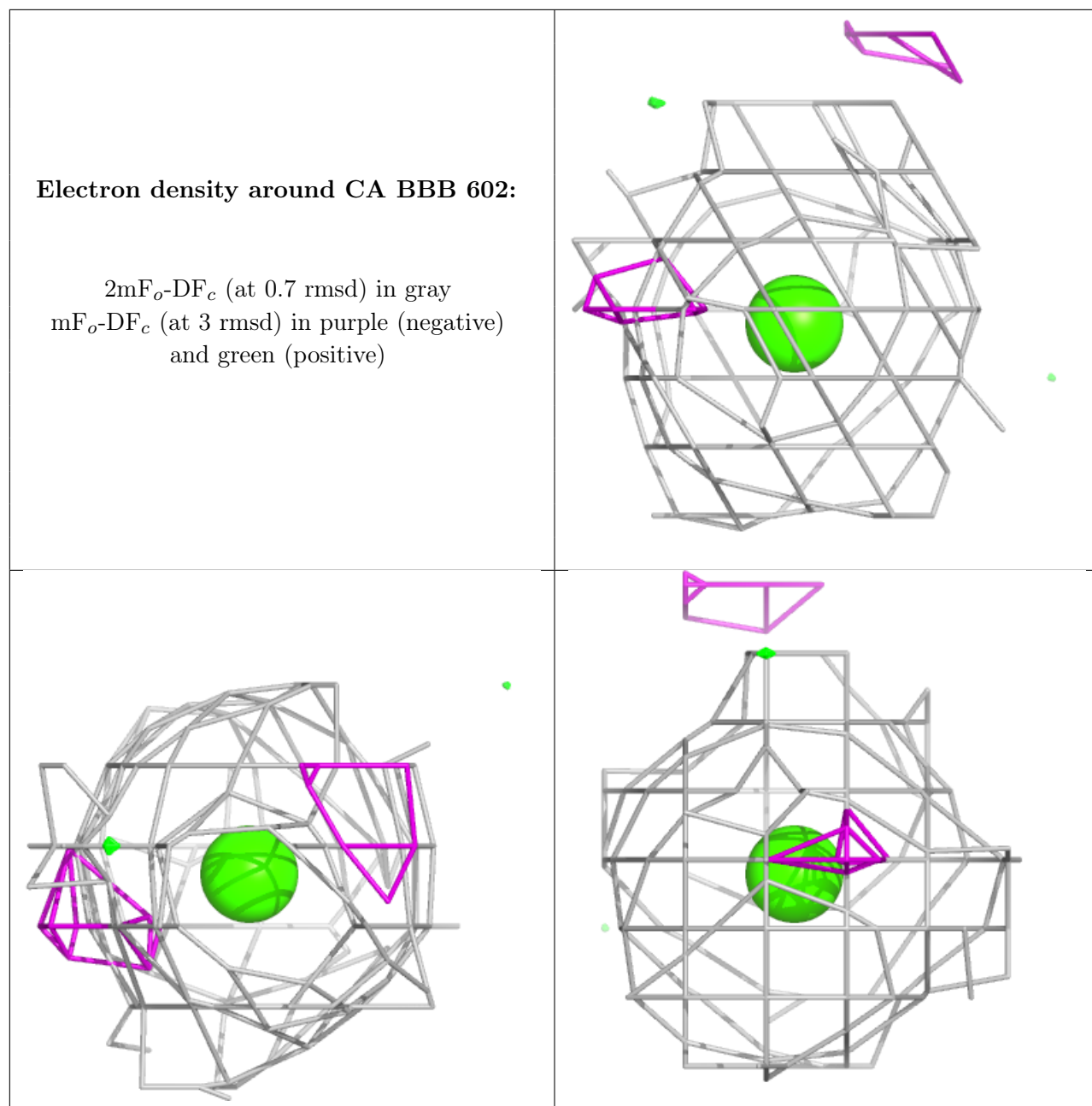


**Electron density around BR DDD 605:**

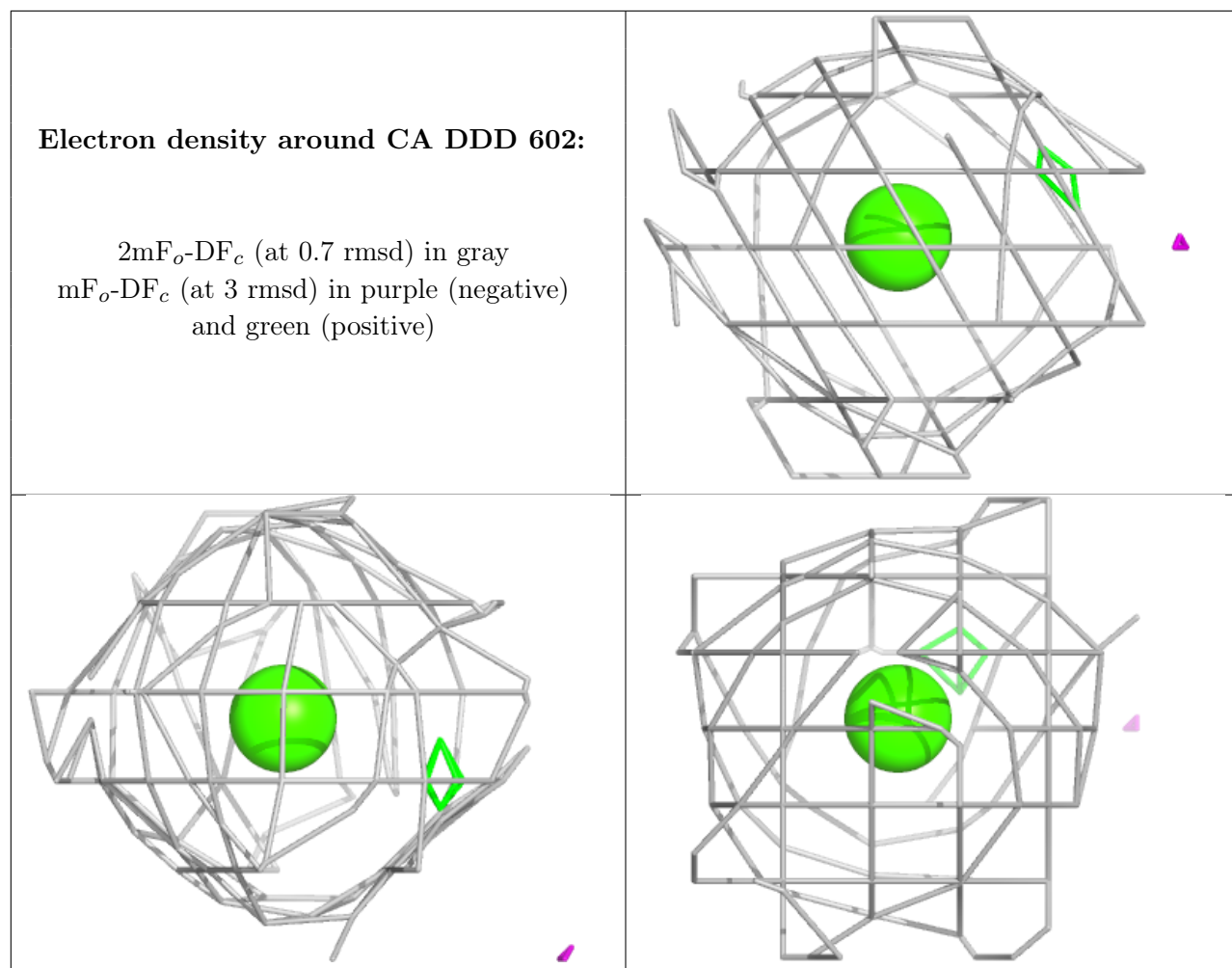
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





