



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 7QVW / pdb_00007qvw
Title : R396W mutant of the vanadium-dependent bromoperoxidase from *Corallina pilulifera*
Authors : Isupov, M.N.; Mitchell, D.; Littelchild, J.A.; Garcia-Rodriguez, E.
Deposited on : 2022-01-23
Resolution : 1.92 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

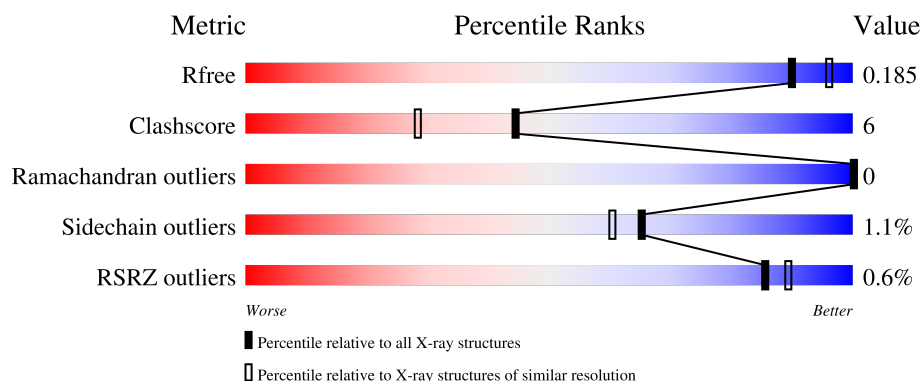
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	90% 9%
1	BBB	598	92% 8%
1	CCC	598	91% 9%
1	DDD	598	92% 7%

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	GOL	AAA	616	-	-	X	-
4	GOL	AAA	619	-	-	X	-
4	GOL	AAA	620	-	-	X	-
4	GOL	AAA	621	-	-	X	-
4	GOL	BBB	601	-	-	X	-
4	GOL	BBB	611	-	-	X	-
4	GOL	BBB	617	-	-	X	-
4	GOL	CCC	611	-	-	X	-
4	GOL	CCC	617	-	-	X	-
4	GOL	DDD	601	-	-	X	-
4	GOL	DDD	616	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22996 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
1	AAA	597	Total	Br	C	N	O	S	0	44	0
			4849	2	3120	781	939	7			
1	BBB	597	Total	Br	C	N	O	S	0	44	0
			4845	2	3118	782	936	7			
1	CCC	597	Total	Br	C	N	O	S	0	50	0
			4877	2	3139	782	947	7			
1	DDD	597	Total	Br	C	N	O	S	0	42	0
			4834	2	3106	780	939	7			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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

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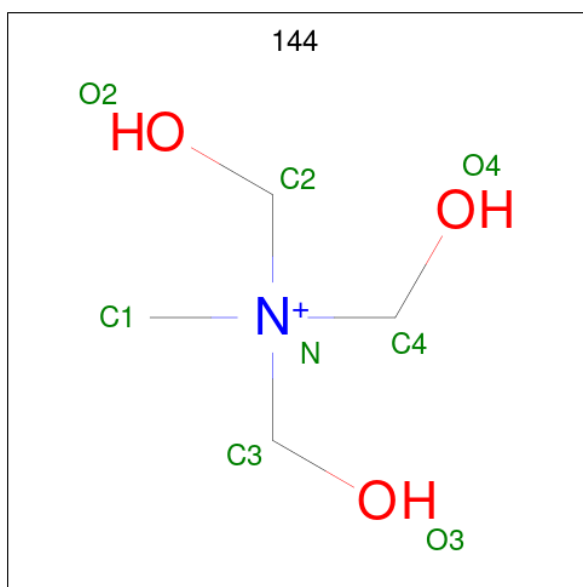
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	DDD	1	Total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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	2	Total Na 2 2	0	0
5	BBB	2	Total Na 2 2	0	0
5	CCC	3	Total Na 3 3	0	0
5	DDD	3	Total Na 3 3	0	0

- Molecule 6 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	CCC	1	Total	C	N	O	0	0
			8	4	1	3		

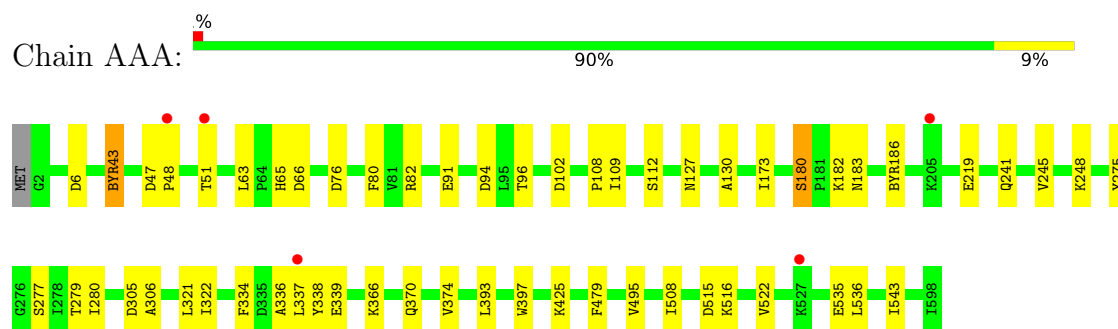
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	785	Total	O	1	0
			785	785		
7	BBB	788	Total	O	0	0
			788	788		
7	CCC	806	Total	O	0	0
			806	806		
7	DDD	768	Total	O	0	0
			768	768		

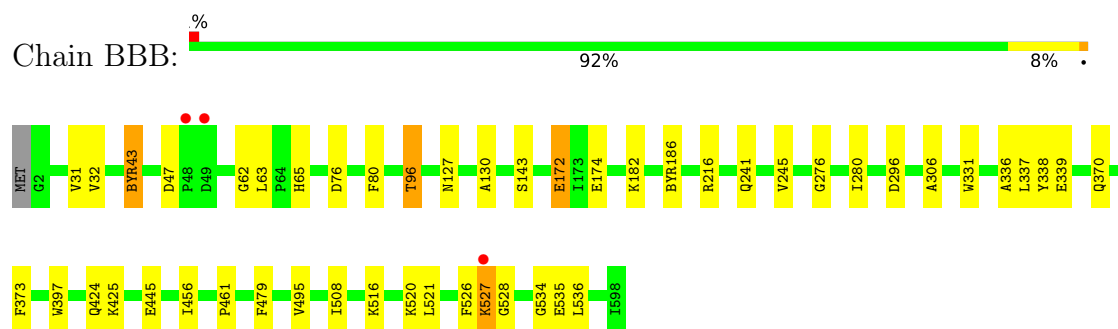
3 Residue-property plots [i](#)

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.

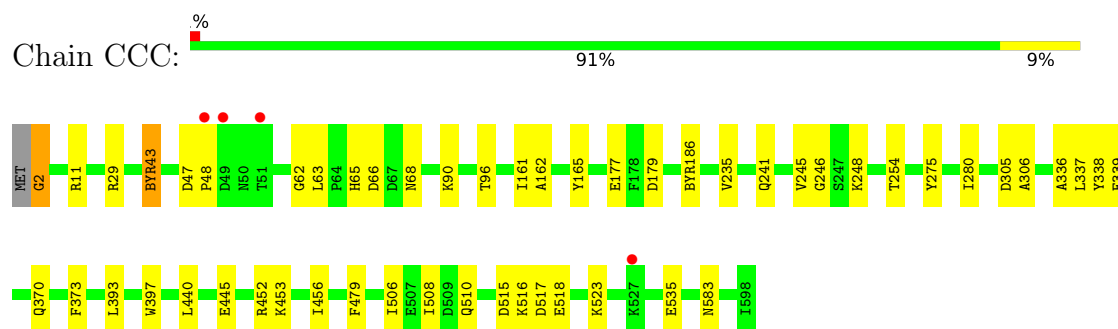
- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	182.15Å 182.15Å 177.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.60 – 1.92 49.60 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.60-1.92) 97.0 (49.60-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.153 , 0.185 0.153 , 0.185	Depositor DCC
R_{free} test set	2477 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22996	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BYR, NA, GOL, 144, PO4, CA

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	0.65	0/5038	0.96	4/6840 (0.1%)
1	BBB	0.63	0/5034	0.94	2/6834 (0.0%)
1	CCC	0.66	1/5082 (0.0%)	0.95	2/6901 (0.0%)
1	DDD	0.64	0/5014	0.94	2/6811 (0.0%)
All	All	0.65	1/20168 (0.0%)	0.95	10/27386 (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	BBB	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	2	GLY	N-CA	5.80	1.54	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	108	PRO	CB-CA-C	-6.52	103.48	111.11
1	DDD	96	THR	CA-CB-OG1	-5.56	101.26	109.60
1	BBB	96	THR	CA-CB-OG1	-5.32	101.62	109.60
1	CCC	254	THR	CA-CB-OG1	-5.29	101.66	109.60
1	AAA	80	PHE	CA-CB-CG	5.29	119.09	113.80
1	DDD	80	PHE	CA-CB-CG	5.11	118.91	113.80
1	CCC	96	THR	CA-CB-OG1	-5.05	102.02	109.60
1	AAA	96	THR	CA-CB-OG1	-5.03	102.06	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	6	ASP	CA-CB-CG	-5.01	107.59	112.60
1	BBB	80	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	527[A]	LYS	Peptide

5.2 Too-close contacts

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	4849	0	4863	57	0
1	BBB	4845	0	4865	53	0
1	CCC	4877	0	4892	66	0
1	DDD	4834	0	4827	53	0
2	AAA	15	0	0	0	0
2	BBB	10	0	0	0	0
2	CCC	10	0	0	0	0
2	DDD	15	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	102	0	134	35	0
4	BBB	90	0	118	22	0
4	CCC	84	0	110	22	0
4	DDD	96	0	127	21	0
5	AAA	2	0	0	0	0
5	BBB	2	0	0	0	0
5	CCC	3	0	0	0	0
5	DDD	3	0	0	0	0
6	CCC	8	0	12	5	0
7	AAA	785	0	0	16	0
7	BBB	788	0	0	14	1
7	CCC	806	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	DDD	768	0	0	11	0
All	All	22996	0	19948	237	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 6.