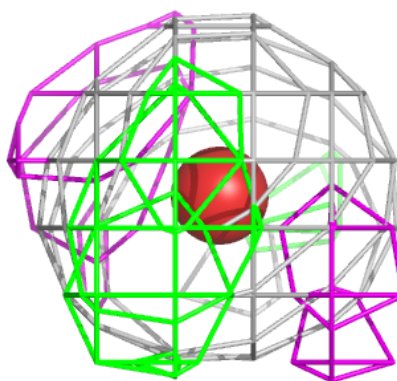
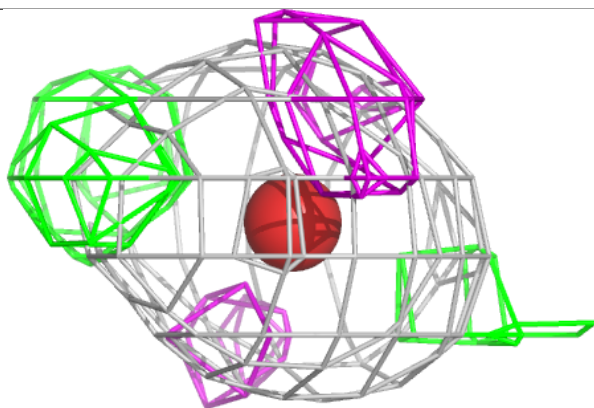
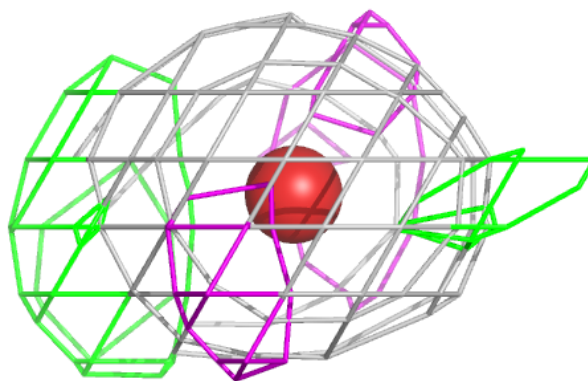




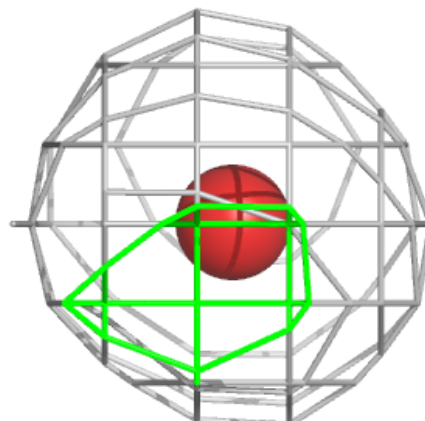
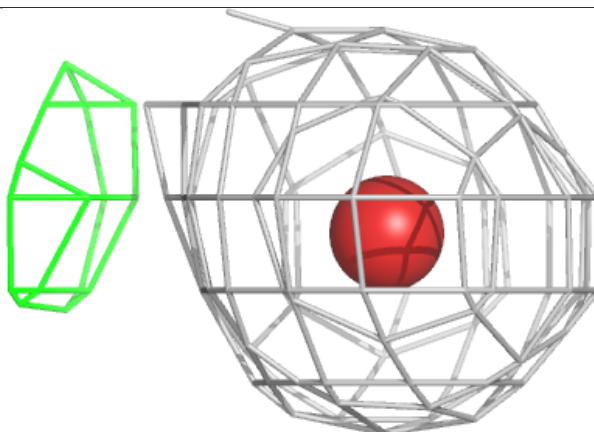
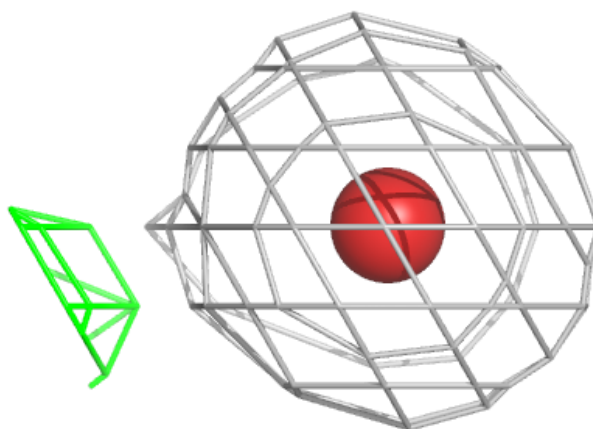


**Electron density around BR AAA 604:**

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

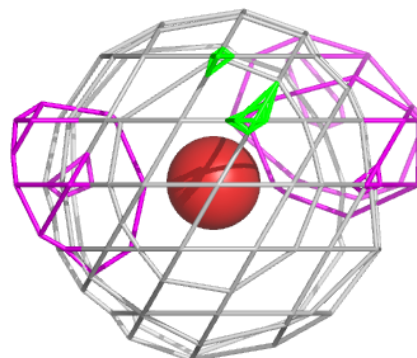
**Electron density around BR AAA 605:**

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

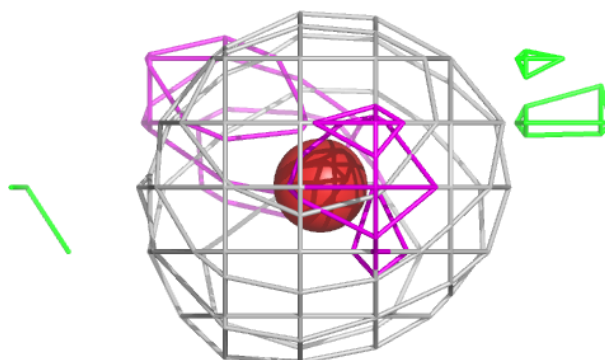
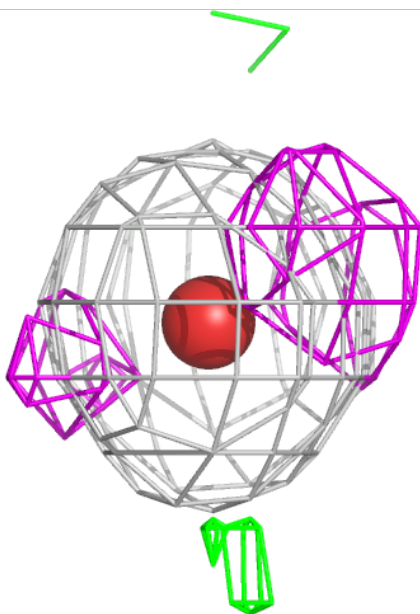