All (237) 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:DDD:47[B]:ASP:OD1	1:DDD:49[B]:ASP:OD1	1.63	1.16
1:BBB:424[B]:GLN:HE21	1:BBB:425[B]:LYS:NZ	1.43	1.15
1:CCC:68:ASN:HB2	4:CCC:611:GOL:O3	1.53	1.06
4:CCC:614:GOL:H11	1:DDD:583:ASN:HD22	1.18	1.05
1:CCC:280:ILE:HG12	1:DDD:280[B]:ILE:CD1	1.91	1.01
1:AAA:280[B]:ILE:CD1	1:BBB:280:ILE:HG12	1.94	0.98
1:DDD:47[B]:ASP:CG	1:DDD:49[B]:ASP:OD1	2.06	0.97
1:BBB:31[B]:VAL:HG23	1:BBB:143:SER:HA	1.47	0.96
1:CCC:68:ASN:HD22	4:CCC:611:GOL:H31	1.29	0.95
1:CCC:337[B]:LEU:HD21	7:CCC:716:HOH:O	1.66	0.95
1:CCC:280:ILE:HG12	1:DDD:280[B]:ILE:HD12	1.47	0.95
4:AAA:621:GOL:H31	1:CCC:583:ASN:HB2	1.47	0.94
1:DDD:51:THR:HG22	7:DDD:1337:HOH:O	1.67	0.94
1:BBB:337[B]:LEU:HD21	7:BBB:728:HOH:O	1.66	0.94
1:BBB:424[B]:GLN:NE2	1:BBB:425[B]:LYS:NZ	2.15	0.94
1:DDD:275:TYR:CD2	1:DDD:280[B]:ILE:HD11	2.04	0.92
1:DDD:337[B]:LEU:HD13	7:DDD:1150:HOH:O	1.69	0.91
1:CCC:179[B]:ASP:OD1	7:CCC:702:HOH:O	1.91	0.88
1:DDD:429[A]:ILE:HD12	7:DDD:1023:HOH:O	1.72	0.88
1:CCC:336[A]:ALA:HB2	4:CCC:617:GOL:H31	1.55	0.87
1:CCC:336[A]:ALA:HA	4:CCC:617:GOL:H11	1.56	0.87
1:BBB:424[B]:GLN:HE21	1:BBB:425[B]:LYS:HZ3	0.92	0.86
1:AAA:280[B]:ILE:HD12	1:BBB:280:ILE:HG12	1.56	0.84
1:DDD:43:BYR:BR	7:DDD:1389:HOH:O	2.50	0.84
1:BBB:336[A]:ALA:HB2	4:BBB:601:GOL:H31	1.60	0.83
4:AAA:621:GOL:H31	1:CCC:583:ASN:CB	2.07	0.83
1:AAA:275:TYR:CD2	1:AAA:280[B]:ILE:HD11	2.14	0.82
4:BBB:611:GOL:H2	7:BBB:1213:HOH:O	1.79	0.81
4:AAA:621:GOL:H11	1:CCC:583:ASN:HD22	1.44	0.81
1:AAA:336[B]:ALA:HB3	1:AAA:339:GLU:HB2	1.63	0.80
4:DDD:605:GOL:H11	7:DDD:1168:HOH:O	1.80	0.80
6:CCC:618:144:H42	7:CCC:1224:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:336[A]:ALA:HA	4:AAA:619:GOL:H32	1.65	0.78
1:BBB:43:BYR:BR	7:BBB:1420:HOH:O	2.57	0.77
1:CCC:280:ILE:CG1	1:DDD:280[B]:ILE:HD12	2.14	0.77
1:BBB:336[A]:ALA:HB2	4:BBB:601:GOL:C3	2.15	0.76
1:CCC:90[B]:LYS:HG3	7:CCC:764:HOH:O	1.86	0.76
1:DDD:336[A]:ALA:HB2	4:DDD:601:GOL:H31	1.66	0.76
1:AAA:280[B]:ILE:HD11	1:BBB:280:ILE:HG12	1.66	0.76
1:BBB:445[A]:GLU:HG2	7:BBB:910:HOH:O	1.86	0.76
1:CCC:336[A]:ALA:HB2	4:CCC:617:GOL:C3	2.15	0.76
1:AAA:337[B]:LEU:HD13	7:AAA:950:HOH:O	1.86	0.75
1:DDD:429[A]:ILE:CD1	7:DDD:1023:HOH:O	2.32	0.75
1:AAA:280[B]:ILE:HD12	1:BBB:280:ILE:CG1	2.16	0.75
1:BBB:424[B]:GLN:NE2	1:BBB:425[B]:LYS:HZ3	1.77	0.74
1:CCC:445[A]:GLU:HG2	7:CCC:717:HOH:O	1.86	0.74
4:DDD:613:GOL:H2	7:DDD:1189:HOH:O	1.86	0.74
1:BBB:336[A]:ALA:HA	4:BBB:601:GOL:H11	1.70	0.73
1:AAA:516:LYS:HD3	4:AAA:616:GOL:H12	1.69	0.73
1:CCC:66:ASP:OD2	4:CCC:611:GOL:H32	1.88	0.73
1:BBB:520[B]:LYS:HG2	1:BBB:521:LEU:N	2.05	0.72
1:BBB:31[B]:VAL:HG23	1:BBB:143:SER:CA	2.21	0.71
4:CCC:614:GOL:H11	1:DDD:583:ASN:ND2	2.00	0.71
4:CCC:607:GOL:H11	7:CCC:756:HOH:O	1.89	0.70
1:AAA:277[B]:SER:OG	1:BBB:331:TRP:HA	1.91	0.70
1:AAA:66:ASP:HA	4:AAA:618:GOL:H2	1.72	0.70
4:CCC:612:GOL:H31	7:CCC:1003:HOH:O	1.91	0.70
1:BBB:31[B]:VAL:HG21	7:BBB:921:HOH:O	1.92	0.70
1:AAA:43:BYR:BR	7:AAA:1425:HOH:O	2.64	0.70
1:CCC:337[B]:LEU:HD22	1:DDD:373:PHE:HZ	1.55	0.69
1:AAA:336[A]:ALA:HB2	4:AAA:619:GOL:C1	2.23	0.69
1:DDD:336[A]:ALA:HA	4:DDD:601:GOL:H11	1.73	0.68
1:CCC:161[B]:ILE:HD12	1:CCC:165:TYR:CE2	2.29	0.68
1:DDD:296[B]:ASP:OD2	4:DDD:615:GOL:O2	2.11	0.67
1:BBB:296[B]:ASP:OD2	4:BBB:612:GOL:O2	2.10	0.67
1:CCC:43:BYR:BR	7:CCC:1417:HOH:O	2.67	0.67
4:AAA:621:GOL:H11	1:CCC:583:ASN:HB3	1.75	0.67
4:AAA:616:GOL:H32	7:AAA:1212:HOH:O	1.95	0.67
1:BBB:43:BYR:BR	7:BBB:1482:HOH:O	2.67	0.66
1:CCC:161[B]:ILE:CD1	1:CCC:165:TYR:CE2	2.78	0.66
1:AAA:336[A]:ALA:HB2	4:AAA:619:GOL:H11	1.77	0.66
1:BBB:31[B]:VAL:CG2	1:BBB:143:SER:HA	2.24	0.66
1:CCC:29:ARG:HE	6:CCC:618:144:H12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:174:GLU:HG3	4:BBB:617:GOL:H11	1.78	0.65
1:CCC:43:BYR:BR	7:CCC:1498:HOH:O	2.69	0.65
1:BBB:182:LYS:NZ	4:BBB:617:GOL:H12	2.13	0.64
1:CCC:337[B]:LEU:HD22	1:DDD:373:PHE:CZ	2.32	0.64
1:BBB:216:ARG:HH22	4:BBB:614:GOL:H12	1.63	0.64
4:DDD:607:GOL:H11	4:DDD:608:GOL:O3	1.98	0.64
1:BBB:31[B]:VAL:CG2	7:BBB:921:HOH:O	2.46	0.63
1:BBB:172:GLU:O	4:BBB:617:GOL:H2	1.99	0.63
1:DDD:298[B]:LYS:HE3	7:DDD:1325:HOH:O	1.98	0.63
1:DDD:336[A]:ALA:HB2	4:DDD:601:GOL:C3	2.29	0.63
1:CCC:68:ASN:HD22	4:CCC:611:GOL:C3	2.10	0.62
1:DDD:2:GLY:N	4:DDD:613:GOL:H11	2.15	0.62
1:CCC:336[A]:ALA:CA	4:CCC:617:GOL:H11	2.28	0.61
1:DDD:338[B]:TYR:C	1:DDD:338[B]:TYR:CD1	2.79	0.61
4:AAA:612:GOL:H12	7:AAA:892:HOH:O	2.02	0.60
4:CCC:612:GOL:H2	7:CCC:1295:HOH:O	2.03	0.59
1:DDD:338[B]:TYR:C	1:DDD:338[B]:TYR:HD1	2.10	0.59
1:BBB:424[B]:GLN:NE2	1:BBB:425[B]:LYS:HZ1	2.01	0.59
4:AAA:621:GOL:H11	1:CCC:583:ASN:ND2	2.17	0.58
1:BBB:516:LYS:HE3	7:BBB:1289:HOH:O	2.03	0.58
1:BBB:508[A]:ILE:HD13	1:BBB:535:GLU:HG3	1.88	0.56
1:BBB:76:ASP:OD2	4:BBB:615:GOL:H32	2.05	0.56
1:CCC:510[B]:GLN:NE2	1:CCC:523:LYS:HD3	2.21	0.55
1:AAA:102:ASP:HB2	1:AAA:109:ILE:HD11	1.89	0.55
7:BBB:1097:HOH:O	4:CCC:612:GOL:H32	2.07	0.55
1:CCC:453[B]:LYS:NZ	7:CCC:705:HOH:O	2.34	0.54
1:AAA:91:GLU:OE2	4:AAA:621:GOL:H12	2.07	0.54
1:CCC:29:ARG:HE	6:CCC:618:144:C1	2.20	0.54
4:AAA:616:GOL:C3	7:AAA:1212:HOH:O	2.54	0.54
1:AAA:275:TYR:CD2	1:AAA:280[B]:ILE:CD1	2.89	0.54
4:AAA:621:GOL:H11	1:CCC:583:ASN:CB	2.38	0.54
1:CCC:280:ILE:HG12	1:DDD:280[B]:ILE:HD11	1.88	0.54
1:DDD:70:ALA:HB3	4:DDD:612:GOL:H32	1.90	0.54
1:DDD:91:GLU:OE2	4:DDD:616:GOL:H12	2.08	0.54
1:AAA:182[B]:LYS:HE3	7:AAA:1238:HOH:O	2.09	0.53
1:AAA:337[B]:LEU:HD23	1:AAA:393:LEU:HD21	1.91	0.53
1:DDD:508[B]:ILE:HD12	1:DDD:535:GLU:HG3	1.89	0.53
4:AAA:619:GOL:H31	7:AAA:1241:HOH:O	2.07	0.53
1:BBB:495[B]:VAL:HG13	1:BBB:536:LEU:HB3	1.91	0.53
4:AAA:621:GOL:H31	1:CCC:583:ASN:HB3	1.90	0.53
1:DDD:534:GLY:HA3	4:DDD:607:GOL:C3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:336[A]:ALA:HB2	4:AAA:619:GOL:H12	1.90	0.53
4:AAA:603:GOL:C2	7:AAA:946:HOH:O	2.57	0.53
1:CCC:161[B]:ILE:HD12	1:CCC:165:TYR:CD2	2.44	0.53
1:AAA:508[A]:ILE:HD13	1:AAA:535:GLU:HG3	1.90	0.52
1:CCC:161[B]:ILE:HD12	1:CCC:165:TYR:HE2	1.71	0.52
1:BBB:336[A]:ALA:HB2	4:BBB:601:GOL:H32	1.92	0.51
1:CCC:66:ASP:OD2	4:CCC:611:GOL:C3	2.57	0.51
1:AAA:336[A]:ALA:CA	4:AAA:619:GOL:H32	2.39	0.51
1:DDD:275:TYR:CD2	1:DDD:280[B]:ILE:CD1	2.85	0.51
4:AAA:619:GOL:H2	7:AAA:1189:HOH:O	2.11	0.51
1:CCC:177:GLU:OE2	1:CCC:516:LYS:HG2	2.11	0.51
4:AAA:621:GOL:C1	1:CCC:583:ASN:HD22	2.17	0.50
1:BBB:31[B]:VAL:HG22	1:BBB:32:VAL:N	2.26	0.50
4:CCC:614:GOL:H2	7:CCC:764:HOH:O	2.09	0.50
4:AAA:603:GOL:H2	7:AAA:946:HOH:O	2.11	0.50
1:CCC:161[B]:ILE:CD1	1:CCC:165:TYR:CD2	2.95	0.49
1:AAA:337[B]:LEU:HD21	7:AAA:830:HOH:O	2.10	0.49
1:AAA:366:LYS:NZ	7:AAA:708:HOH:O	2.44	0.49
1:CCC:2:GLY:N	4:CCC:604:GOL:HO2	2.10	0.49
1:DDD:91:GLU:CD	4:DDD:616:GOL:H12	2.37	0.49
1:DDD:47[B]:ASP:OD2	1:DDD:49[B]:ASP:OD1	2.30	0.49
1:AAA:241:GLN:O	1:AAA:245[A]:VAL:HG22	2.13	0.48
1:DDD:112:SER:HB2	4:DDD:615:GOL:H2	1.94	0.48
4:AAA:612:GOL:H2	7:AAA:1274:HOH:O	2.13	0.48
1:DDD:241:GLN:O	1:DDD:245[A]:VAL:HG22	2.13	0.48
1:CCC:161[B]:ILE:CD1	1:CCC:165:TYR:HE2	2.22	0.47
1:AAA:51:THR:HB	1:CCC:506:ILE:CD1	2.44	0.47
1:CCC:452:ARG:O	1:CCC:456[B]:ILE:HG12	2.14	0.47
7:CCC:1155:HOH:O	4:DDD:619:GOL:H31	2.15	0.47
1:DDD:336[A]:ALA:CA	4:DDD:601:GOL:H11	2.43	0.47
1:CCC:508[A]:ILE:HD13	1:CCC:535:GLU:HG3	1.96	0.47
1:DDD:453[A]:LYS:HG3	7:DDD:1034:HOH:O	2.15	0.47
1:AAA:248:LYS:NZ	7:AAA:707:HOH:O	2.41	0.47
1:BBB:241:GLN:O	1:BBB:245[A]:VAL:HG22	2.15	0.47
1:CCC:162:ALA:HA	1:CCC:440[B]:LEU:HD21	1.97	0.47
1:AAA:82:ARG:NE	4:AAA:620:GOL:H12	2.30	0.46
1:BBB:182:LYS:HZ1	4:BBB:617:GOL:H12	1.78	0.46
1:CCC:241:GLN:O	1:CCC:245[A]:VAL:HG22	2.15	0.46
1:AAA:495[B]:VAL:HG13	1:AAA:536:LEU:HB3	1.96	0.46
1:CCC:245[B]:VAL:HG12	1:CCC:246:GLY:O	2.15	0.46
1:CCC:11:ARG:H	4:CCC:601:GOL:H32	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CCC:601:GOL:C1	7:CCC:955:HOH:O	2.62	0.46
1:DDD:47[B]:ASP:OD1	1:DDD:48:PRO:HD2	2.15	0.46
1:AAA:336[B]:ALA:O	1:AAA:337[B]:LEU:C	2.58	0.46
1:CCC:339:GLU:HG3	1:DDD:275:TYR:CZ	2.51	0.46
1:AAA:180[A]:SER:HB2	4:AAA:616:GOL:H11	1.97	0.46
6:CCC:618:144:H21	7:CCC:802:HOH:O	2.15	0.45
4:BBB:611:GOL:H11	7:BBB:905:HOH:O	2.15	0.45
1:BBB:182:LYS:HZ2	4:BBB:617:GOL:H12	1.81	0.45
1:DDD:91:GLU:OE1	4:DDD:616:GOL:H12	2.17	0.45
1:AAA:82:ARG:HE	4:AAA:620:GOL:H12	1.81	0.45
1:BBB:96:THR:HG21	4:BBB:615:GOL:H31	1.98	0.45
4:BBB:611:GOL:C2	7:BBB:1213:HOH:O	2.50	0.45
1:CCC:517:ASP:HB3	1:CCC:518[B]:GLU:OE1	2.17	0.45
1:AAA:94:ASP:OD2	1:DDD:90[A]:LYS:HE2	2.17	0.44
1:AAA:425[B]:LYS:HB3	1:AAA:425[B]:LYS:HE3	1.77	0.44
1:AAA:76:ASP:OD1	4:AAA:617:GOL:H2	2.17	0.44
4:BBB:611:GOL:C1	7:BBB:905:HOH:O	2.65	0.44
1:CCC:338[B]:TYR:C	1:CCC:338[B]:TYR:CD1	2.95	0.44
1:CCC:161[B]:ILE:HD11	1:CCC:165:TYR:CE2	2.53	0.44
4:DDD:605:GOL:H2	7:DDD:1232:HOH:O	2.16	0.44
1:AAA:425[A]:LYS:HE2	7:AAA:1360:HOH:O	2.18	0.43
1:AAA:180[B]:SER:OG	4:AAA:616:GOL:H11	2.18	0.43
1:CCC:337[B]:LEU:HD23	1:CCC:393:LEU:HD21	2.01	0.43
1:CCC:373:PHE:CZ	1:DDD:337[B]:LEU:HD22	2.53	0.43
1:AAA:305:ASP:O	1:AAA:306:ALA:HB3	2.18	0.43
1:BBB:456[B]:ILE:HD11	1:BBB:461:PRO:O	2.18	0.43
1:DDD:104:GLU:HB2	7:DDD:1015:HOH:O	2.17	0.43
1:AAA:180[A]:SER:OG	1:AAA:182[A]:LYS:HG2	2.19	0.43
1:CCC:305:ASP:O	1:CCC:306:ALA:HB3	2.19	0.43
1:AAA:91:GLU:CD	4:AAA:621:GOL:H12	2.44	0.43
1:CCC:29:ARG:HG2	6:CCC:618:144:H13	2.01	0.43
1:AAA:82:ARG:HH21	4:AAA:620:GOL:C1	2.32	0.43
1:AAA:275:TYR:HD2	1:AAA:280[B]:ILE:HD11	1.79	0.43
1:AAA:82:ARG:NH2	4:AAA:620:GOL:H12	2.34	0.42
4:BBB:601:GOL:H12	7:BBB:1265:HOH:O	2.18	0.42
1:BBB:456[B]:ILE:CD1	1:BBB:461:PRO:O	2.67	0.42
1:DDD:70:ALA:CB	4:DDD:612:GOL:H32	2.48	0.42
1:AAA:47[B]:ASP:HA	1:AAA:48:PRO:HD3	1.90	0.42
1:BBB:47:ASP:OD1	1:BBB:47:ASP:C	2.62	0.42
1:CCC:248:LYS:NZ	7:CCC:708:HOH:O	2.37	0.42
1:DDD:305:ASP:O	1:DDD:306:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:526:PHE:CZ	1:BBB:528[A]:GLY:HA3	2.54	0.42
1:AAA:82:ARG:HH21	4:AAA:620:GOL:H12	1.85	0.42
1:CCC:11:ARG:N	4:CCC:601:GOL:H32	2.34	0.42
1:DDD:47[A]:ASP:HA	1:DDD:48:PRO:HD3	1.88	0.42
1:BBB:336[B]:ALA:HB3	1:BBB:339:GLU:HB2	2.01	0.42
1:CCC:47:ASP:HA	1:CCC:48:PRO:HD3	1.88	0.42
1:CCC:235[B]:VAL:HG11	4:CCC:607:GOL:H31	2.01	0.42
1:CCC:63:LEU:O	1:CCC:65:HIS:CE1	2.74	0.41
1:CCC:515[B]:ASP:OD1	1:CCC:516:LYS:N	2.53	0.41
1:BBB:296[A]:ASP:CG	4:BBB:612:GOL:HO2	2.26	0.41
1:DDD:505:GLY:HA2	4:DDD:606:GOL:H31	2.02	0.41
1:DDD:483:TYR:HA	1:DDD:484:GLY:HA2	1.88	0.41
1:AAA:337[B]:LEU:CD2	1:AAA:393:LEU:HD21	2.50	0.41
1:BBB:127:ASN:HB3	1:BBB:130:ALA:HB2	2.03	0.41
1:AAA:127:ASN:HB3	1:AAA:130:ALA:HB2	2.03	0.41
1:BBB:62:GLY:HA2	1:BBB:306:ALA:HB2	2.02	0.41
1:AAA:112:SER:HB2	4:AAA:614:GOL:H2	2.03	0.41
1:AAA:337[B]:LEU:HD22	1:BBB:373:PHE:CZ	2.55	0.41
1:BBB:534:GLY:HA3	4:BBB:606:GOL:C3	2.51	0.41
1:DDD:62:GLY:HA2	1:DDD:306:ALA:HB2	2.03	0.41
1:AAA:515:ASP:OD1	1:AAA:522[A]:VAL:HG11	2.20	0.41
1:BBB:63:LEU:O	1:BBB:65:HIS:CE1	2.74	0.41
1:CCC:373:PHE:HZ	1:DDD:337[B]:LEU:HD22	1.86	0.41
1:AAA:63:LEU:O	1:AAA:65:HIS:CE1	2.74	0.41
1:AAA:321:LEU:O	1:AAA:322:ILE:C	2.64	0.41
1:CCC:275:TYR:CZ	1:DDD:339:GLU:HG3	2.56	0.41
1:BBB:216:ARG:NH2	4:BBB:614:GOL:H12	2.32	0.41
1:CCC:336[A]:ALA:HB2	4:CCC:617:GOL:H32	1.99	0.41
1:AAA:279:THR:C	1:AAA:280[B]:ILE:HD13	2.46	0.40
4:AAA:614:GOL:H12	7:AAA:862:HOH:O	2.20	0.40
1:BBB:424[B]:GLN:HG3	7:BBB:1195:HOH:O	2.21	0.40
1:AAA:334:PHE:O	1:BBB:276:GLY:HA2	2.21	0.40
1:BBB:216:ARG:HH22	4:BBB:614:GOL:C1	2.31	0.40
1:CCC:62:GLY:HA2	1:CCC:306:ALA:HB2	2.03	0.40
1:DDD:63:LEU:O	1:DDD:65:HIS:CE1	2.73	0.40
1:DDD:91:GLU:OE2	4:DDD:616:GOL:C3	2.70	0.40
1:AAA:173[B]:ILE:CD1	1:AAA:183:ASN:OD1	2.69	0.40
1:DDD:66:ASP:OD2	4:DDD:612:GOL:C3	2.69	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:1148:HOH:O	7:BBB:1361:HOH:O[3_565]	2.09	0.11