**Electron density around BR AAA 606:**

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



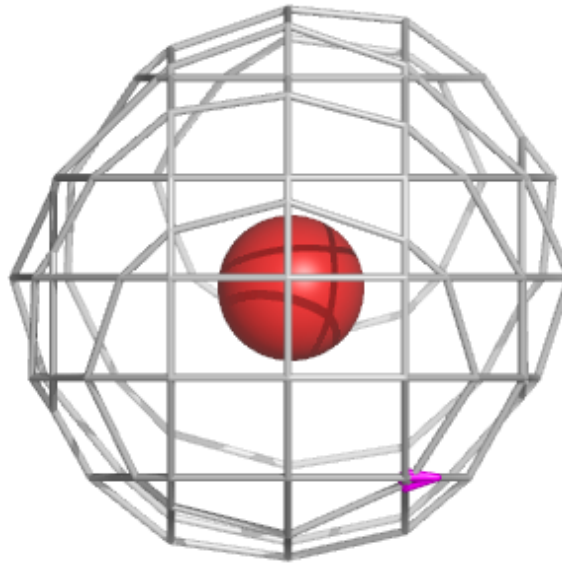
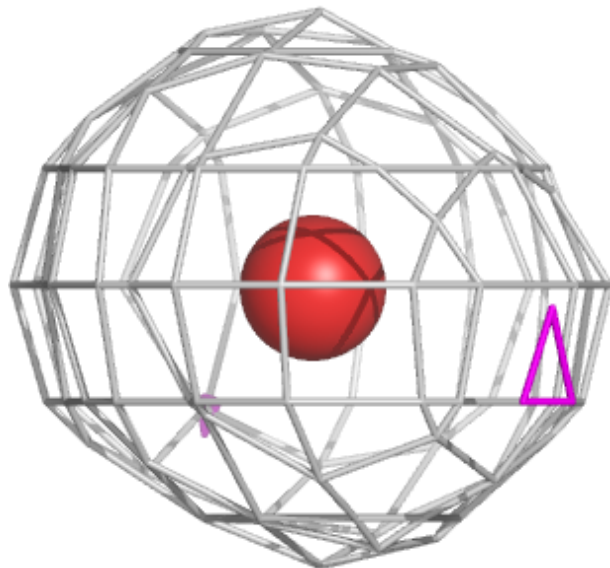
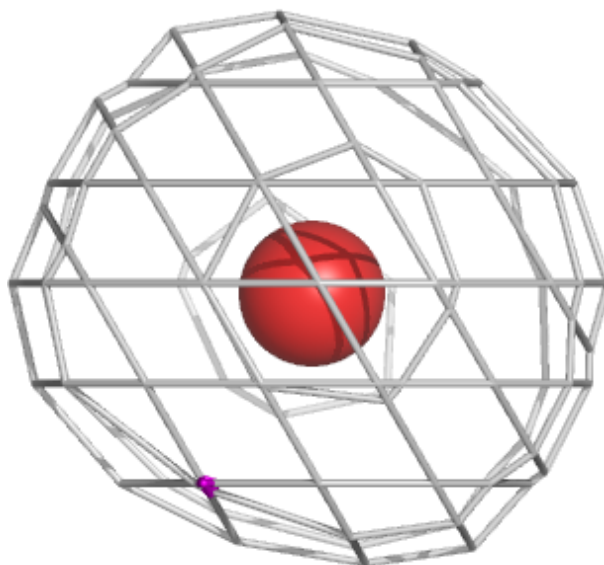
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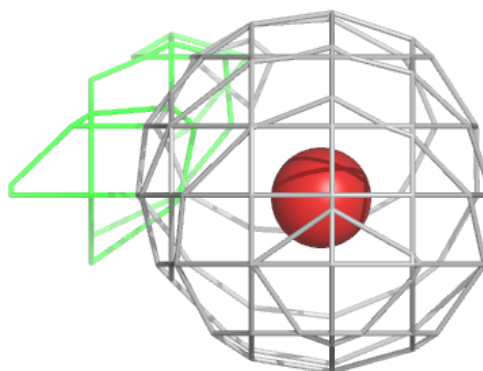
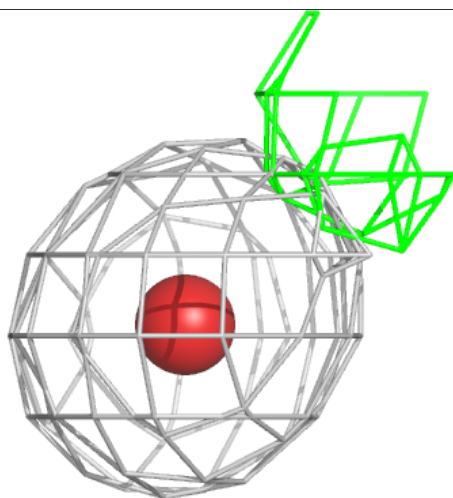
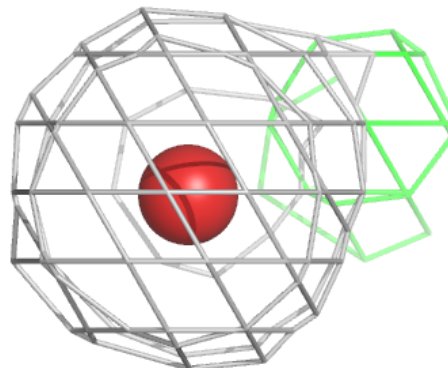
**Electron density around BR AAA 607:**