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	638/598 (107%)	627 (98%)	11 (2%)	0	100	100
1	BBB	637/598 (106%)	626 (98%)	11 (2%)	0	100	100
1	CCC	643/598 (108%)	634 (99%)	9 (1%)	0	100	100
1	DDD	635/598 (106%)	623 (98%)	12 (2%)	0	100	100
All	All	2553/2392 (107%)	2510 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	531/489 (109%)	520 (98%)	11 (2%)	47	33
1	BBB	530/489 (108%)	522 (98%)	8 (2%)	57	47
1	CCC	536/489 (110%)	533 (99%)	3 (1%)	78	75
1	DDD	528/489 (108%)	520 (98%)	8 (2%)	57	47
All	All	2125/1956 (109%)	2095 (99%)	30 (1%)	65	50

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	180[A]	SER
1	AAA	180[B]	SER
1	AAA	338[A]	TYR
1	AAA	338[B]	TYR
1	AAA	370	GLN
1	AAA	374[A]	VAL
1	AAA	374[B]	VAL
1	AAA	397	TRP
1	AAA	479	PHE
1	AAA	543[A]	ILE
1	AAA	543[B]	ILE
1	BBB	172	GLU
1	BBB	338[A]	TYR
1	BBB	338[B]	TYR
1	BBB	370	GLN
1	BBB	397	TRP
1	BBB	479	PHE
1	BBB	527[A]	LYS
1	BBB	527[B]	LYS
1	CCC	370	GLN
1	CCC	397	TRP
1	CCC	479	PHE
1	DDD	172	GLU
1	DDD	180[A]	SER
1	DDD	180[B]	SER
1	DDD	338[A]	TYR
1	DDD	338[B]	TYR
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 ⓘ

There are no RNA molecules in this entry.

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

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	AAA	186	1	12,13,14	0.65	0	12,17,19	1.76	1 (8%)
1	BYR	CCC	43	1	12,13,14	0.87	0	12,17,19	1.31	2 (16%)
1	BYR	CCC	186	1	12,13,14	0.95	0	12,17,19	1.62	1 (8%)
1	BYR	BBB	43	1	12,13,14	1.20	1 (8%)	12,17,19	1.81	3 (25%)
1	BYR	DDD	186	1	12,13,14	0.62	0	12,17,19	1.36	1 (8%)
1	BYR	DDD	43	1	12,13,14	0.85	0	12,17,19	1.48	2 (16%)
1	BYR	BBB	186	1	12,13,14	0.72	0	12,17,19	1.40	1 (8%)
1	BYR	AAA	43	1	12,13,14	0.95	1 (8%)	12,17,19	1.32	2 (16%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	43	BYR	CD1-CE1	2.38	1.42	1.38
1	AAA	43	BYR	CD1-CE1	2.13	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	186	BYR	BR-CE2-CZ	4.85	123.10	119.38
1	CCC	186	BYR	BR-CE2-CZ	4.79	123.05	119.38
1	DDD	186	BYR	BR-CE2-CZ	4.08	122.51	119.38
1	BBB	186	BYR	BR-CE2-CZ	3.96	122.41	119.38
1	BBB	43	BYR	CD1-CE1-CZ	-3.28	117.22	120.50
1	BBB	43	BYR	CE1-CZ-CE2	3.10	120.41	118.07
1	DDD	43	BYR	CD1-CE1-CZ	-2.88	117.61	120.50
1	DDD	43	BYR	CD2-CE2-CZ	2.60	122.94	120.95
1	BBB	43	BYR	CD2-CE2-CZ	2.50	122.86	120.95
1	AAA	43	BYR	CD1-CE1-CZ	-2.38	118.12	120.50
1	CCC	43	BYR	CD2-CE2-CZ	2.28	122.69	120.95
1	CCC	43	BYR	CD1-CE1-CZ	-2.27	118.22	120.50
1	AAA	43	BYR	CD2-CE2-CZ	2.22	122.64	120.95

There are no chirality outliers.

All (2) 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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 87 ligands modelled in this entry, 14 are monoatomic - leaving 73 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
4	GOL	AAA	617	-	5,5,5	0.10	0	5,5,5	0.24	0
4	GOL	AAA	616	-	5,5,5	0.10	0	5,5,5	0.42	0
4	GOL	AAA	615	-	5,5,5	0.18	0	5,5,5	0.34	0
2	PO4	AAA	608	-	4,4,4	1.71	1 (25%)	6,6,6	0.57	0
2	PO4	DDD	603	-	4,4,4	1.91	2 (50%)	6,6,6	0.79	0
4	GOL	DDD	611	-	5,5,5	0.18	0	5,5,5	0.29	0
2	PO4	BBB	602	-	4,4,4	1.20	0	6,6,6	0.84	0
4	GOL	DDD	605	-	5,5,5	0.15	0	5,5,5	0.62	0
4	GOL	CCC	601	-	5,5,5	0.25	0	5,5,5	0.48	0
4	GOL	AAA	612	-	5,5,5	0.21	0	5,5,5	0.49	0
4	GOL	DDD	602	-	5,5,5	0.17	0	5,5,5	0.51	0
4	GOL	DDD	615	-	5,5,5	0.17	0	5,5,5	0.42	0
6	144	CCC	618	-	1,7,7	0.24	0	3,9,9	2.67	2 (66%)
2	PO4	BBB	607	-	4,4,4	0.63	0	6,6,6	0.65	0
4	GOL	AAA	603	-	5,5,5	0.14	0	5,5,5	0.63	0
4	GOL	BBB	614	-	5,5,5	0.22	0	5,5,5	0.53	0
4	GOL	CCC	613	-	5,5,5	0.19	0	5,5,5	0.53	0
4	GOL	AAA	605	-	5,5,5	0.19	0	5,5,5	0.60	0
4	GOL	BBB	615	-	5,5,5	0.18	0	5,5,5	0.36	0
4	GOL	DDD	608	-	5,5,5	0.15	0	5,5,5	0.47	0
4	GOL	BBB	605	-	5,5,5	0.11	0	5,5,5	0.34	0
2	PO4	CCC	602	-	4,4,4	1.45	1 (25%)	6,6,6	0.81	0
4	GOL	BBB	601	5	5,5,5	0.15	0	5,5,5	0.31	0
4	GOL	DDD	616	-	5,5,5	0.48	0	5,5,5	0.83	0
4	GOL	DDD	617	-	5,5,5	0.24	0	5,5,5	0.40	0
4	GOL	DDD	612	-	5,5,5	0.18	0	5,5,5	0.37	0
4	GOL	DDD	601	-	5,5,5	0.25	0	5,5,5	0.67	0
4	GOL	DDD	606	5	5,5,5	0.53	0	5,5,5	0.66	0
4	GOL	AAA	606	-	5,5,5	0.10	0	5,5,5	0.41	0
4	GOL	BBB	604	5	5,5,5	0.47	0	5,5,5	0.71	0
4	GOL	BBB	609	-	5,5,5	0.23	0	5,5,5	0.58	0
4	GOL	AAA	620	-	5,5,5	0.11	0	5,5,5	0.43	0
4	GOL	BBB	618	-	5,5,5	0.10	0	5,5,5	0.42	0
4	GOL	CCC	605	5	5,5,5	0.39	0	5,5,5	0.60	0
4	GOL	BBB	612	-	5,5,5	0.22	0	5,5,5	0.41	0
4	GOL	DDD	619	-	5,5,5	0.20	0	5,5,5	0.39	0
4	GOL	DDD	618	-	5,5,5	0.13	0	5,5,5	0.38	0
4	GOL	AAA	610	-	5,5,5	0.16	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	AAA	601	-	4,4,4	0.94	0	6,6,6	0.75	0
4	GOL	BBB	617	-	5,5,5	0.17	0	5,5,5	0.69	0
4	GOL	BBB	611	-	5,5,5	0.22	0	5,5,5	0.57	0
4	GOL	CCC	609	-	5,5,5	0.34	0	5,5,5	0.54	0
4	GOL	AAA	614	-	5,5,5	0.22	0	5,5,5	0.63	0
4	GOL	CCC	616	-	5,5,5	0.24	0	5,5,5	0.48	0
4	GOL	CCC	617	5	5,5,5	0.18	0	5,5,5	0.51	0
4	GOL	AAA	621	-	5,5,5	0.52	0	5,5,5	1.08	0
2	PO4	DDD	609	-	4,4,4	1.12	0	6,6,6	0.81	0
4	GOL	CCC	615	-	5,5,5	0.15	0	5,5,5	0.36	0
4	GOL	DDD	610	-	5,5,5	0.22	0	5,5,5	0.55	0
4	GOL	AAA	604	5	5,5,5	0.46	0	5,5,5	0.54	0
4	GOL	BBB	606	-	5,5,5	0.24	0	5,5,5	0.50	0
4	GOL	CCC	607	-	5,5,5	0.15	0	5,5,5	0.47	0
4	GOL	AAA	618	-	5,5,5	0.23	0	5,5,5	0.43	0
2	PO4	CCC	608	-	4,4,4	1.23	0	6,6,6	0.86	0
4	GOL	AAA	613	-	5,5,5	0.33	0	5,5,5	0.56	0
4	GOL	BBB	608	-	5,5,5	0.30	0	5,5,5	0.47	0
4	GOL	BBB	610	-	5,5,5	0.24	0	5,5,5	0.71	0
4	GOL	CCC	614	-	5,5,5	0.41	0	5,5,5	1.11	0
4	GOL	DDD	607	-	5,5,5	0.16	0	5,5,5	0.36	0
4	GOL	DDD	614	-	5,5,5	0.29	0	5,5,5	0.74	0
4	GOL	CCC	604	-	5,5,5	0.15	0	5,5,5	0.45	0
4	GOL	AAA	609	-	5,5,5	0.40	0	5,5,5	0.63	0
4	GOL	CCC	612	-	5,5,5	0.18	0	5,5,5	0.48	0
4	GOL	AAA	619	5	5,5,5	0.14	0	5,5,5	0.35	0
4	GOL	BBB	616	-	5,5,5	0.19	0	5,5,5	0.47	0
4	GOL	CCC	611	-	5,5,5	0.24	0	5,5,5	0.44	0
4	GOL	AAA	611	-	5,5,5	0.23	0	5,5,5	0.52	0
4	GOL	BBB	613	-	5,5,5	0.26	0	5,5,5	0.94	0
2	PO4	DDD	623	-	4,4,4	1.19	1 (25%)	6,6,6	0.39	0
4	GOL	DDD	613	-	5,5,5	0.13	0	5,5,5	0.40	0
2	PO4	AAA	607	-	4,4,4	1.77	1 (25%)	6,6,6	0.74	0
4	GOL	CCC	606	-	5,5,5	0.24	0	5,5,5	0.90	0
4	GOL	CCC	610	-	5,5,5	0.14	0	5,5,5	0.44	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
4	GOL	AAA	617	-	-	4/4/4/4	-
4	GOL	AAA	616	-	-	3/4/4/4	-
4	GOL	AAA	615	-	-	2/4/4/4	-
4	GOL	DDD	611	-	-	0/4/4/4	-
4	GOL	DDD	605	-	-	2/4/4/4	-
4	GOL	CCC	601	-	-	4/4/4/4	-
4	GOL	AAA	612	-	-	2/4/4/4	-
4	GOL	DDD	602	-	-	0/4/4/4	-
4	GOL	DDD	615	-	-	4/4/4/4	-
6	144	CCC	618	-	-	0/0/9/9	-
4	GOL	AAA	603	-	-	4/4/4/4	-
4	GOL	BBB	614	-	-	4/4/4/4	-
4	GOL	CCC	613	-	-	1/4/4/4	-
4	GOL	AAA	605	-	-	2/4/4/4	-
4	GOL	BBB	615	-	-	2/4/4/4	-
4	GOL	DDD	608	-	-	1/4/4/4	-
4	GOL	BBB	605	-	-	2/4/4/4	-
4	GOL	BBB	601	5	-	2/4/4/4	-
4	GOL	DDD	616	-	-	4/4/4/4	-
4	GOL	DDD	617	-	-	1/4/4/4	-
4	GOL	DDD	612	-	-	2/4/4/4	-
4	GOL	DDD	601	-	-	2/4/4/4	-
4	GOL	DDD	606	5	-	0/4/4/4	-
4	GOL	AAA	606	-	-	2/4/4/4	-
4	GOL	BBB	604	5	-	0/4/4/4	-
4	GOL	BBB	609	-	-	0/4/4/4	-
4	GOL	AAA	620	-	-	2/4/4/4	-
4	GOL	BBB	618	-	-	3/4/4/4	-
4	GOL	CCC	605	5	-	0/4/4/4	-
4	GOL	BBB	612	-	-	2/4/4/4	-
4	GOL	DDD	619	-	-	2/4/4/4	-
4	GOL	DDD	618	-	-	4/4/4/4	-
4	GOL	AAA	610	-	-	0/4/4/4	-
4	GOL	CCC	609	-	-	0/4/4/4	-
4	GOL	BBB	617	-	-	2/4/4/4	-
4	GOL	BBB	611	-	-	4/4/4/4	-
4	GOL	CCC	616	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	AAA	614	-	-	4/4/4/4	-
4	GOL	CCC	617	5	-	2/4/4/4	-
4	GOL	AAA	621	-	-	4/4/4/4	-
4	GOL	CCC	615	-	-	2/4/4/4	-
4	GOL	DDD	610	-	-	0/4/4/4	-
4	GOL	AAA	604	5	-	0/4/4/4	-
4	GOL	BBB	606	-	-	4/4/4/4	-
4	GOL	CCC	607	-	-	2/4/4/4	-
4	GOL	AAA	618	-	-	3/4/4/4	-
4	GOL	AAA	613	-	-	4/4/4/4	-
4	GOL	BBB	608	-	-	0/4/4/4	-
4	GOL	BBB	610	-	-	3/4/4/4	-
4	GOL	CCC	614	-	-	2/4/4/4	-
4	GOL	DDD	607	-	-	4/4/4/4	-
4	GOL	DDD	614	-	-	3/4/4/4	-
4	GOL	CCC	604	-	-	2/4/4/4	-
4	GOL	AAA	609	-	-	0/4/4/4	-
4	GOL	CCC	612	-	-	2/4/4/4	-
4	GOL	AAA	619	5	-	2/4/4/4	-
4	GOL	BBB	616	-	-	0/4/4/4	-
4	GOL	CCC	611	-	-	0/4/4/4	-
4	GOL	AAA	611	-	-	3/4/4/4	-
4	GOL	BBB	613	-	-	4/4/4/4	-
4	GOL	DDD	613	-	-	2/4/4/4	-
4	GOL	CCC	606	-	-	3/4/4/4	-
4	GOL	CCC	610	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	608	PO4	P-O1	3.11	1.57	1.50
2	DDD	603	PO4	P-O1	3.04	1.57	1.50
2	AAA	607	PO4	P-O1	2.92	1.57	1.50
2	DDD	603	PO4	P-O2	-2.31	1.47	1.54
2	CCC	602	PO4	P-O1	2.30	1.56	1.50
2	DDD	623	PO4	P-O1	2.16	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	CCC	618	144	C1-N-C4	-3.69	99.89	109.30
6	CCC	618	144	C1-N-C3	2.11	114.69	109.30

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	603	GOL	O1-C1-C2-O2
4	AAA	603	GOL	O1-C1-C2-C3
4	AAA	603	GOL	C1-C2-C3-O3
4	AAA	605	GOL	O1-C1-C2-C3
4	AAA	611	GOL	C1-C2-C3-O3
4	AAA	613	GOL	O1-C1-C2-C3
4	AAA	614	GOL	O1-C1-C2-C3
4	AAA	614	GOL	C1-C2-C3-O3
4	AAA	615	GOL	O1-C1-C2-C3
4	AAA	616	GOL	O1-C1-C2-C3
4	AAA	617	GOL	O1-C1-C2-C3
4	AAA	617	GOL	C1-C2-C3-O3
4	AAA	618	GOL	O1-C1-C2-C3
4	AAA	619	GOL	C1-C2-C3-O3
4	AAA	620	GOL	O1-C1-C2-O2
4	AAA	620	GOL	O1-C1-C2-C3
4	AAA	621	GOL	O1-C1-C2-O2
4	AAA	621	GOL	O1-C1-C2-C3
4	AAA	621	GOL	C1-C2-C3-O3
4	AAA	621	GOL	O2-C2-C3-O3
4	BBB	601	GOL	O1-C1-C2-O2
4	BBB	601	GOL	O1-C1-C2-C3
4	BBB	610	GOL	O1-C1-C2-O2
4	BBB	610	GOL	O1-C1-C2-C3
4	BBB	611	GOL	O1-C1-C2-C3
4	BBB	611	GOL	C1-C2-C3-O3
4	BBB	612	GOL	O1-C1-C2-O2
4	BBB	612	GOL	O1-C1-C2-C3
4	BBB	614	GOL	O1-C1-C2-C3
4	BBB	615	GOL	O1-C1-C2-C3
4	BBB	618	GOL	C1-C2-C3-O3
4	CCC	601	GOL	O1-C1-C2-O2
4	CCC	601	GOL	O1-C1-C2-C3
4	CCC	601	GOL	C1-C2-C3-O3
4	CCC	604	GOL	C1-C2-C3-O3
4	CCC	604	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	CCC	606	GOL	C1-C2-C3-O3
4	CCC	614	GOL	C1-C2-C3-O3
4	CCC	615	GOL	C1-C2-C3-O3
4	CCC	617	GOL	O1-C1-C2-C3
4	DDD	601	GOL	O1-C1-C2-C3
4	DDD	605	GOL	O1-C1-C2-C3
4	DDD	607	GOL	C1-C2-C3-O3
4	DDD	612	GOL	O1-C1-C2-C3
4	DDD	613	GOL	O1-C1-C2-C3
4	DDD	616	GOL	C1-C2-C3-O3
4	DDD	618	GOL	O1-C1-C2-C3
4	DDD	618	GOL	C1-C2-C3-O3
4	DDD	619	GOL	O1-C1-C2-C3
4	AAA	611	GOL	O2-C2-C3-O3
4	AAA	614	GOL	O1-C1-C2-O2
4	AAA	618	GOL	O1-C1-C2-O2
4	BBB	611	GOL	O1-C1-C2-O2
4	BBB	611	GOL	O2-C2-C3-O3
4	CCC	617	GOL	O1-C1-C2-O2
4	DDD	601	GOL	O1-C1-C2-O2
4	DDD	618	GOL	O2-C2-C3-O3
4	AAA	606	GOL	O1-C1-C2-C3
4	AAA	611	GOL	O1-C1-C2-C3
4	AAA	612	GOL	O1-C1-C2-C3
4	AAA	613	GOL	C1-C2-C3-O3
4	BBB	605	GOL	C1-C2-C3-O3
4	BBB	606	GOL	O1-C1-C2-C3
4	BBB	606	GOL	C1-C2-C3-O3
4	BBB	613	GOL	O1-C1-C2-C3
4	BBB	613	GOL	C1-C2-C3-O3
4	BBB	614	GOL	C1-C2-C3-O3
4	BBB	617	GOL	O1-C1-C2-C3
4	CCC	606	GOL	O1-C1-C2-C3
4	CCC	607	GOL	O1-C1-C2-C3
4	CCC	612	GOL	C1-C2-C3-O3
4	DDD	607	GOL	O1-C1-C2-C3
4	DDD	614	GOL	O1-C1-C2-C3
4	DDD	614	GOL	C1-C2-C3-O3
4	DDD	615	GOL	O1-C1-C2-C3
4	DDD	615	GOL	C1-C2-C3-O3
4	DDD	616	GOL	O1-C1-C2-C3
4	AAA	605	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	AAA	606	GOL	O1-C1-C2-O2
4	AAA	613	GOL	O1-C1-C2-O2
4	AAA	614	GOL	O2-C2-C3-O3
4	AAA	615	GOL	O1-C1-C2-O2
4	AAA	616	GOL	O1-C1-C2-O2
4	AAA	617	GOL	O2-C2-C3-O3
4	AAA	619	GOL	O2-C2-C3-O3
4	BBB	606	GOL	O2-C2-C3-O3
4	BBB	613	GOL	O1-C1-C2-O2
4	BBB	613	GOL	O2-C2-C3-O3
4	BBB	614	GOL	O1-C1-C2-O2
4	BBB	615	GOL	O1-C1-C2-O2
4	CCC	601	GOL	O2-C2-C3-O3
4	CCC	607	GOL	O1-C1-C2-O2
4	CCC	612	GOL	O2-C2-C3-O3
4	CCC	614	GOL	O2-C2-C3-O3
4	CCC	615	GOL	O2-C2-C3-O3
4	DDD	612	GOL	O1-C1-C2-O2
4	DDD	615	GOL	O1-C1-C2-O2
4	DDD	616	GOL	O1-C1-C2-O2
4	AAA	603	GOL	O2-C2-C3-O3
4	AAA	613	GOL	O2-C2-C3-O3
4	AAA	617	GOL	O1-C1-C2-O2
4	BBB	606	GOL	O1-C1-C2-O2
4	DDD	605	GOL	O1-C1-C2-O2
4	DDD	607	GOL	O2-C2-C3-O3
4	DDD	613	GOL	O1-C1-C2-O2
4	DDD	614	GOL	O1-C1-C2-O2
4	DDD	619	GOL	O1-C1-C2-O2
4	BBB	618	GOL	O2-C2-C3-O3
4	DDD	616	GOL	O2-C2-C3-O3
4	DDD	617	GOL	O1-C1-C2-O2
4	CCC	606	GOL	O2-C2-C3-O3
4	CCC	616	GOL	O2-C2-C3-O3
4	AAA	618	GOL	C1-C2-C3-O3
4	DDD	608	GOL	O1-C1-C2-C3
4	DDD	618	GOL	O1-C1-C2-O2
4	BBB	614	GOL	O2-C2-C3-O3
4	DDD	615	GOL	O2-C2-C3-O3
4	BBB	610	GOL	C1-C2-C3-O3
4	AAA	616	GOL	O2-C2-C3-O3
4	BBB	617	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	BBB	618	GOL	O1-C1-C2-C3
4	AAA	612	GOL	O1-C1-C2-O2
4	BBB	605	GOL	O2-C2-C3-O3
4	CCC	613	GOL	O2-C2-C3-O3
4	DDD	607	GOL	O1-C1-C2-O2

There are no ring outliers.

34 monomers are involved in 105 short contacts:

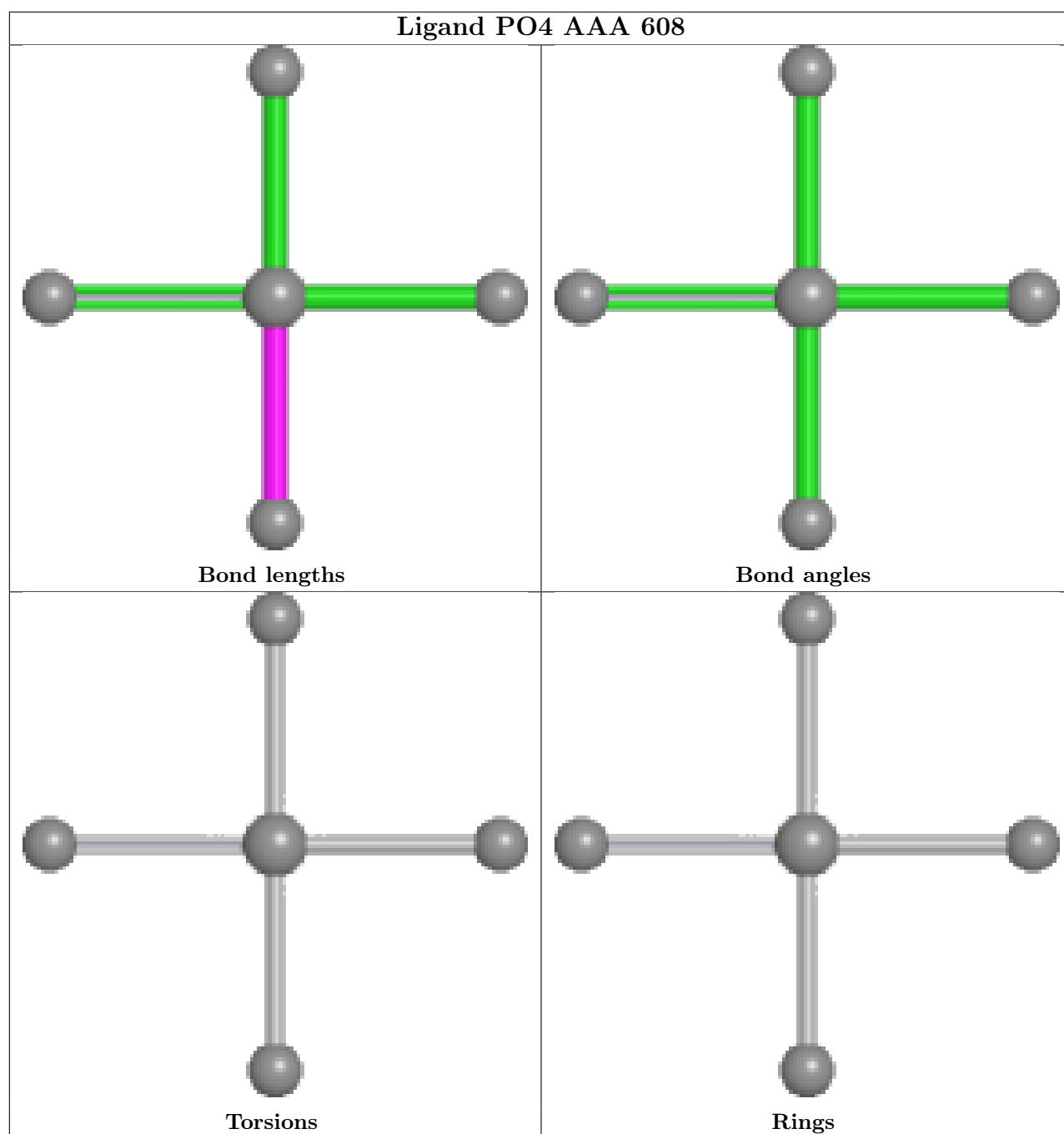
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	617	GOL	1	0
4	AAA	616	GOL	5	0
4	DDD	605	GOL	2	0
4	CCC	601	GOL	3	0
4	AAA	612	GOL	2	0
4	DDD	615	GOL	2	0
6	CCC	618	144	5	0
4	AAA	603	GOL	2	0
4	BBB	614	GOL	3	0
4	BBB	615	GOL	2	0
4	DDD	608	GOL	1	0
4	BBB	601	GOL	5	0
4	DDD	616	GOL	4	0
4	DDD	612	GOL	3	0
4	DDD	601	GOL	4	0
4	DDD	606	GOL	1	0
4	AAA	620	GOL	5	0
4	BBB	612	GOL	2	0
4	DDD	619	GOL	1	0
4	BBB	617	GOL	5	0
4	BBB	611	GOL	4	0
4	AAA	614	GOL	2	0
4	CCC	617	GOL	5	0
4	AAA	621	GOL	10	0
4	BBB	606	GOL	1	0
4	CCC	607	GOL	2	0
4	AAA	618	GOL	1	0
4	CCC	614	GOL	3	0
4	DDD	607	GOL	2	0
4	CCC	604	GOL	1	0
4	CCC	612	GOL	3	0
4	AAA	619	GOL	7	0