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



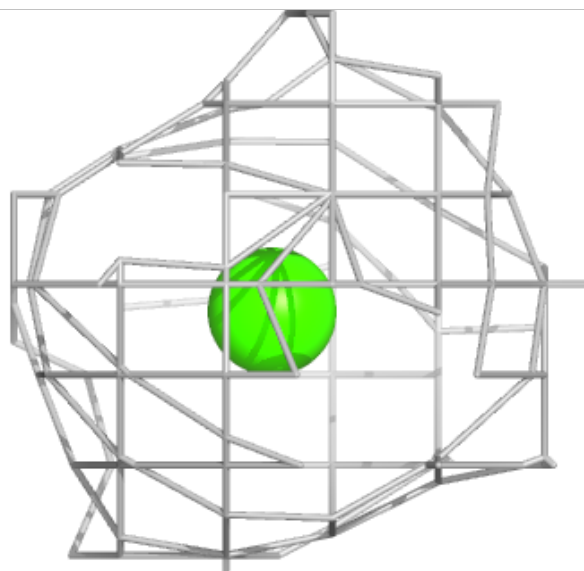
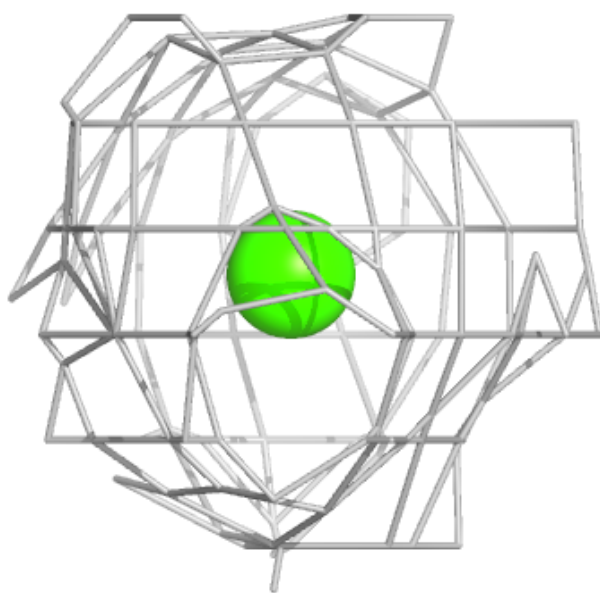
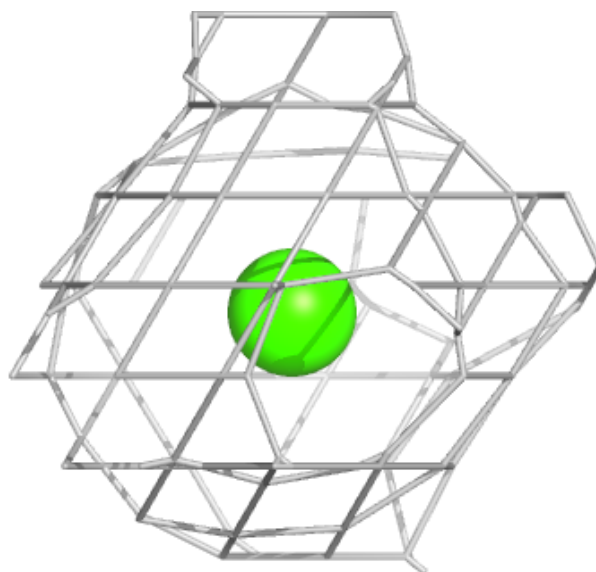
**Electron density around BR CCC 606:**