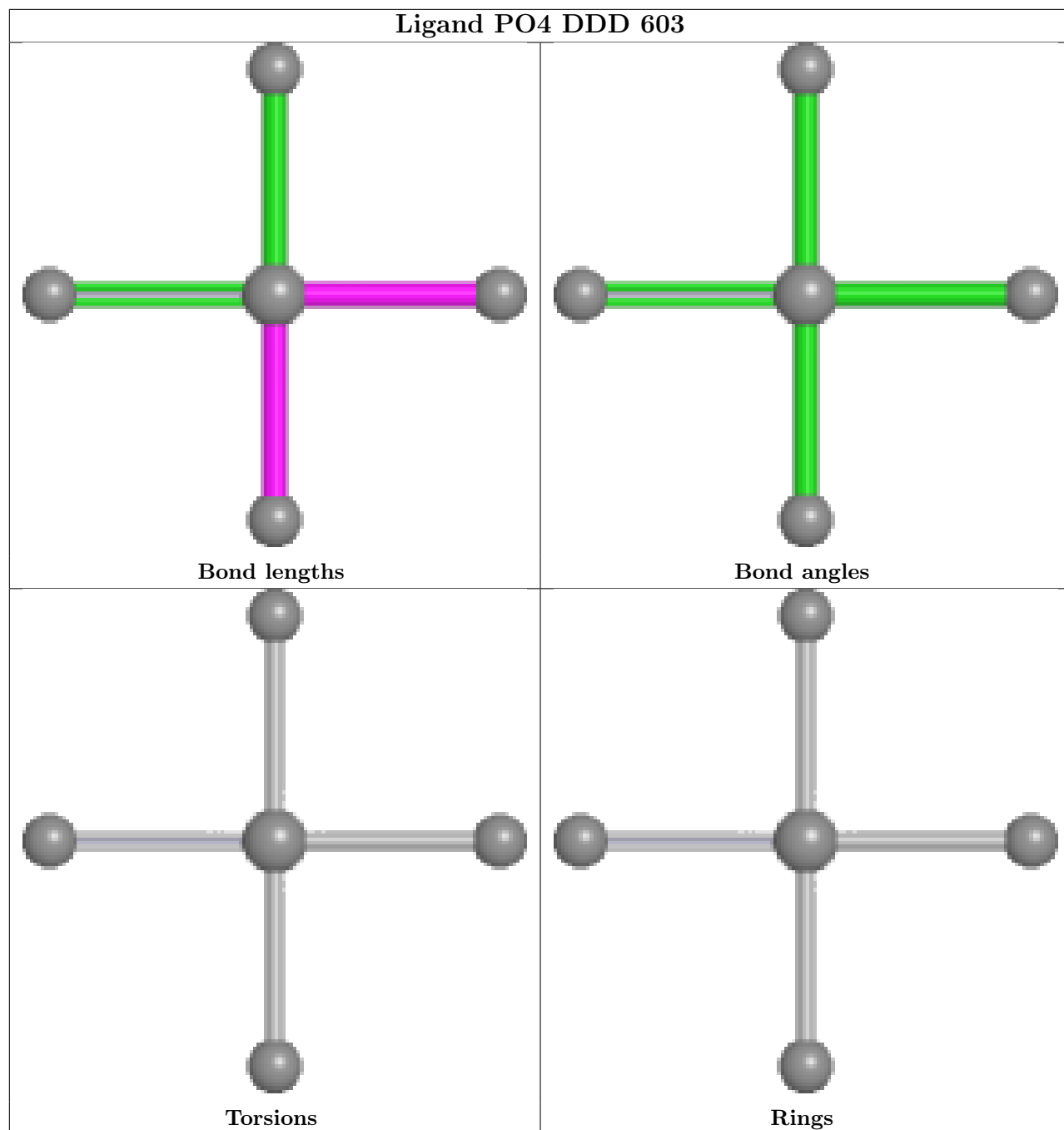
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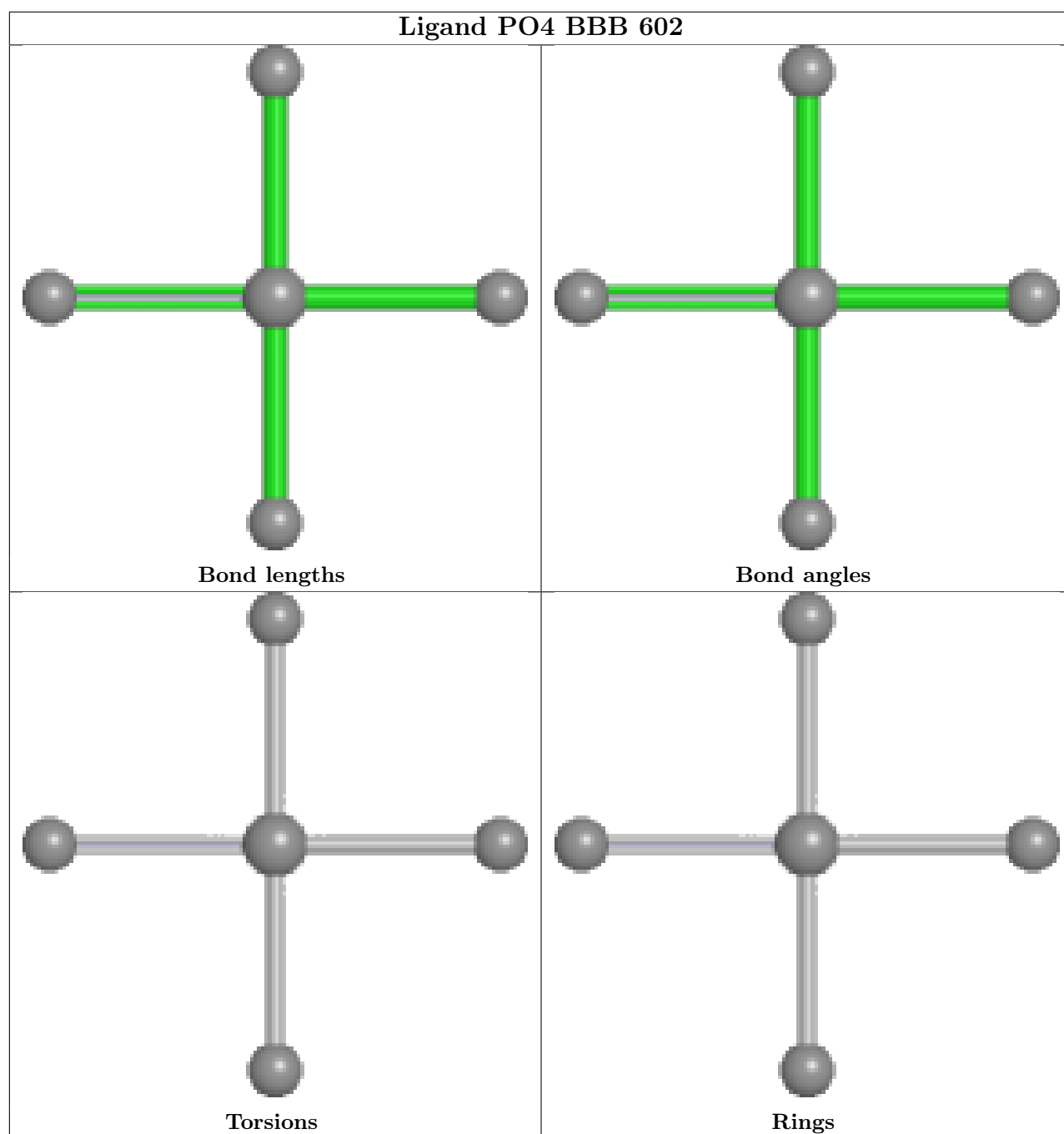
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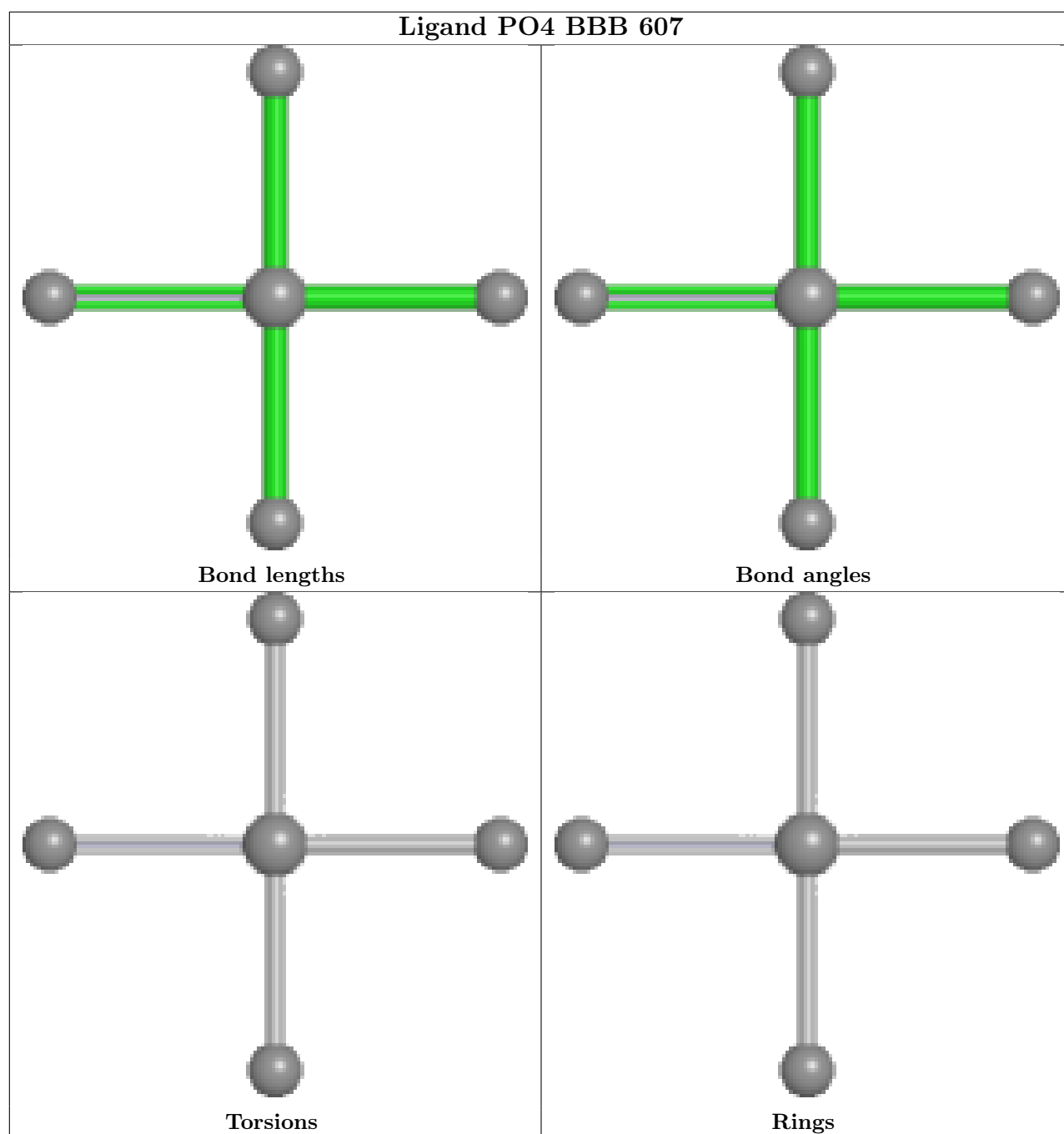
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	611	GOL	5	0
4	DDD	613	GOL	2	0

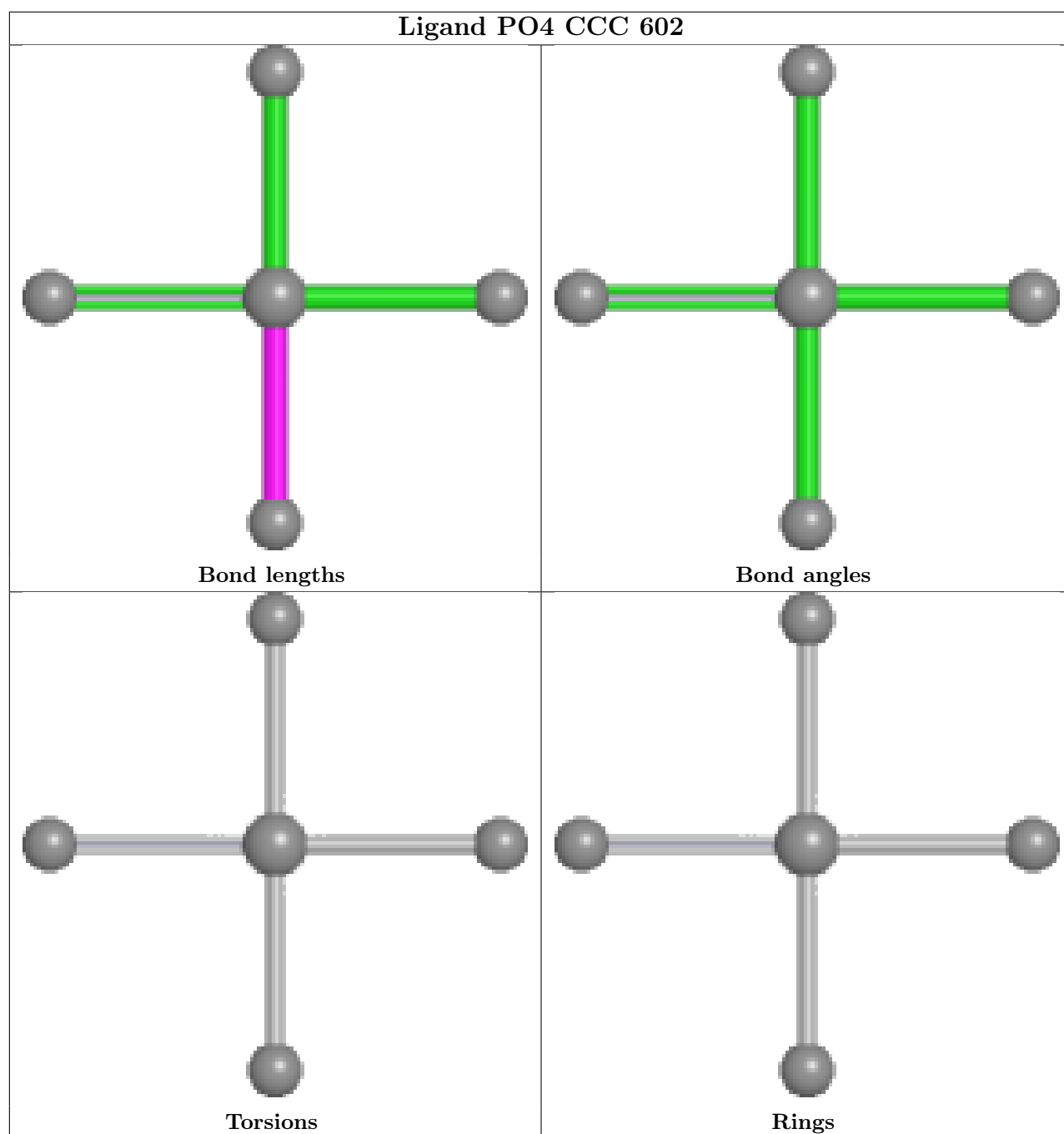
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