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



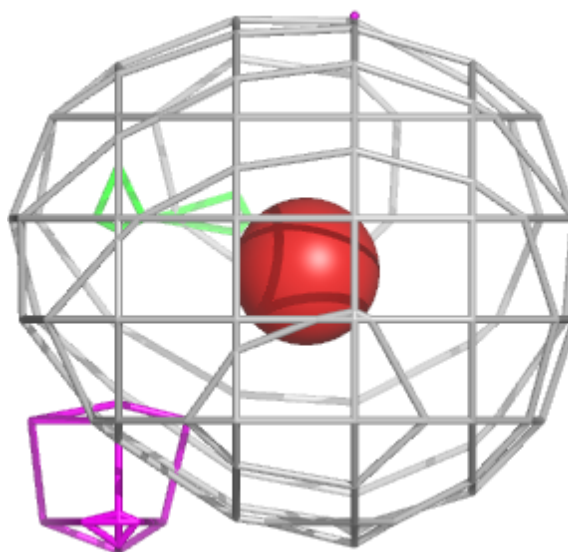
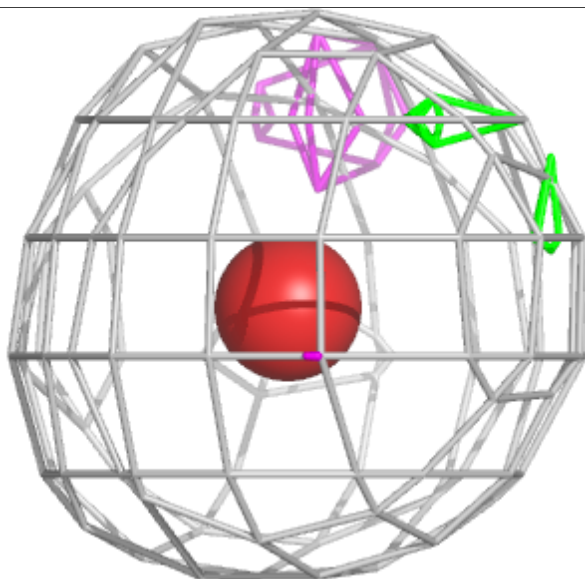
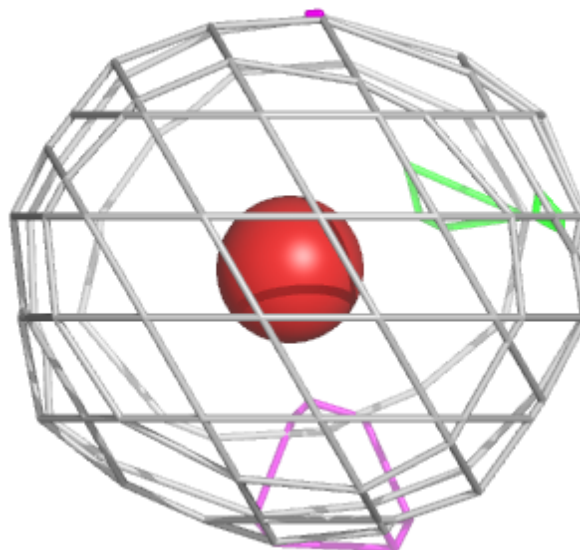
**Electron density around CA AAA 602:**

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



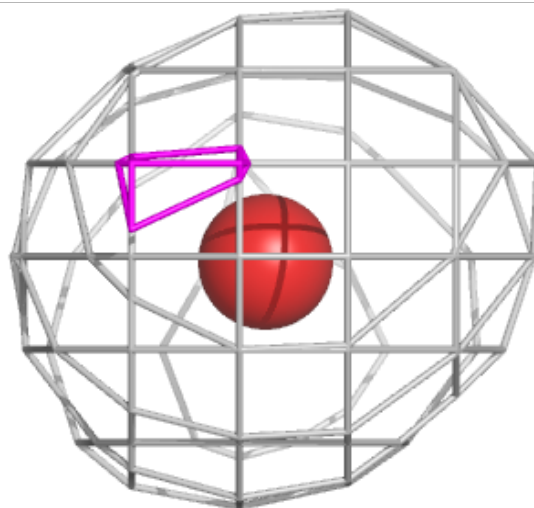
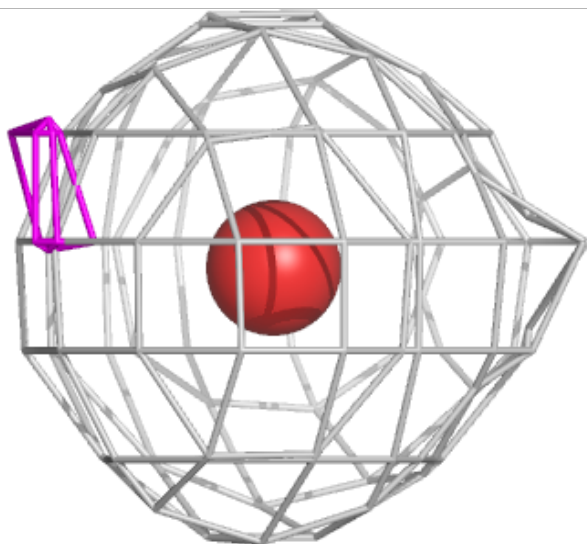
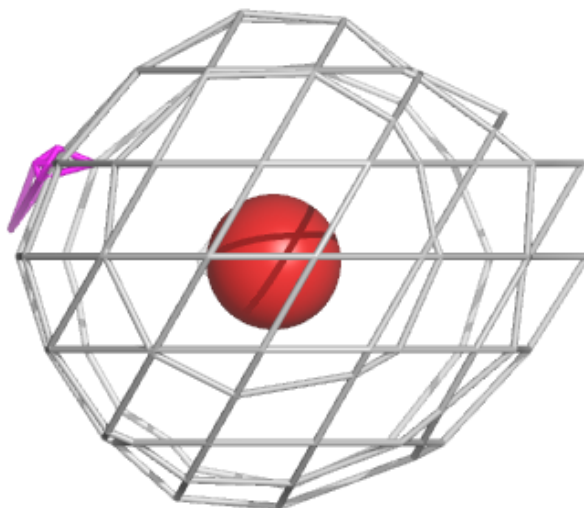
**Electron density around BR DDD 604:**