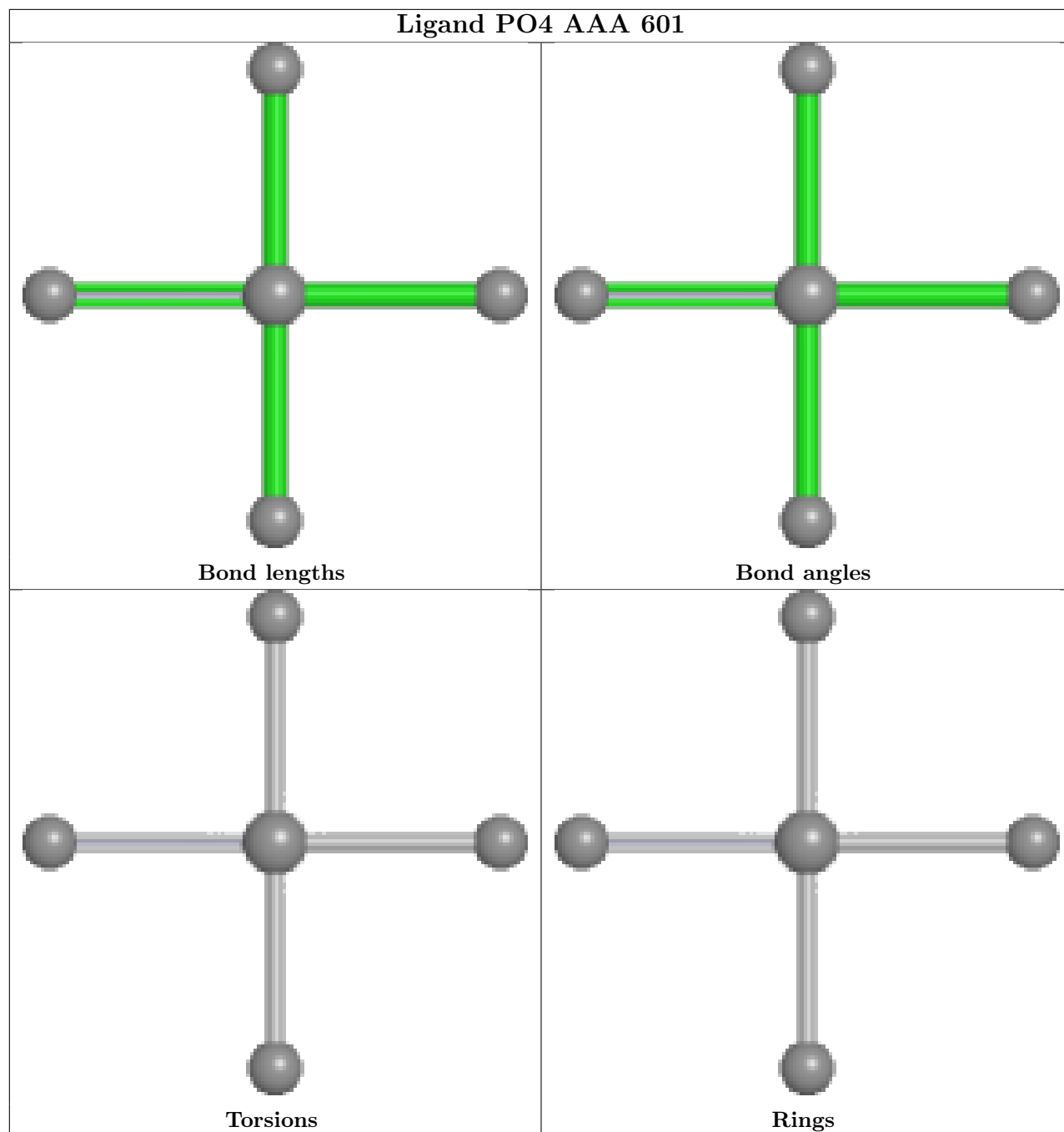


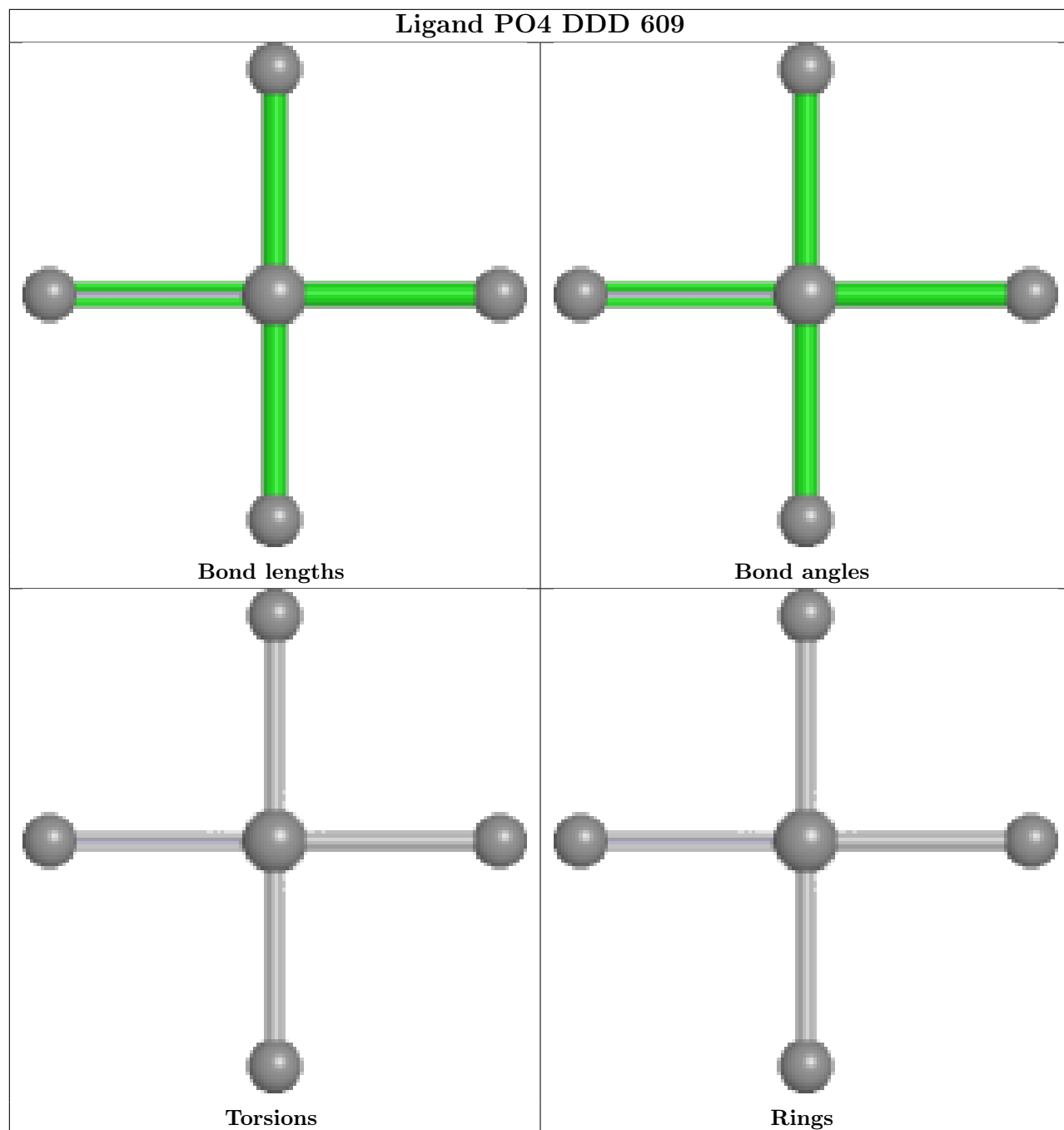


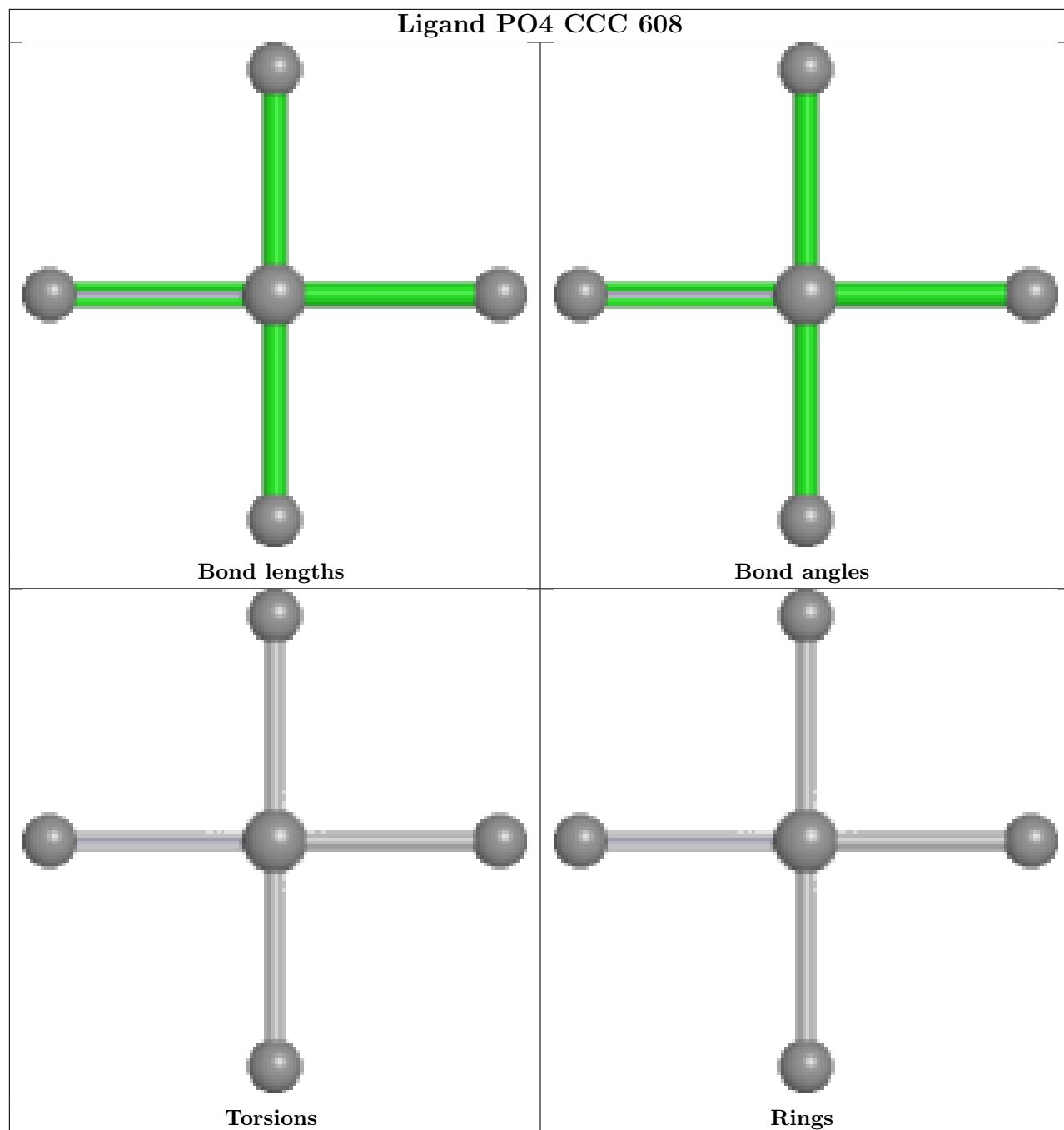


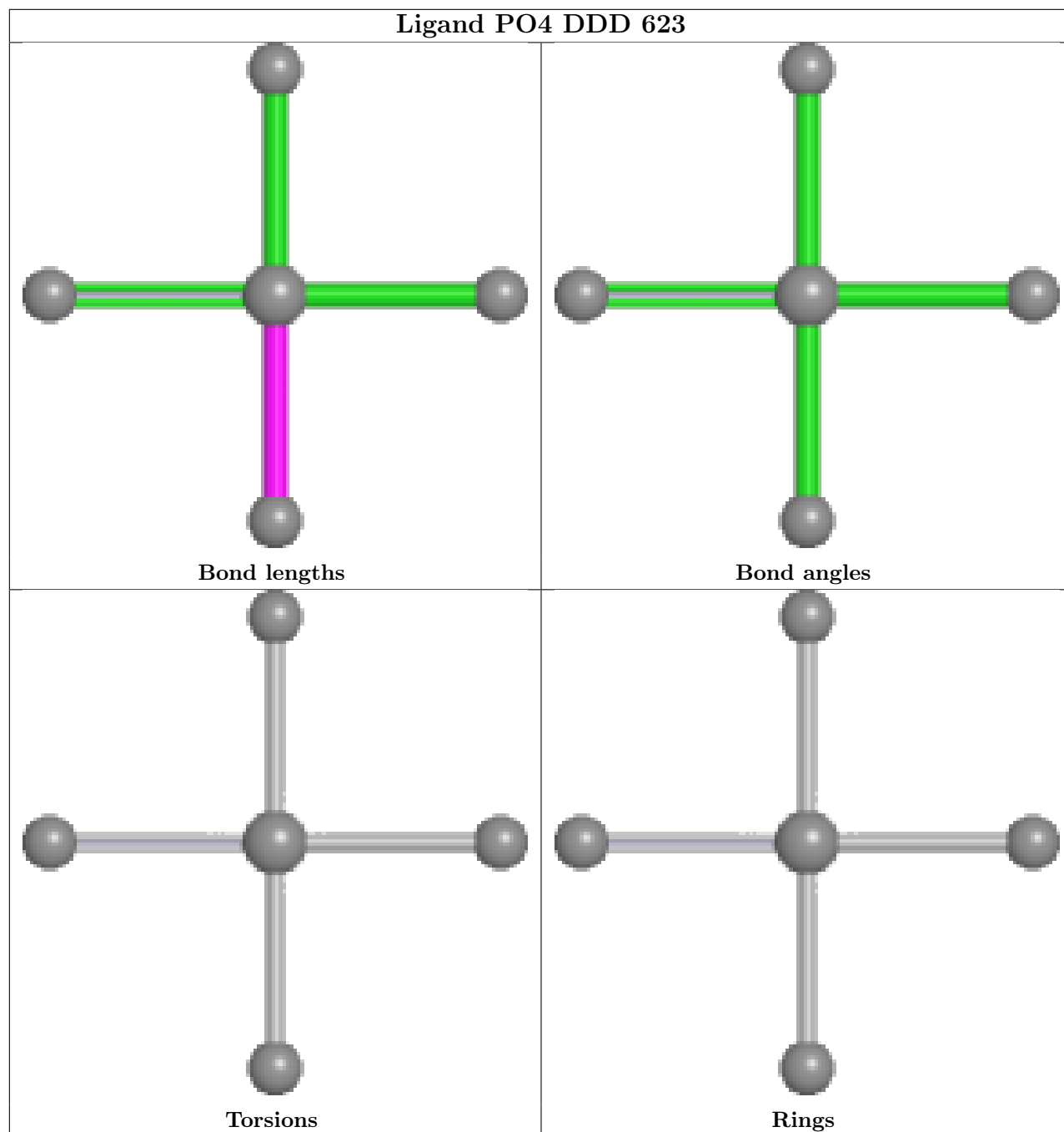


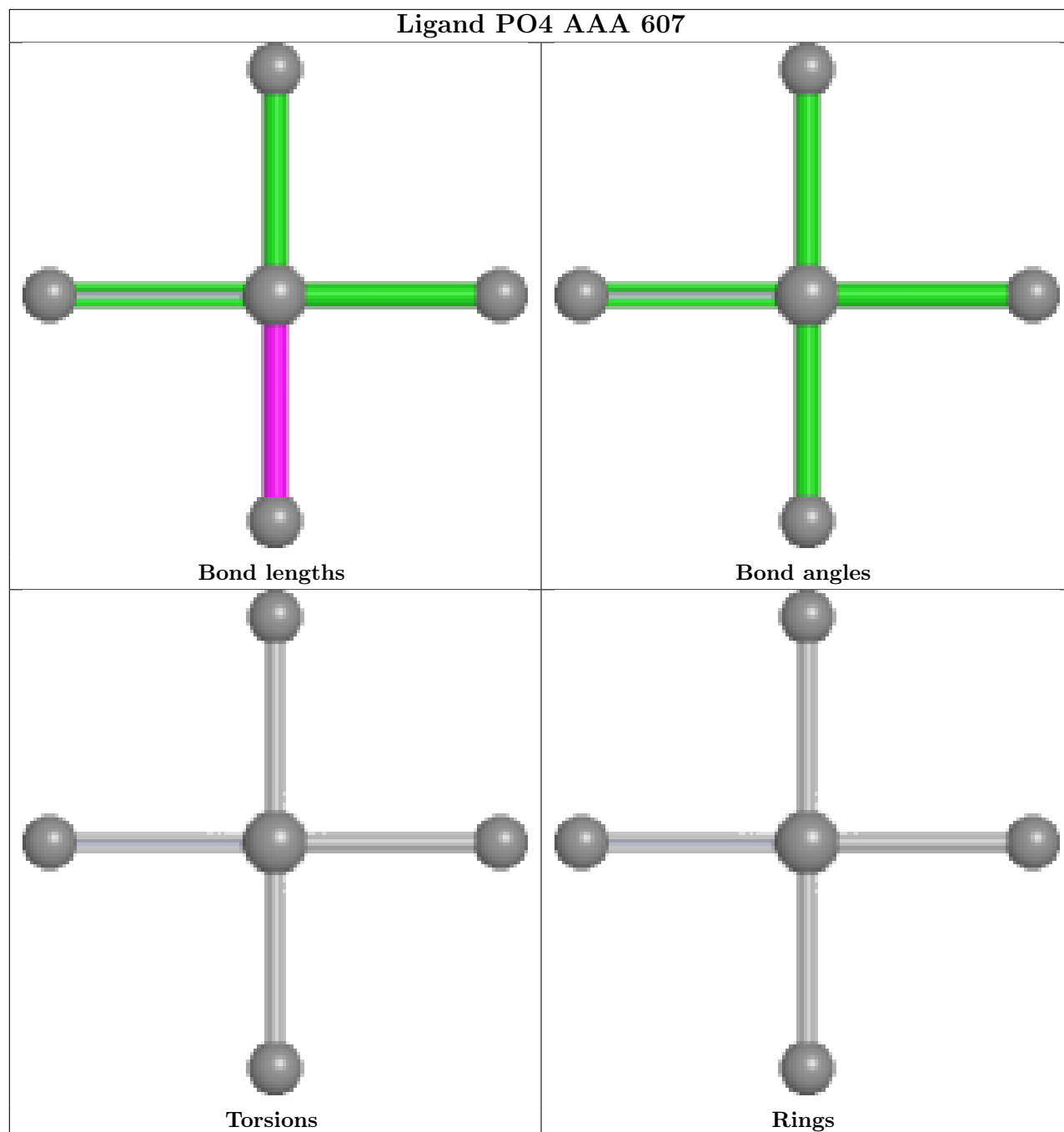












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	595/598 (99%)	-0.49	5 (0%) 82 88	12, 26, 39, 91	44 (7%)
1	BBB	595/598 (99%)	-0.50	3 (0%) 87 91	11, 26, 39, 86	44 (7%)
1	CCC	595/598 (99%)	-0.57	4 (0%) 84 88	8, 24, 36, 106	50 (8%)
1	DDD	595/598 (99%)	-0.51	2 (0%) 90 93	10, 26, 40, 98	42 (7%)
All	All	2380/2392 (99%)	-0.52	14 (0%) 85 89	8, 26, 39, 106	180 (7%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	48	PRO	5.1
1	CCC	48	PRO	4.3
1	CCC	527[A]	LYS	4.0
1	DDD	527[A]	LYS	3.0
1	AAA	527[A]	LYS	2.9
1	CCC	49[A]	ASP	2.7
1	AAA	51	THR	2.7
1	AAA	48	PRO	2.7
1	BBB	527[A]	LYS	2.4
1	CCC	51	THR	2.4
1	BBB	49	ASP	2.4
1	DDD	48	PRO	2.4
1	AAA	205[A]	LYS	2.3
1	AAA	337[A]	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	BYR	CCC	186	13/14	0.94	0.08	32,37,46,49	1
1	BYR	BBB	186	13/14	0.96	0.08	31,35,42,52	1
1	BYR	AAA	186	13/14	0.96	0.08	29,37,43,47	1
1	BYR	DDD	186	13/14	0.97	0.06	25,35,41,44	1
1	BYR	BBB	43	13/14	0.98	0.05	23,26,30,33	1
1	BYR	DDD	43	13/14	0.98	0.05	21,24,28,28	1
1	BYR	AAA	43	13/14	0.98	0.05	18,23,29,31	1
1	BYR	CCC	43	13/14	0.99	0.04	21,22,27,31	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	BBB	618	6/6	0.75	0.22	71,75,92,113	0
4	GOL	DDD	619	6/6	0.75	0.20	60,69,70,128	0
4	GOL	AAA	613	6/6	0.79	0.29	26,39,49,59	6
4	GOL	AAA	621	6/6	0.79	0.20	39,49,88,102	0
4	GOL	AAA	618	6/6	0.80	0.17	43,55,60,112	0
4	GOL	DDD	616	6/6	0.82	0.24	38,45,52,106	0
4	GOL	DDD	618	6/6	0.82	0.18	30,48,51,51	6
4	GOL	BBB	610	6/6	0.82	0.17	45,67,76,80	0
5	NA	AAA	623	1/1	0.84	0.28	46,46,46,46	0
4	GOL	BBB	613	6/6	0.85	0.16	39,50,65,66	0
4	GOL	BBB	615	6/6	0.86	0.14	29,62,75,78	0
4	GOL	BBB	606	6/6	0.86	0.17	27,62,86,86	0
5	NA	CCC	620	1/1	0.86	0.16	60,60,60,60	0
4	GOL	DDD	617	6/6	0.87	0.15	29,57,75,82	0
4	GOL	BBB	609	6/6	0.87	0.13	31,44,77,82	0
4	GOL	CCC	616	6/6	0.87	0.17	35,60,81,84	0
4	GOL	DDD	602	6/6	0.87	0.15	55,62,69,73	0
5	NA	BBB	620	1/1	0.87	0.26	43,43,43,43	0
4	GOL	AAA	620	6/6	0.87	0.15	52,61,77,89	0
6	144	CCC	618	8/8	0.87	0.14	35,69,98,104	0
4	GOL	CCC	610	6/6	0.88	0.14	32,57,86,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	CCC	614	6/6	0.88	0.18	29,48,61,85	0
4	GOL	AAA	616	6/6	0.88	0.11	60,71,73,92	0
4	GOL	BBB	616	6/6	0.88	0.19	51,66,95,98	0
5	NA	CCC	619	1/1	0.88	0.14	61,61,61,61	0
4	GOL	BBB	617	6/6	0.88	0.13	30,58,72,72	0
4	GOL	BBB	605	6/6	0.88	0.15	33,52,65,81	0
2	PO4	DDD	623	5/5	0.89	0.12	31,50,64,65	5
4	GOL	AAA	611	6/6	0.89	0.18	30,53,74,97	0
4	GOL	DDD	614	6/6	0.89	0.14	31,44,63,69	0
4	GOL	CCC	613	6/6	0.90	0.14	38,53,61,61	0
4	GOL	BBB	614	6/6	0.90	0.16	44,47,57,154	0
4	GOL	CCC	615	6/6	0.90	0.14	53,61,78,113	0
4	GOL	CCC	607	6/6	0.90	0.14	25,68,72,74	0
5	NA	CCC	621	1/1	0.90	0.20	44,44,44,44	0
5	NA	DDD	621	1/1	0.90	0.14	62,62,62,62	0
4	GOL	AAA	615	6/6	0.90	0.14	56,58,76,91	0
4	GOL	DDD	607	6/6	0.91	0.14	24,61,73,82	0
4	GOL	DDD	608	6/6	0.91	0.12	37,47,56,65	0
4	GOL	AAA	617	6/6	0.91	0.13	36,55,77,112	0
4	GOL	AAA	614	6/6	0.91	0.12	37,51,76,80	0
4	GOL	CCC	601	6/6	0.91	0.15	27,42,51,113	0
2	PO4	AAA	607	5/5	0.91	0.12	34,34,40,47	5
5	NA	DDD	622	1/1	0.91	0.14	39,39,39,39	0
4	GOL	AAA	605	6/6	0.91	0.14	36,48,56,70	0
4	GOL	BBB	612	6/6	0.92	0.14	33,46,67,75	0
4	GOL	BBB	601	6/6	0.92	0.11	44,53,62,66	0
4	GOL	DDD	615	6/6	0.92	0.10	40,46,53,80	0
4	GOL	CCC	606	6/6	0.93	0.13	32,45,62,80	0
4	GOL	DDD	611	6/6	0.93	0.10	30,41,54,60	0
4	GOL	AAA	619	6/6	0.93	0.15	43,52,77,80	0
4	GOL	AAA	606	6/6	0.93	0.13	19,38,49,54	6
4	GOL	CCC	617	6/6	0.93	0.09	37,47,56,60	0
4	GOL	DDD	601	6/6	0.93	0.13	42,64,70,72	0
4	GOL	CCC	612	6/6	0.93	0.13	37,46,77,91	0
4	GOL	CCC	604	6/6	0.93	0.14	30,41,78,101	0
4	GOL	BBB	611	6/6	0.94	0.12	36,52,77,85	0
4	GOL	DDD	605	6/6	0.94	0.15	23,40,76,112	0
4	GOL	DDD	606	6/6	0.94	0.10	26,29,34,34	0
4	GOL	AAA	612	6/6	0.94	0.11	35,44,66,79	0
4	GOL	AAA	610	6/6	0.94	0.10	33,42,57,74	0
4	GOL	AAA	604	6/6	0.94	0.09	28,32,35,37	0
4	GOL	DDD	613	6/6	0.94	0.14	40,53,62,81	0

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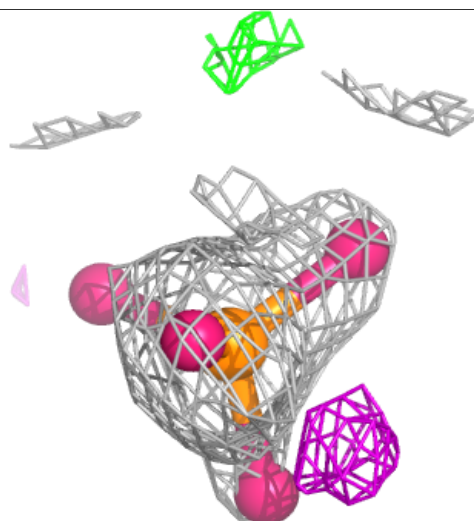
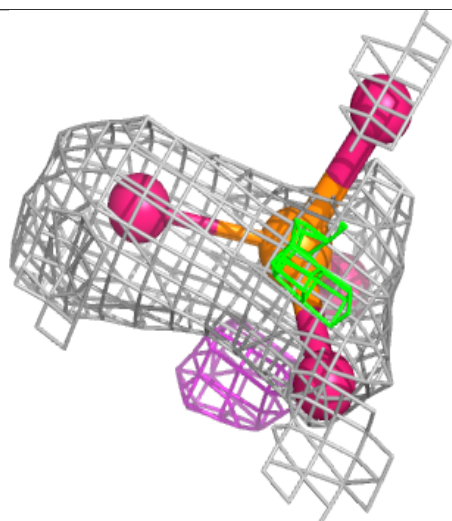
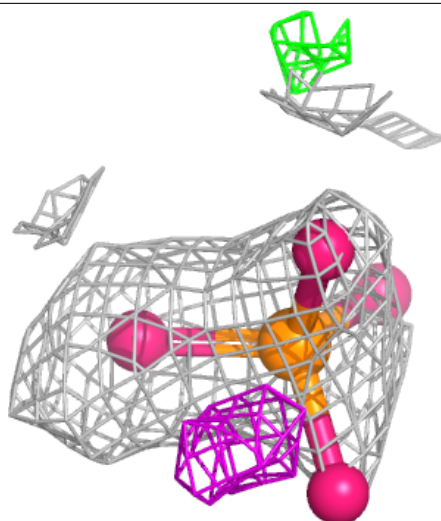
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	AAA	603	6/6	0.95	0.13	24,49,52,112	0
4	GOL	DDD	612	6/6	0.95	0.09	33,47,57,63	0
2	PO4	CCC	608	5/5	0.95	0.08	42,43,57,70	0
5	NA	AAA	622	1/1	0.95	0.20	51,51,51,51	0
4	GOL	BBB	604	6/6	0.96	0.08	29,34,34,37	0
2	PO4	BBB	607	5/5	0.96	0.07	44,44,53,53	0
5	NA	BBB	619	1/1	0.96	0.12	57,57,57,57	0
2	PO4	AAA	608	5/5	0.96	0.07	39,46,53,57	0
4	GOL	CCC	605	6/6	0.96	0.09	25,31,34,39	0
2	PO4	DDD	609	5/5	0.97	0.07	40,45,57,84	0
4	GOL	CCC	611	6/6	0.97	0.10	21,37,54,102	0
4	GOL	AAA	609	6/6	0.97	0.10	31,35,36,41	0
5	NA	DDD	620	1/1	0.97	0.06	49,49,49,49	0
4	GOL	BBB	608	6/6	0.97	0.07	26,33,40,40	0
4	GOL	DDD	610	6/6	0.97	0.07	26,40,43,46	0
4	GOL	CCC	609	6/6	0.97	0.08	27,32,33,36	0
2	PO4	DDD	603	5/5	0.98	0.05	29,29,30,32	0
3	CA	AAA	602	1/1	0.99	0.03	27,27,27,27	0
3	CA	BBB	603	1/1	0.99	0.03	27,27,27,27	0
3	CA	CCC	603	1/1	0.99	0.02	28,28,28,28	0
3	CA	DDD	604	1/1	0.99	0.02	25,25,25,25	0
2	PO4	AAA	601	5/5	0.99	0.04	25,26,28,36	0
2	PO4	CCC	602	5/5	0.99	0.04	24,25,27,27	0
2	PO4	BBB	602	5/5	0.99	0.04	27,28,30,36	0