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



**Electron density around BR BBB 606:**

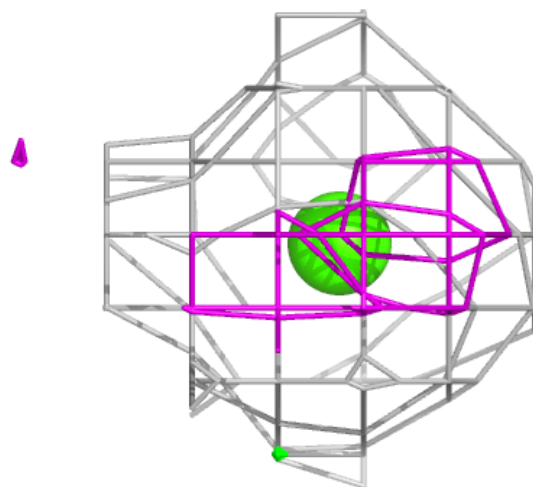
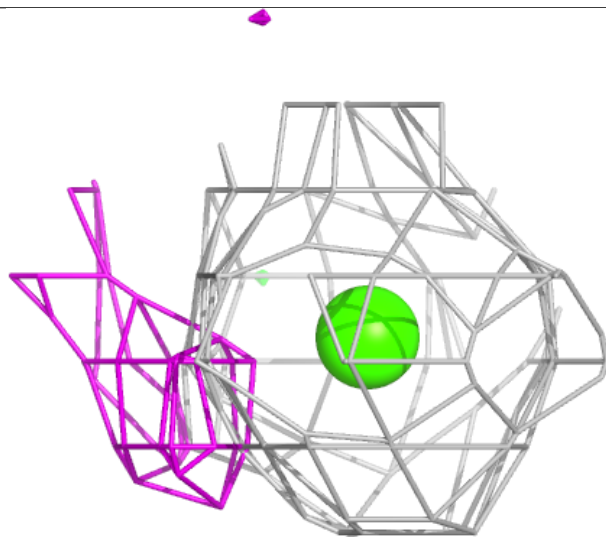
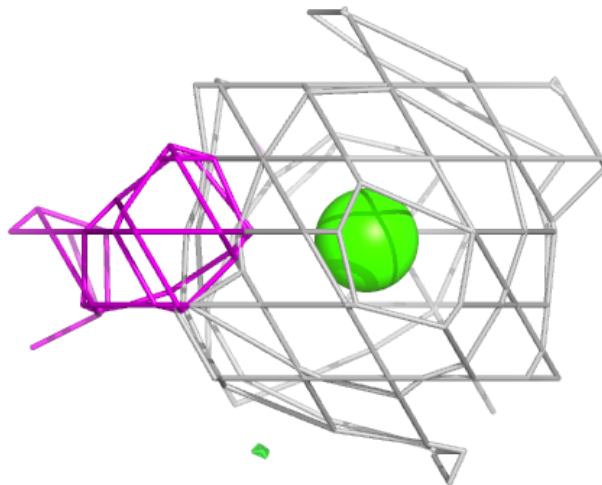
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





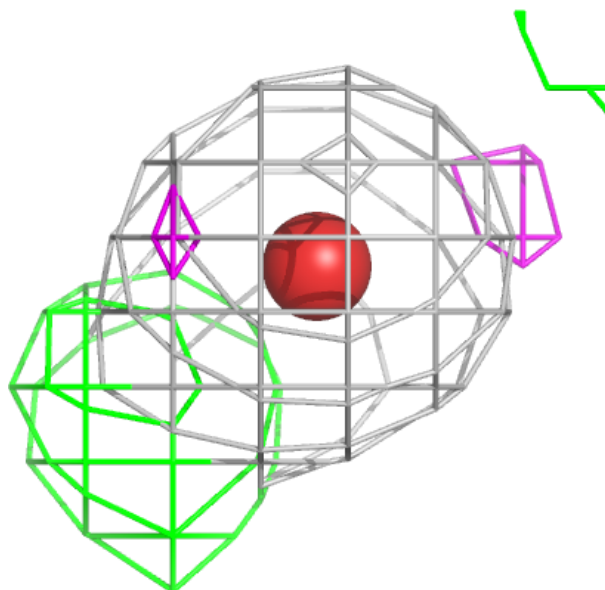
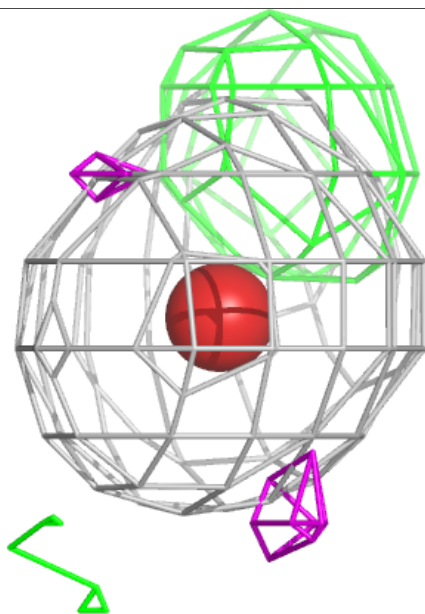
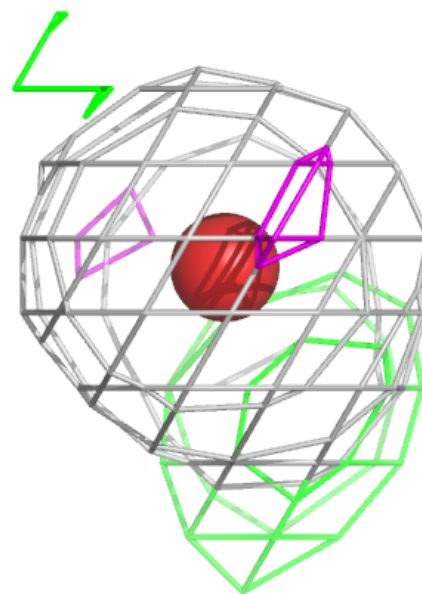
**Electron density around CA CCC 602:**

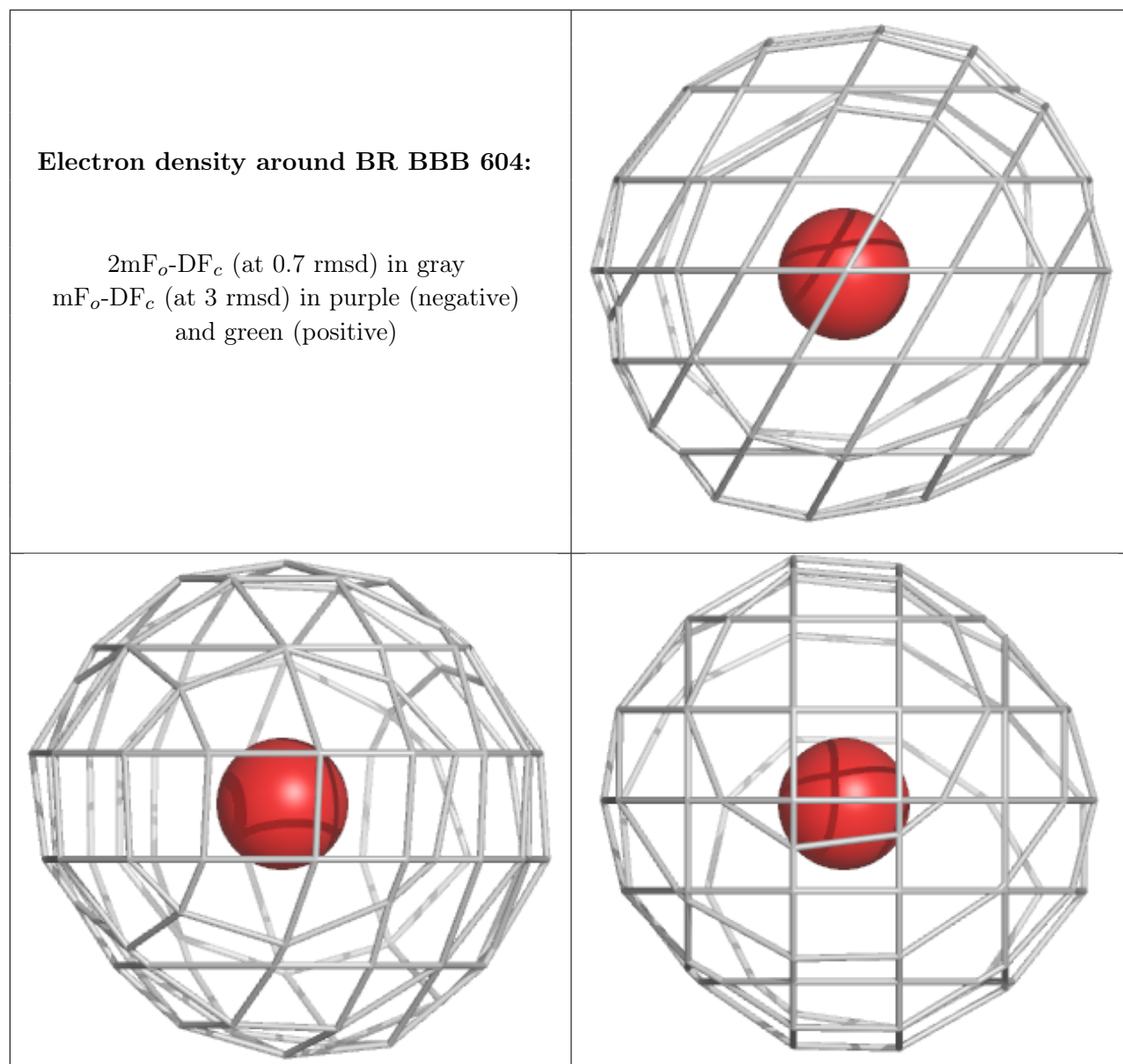
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BR CCC 604:**

$2mF_o-DF_c$  (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.