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

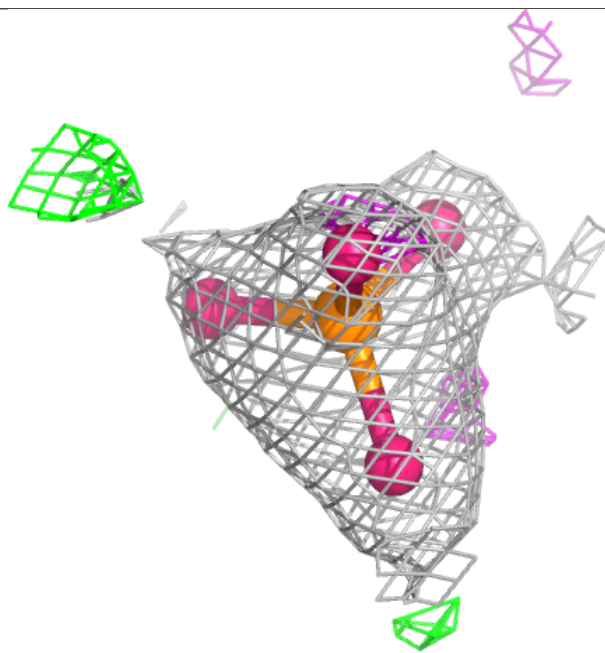
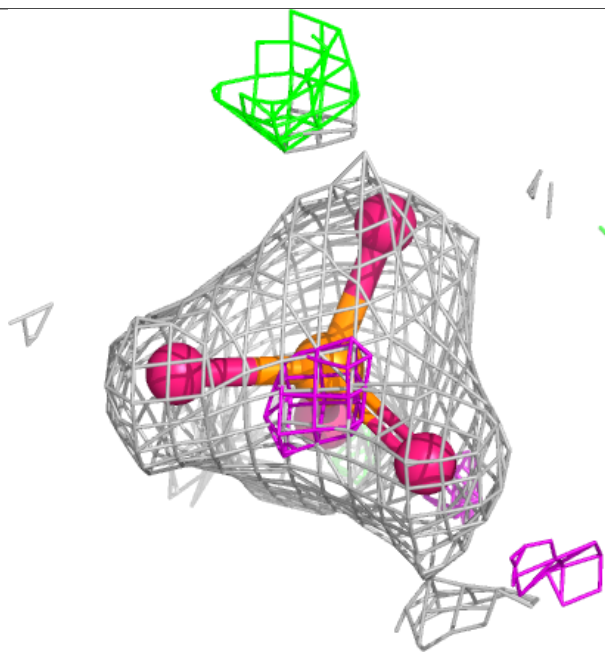
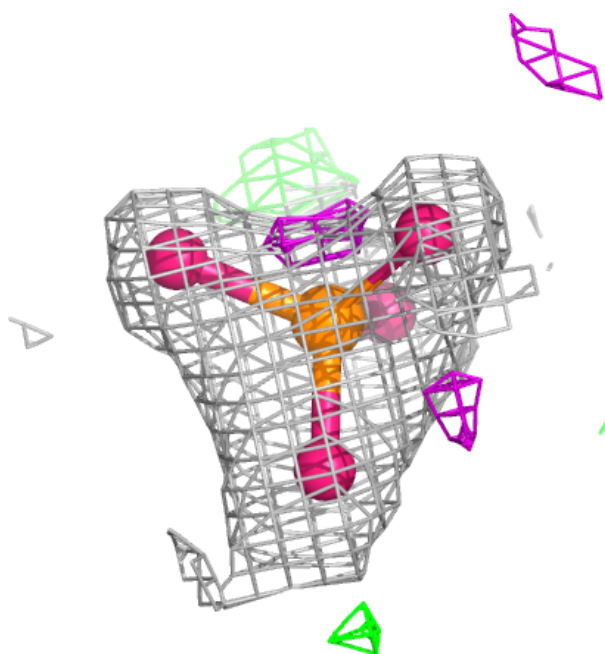
Electron density around PO4 DDD 623:

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



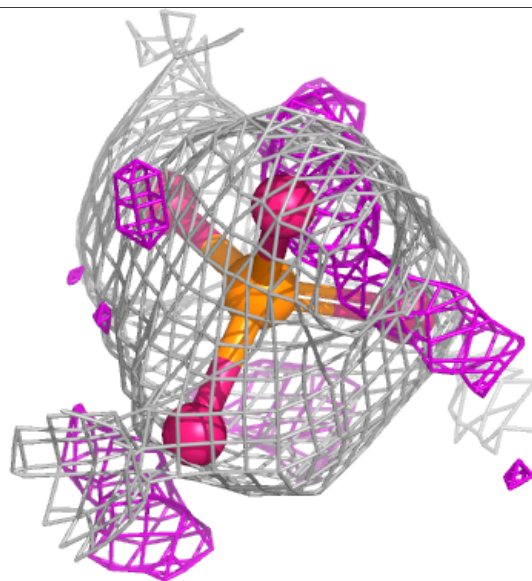
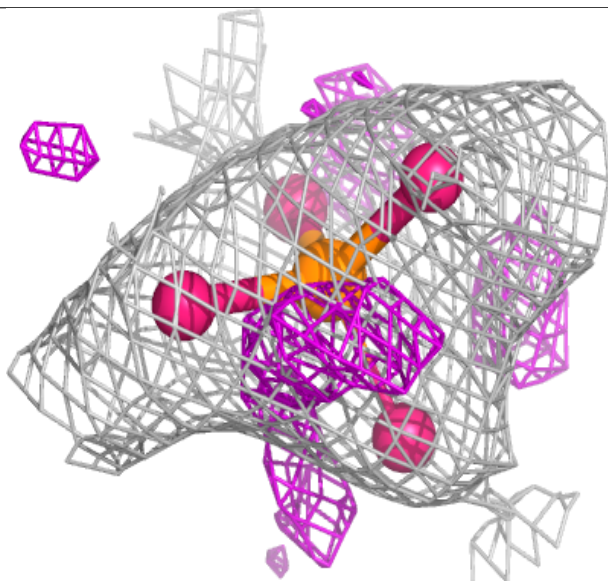
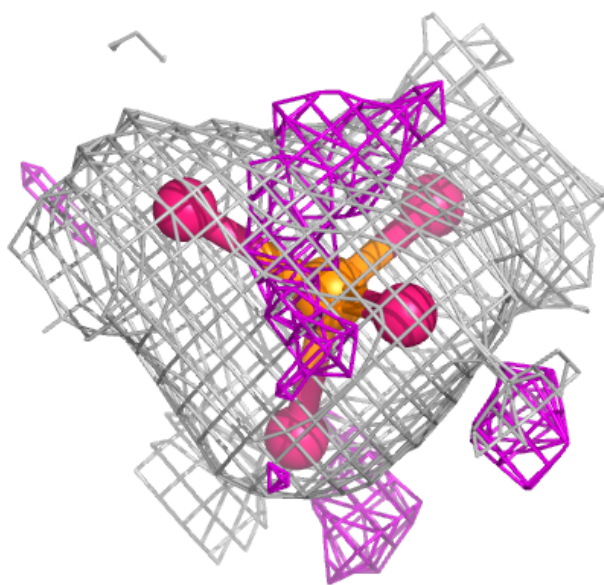
Electron density around PO4 AAA 607:

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



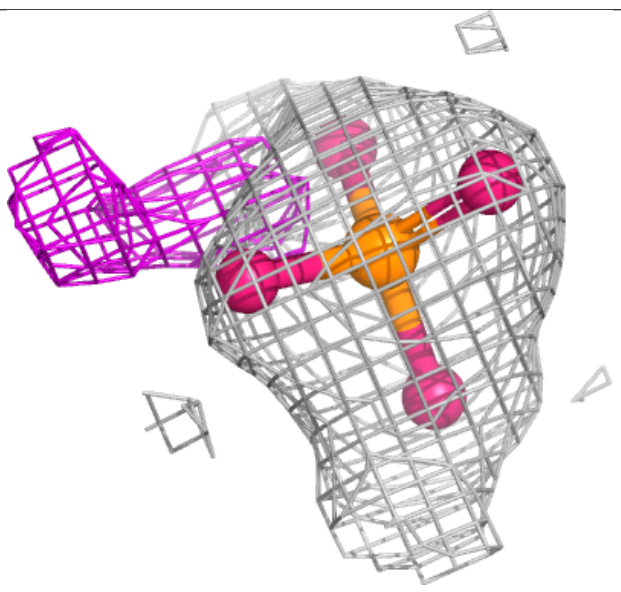
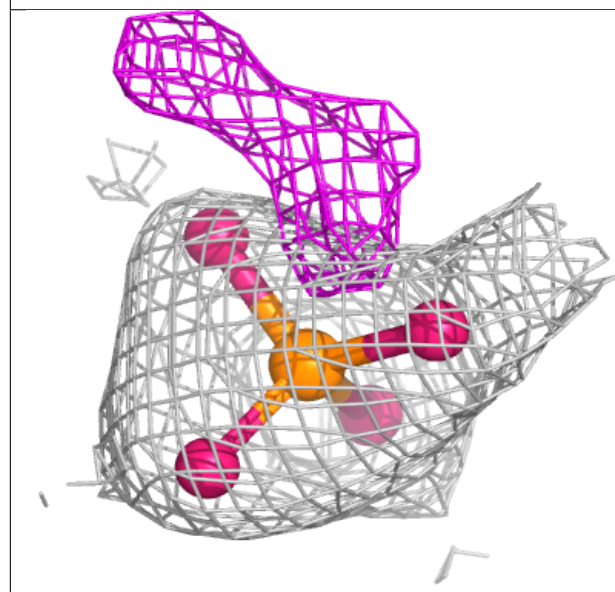
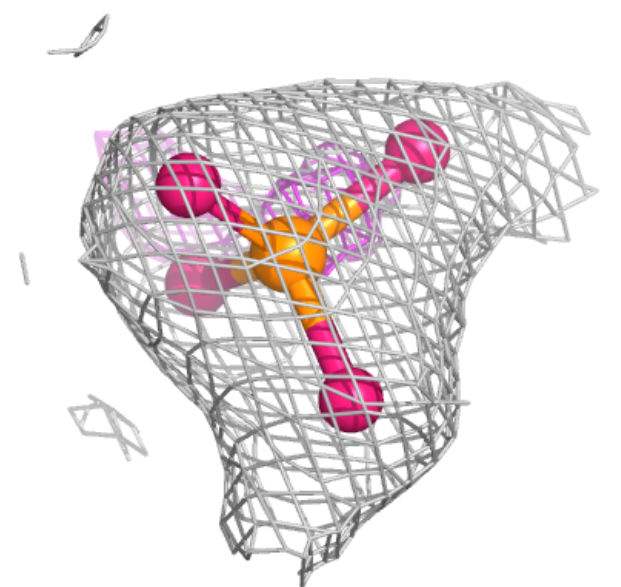
Electron density around PO4 CCC 608:

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



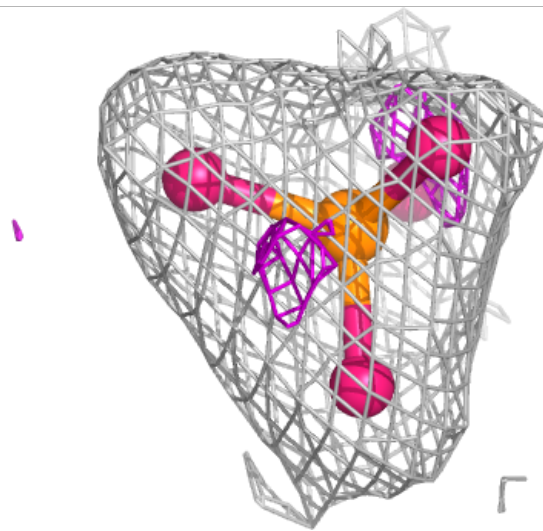
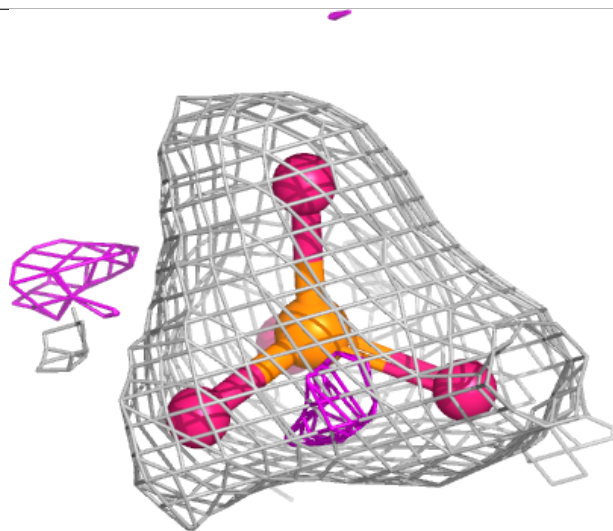
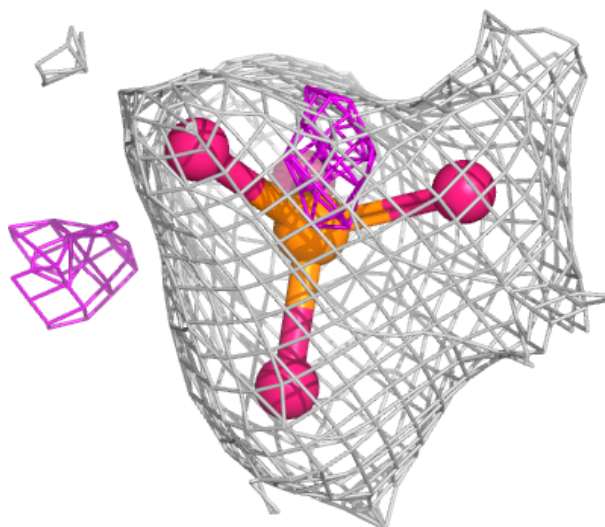
Electron density around PO4 BBB 607:

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



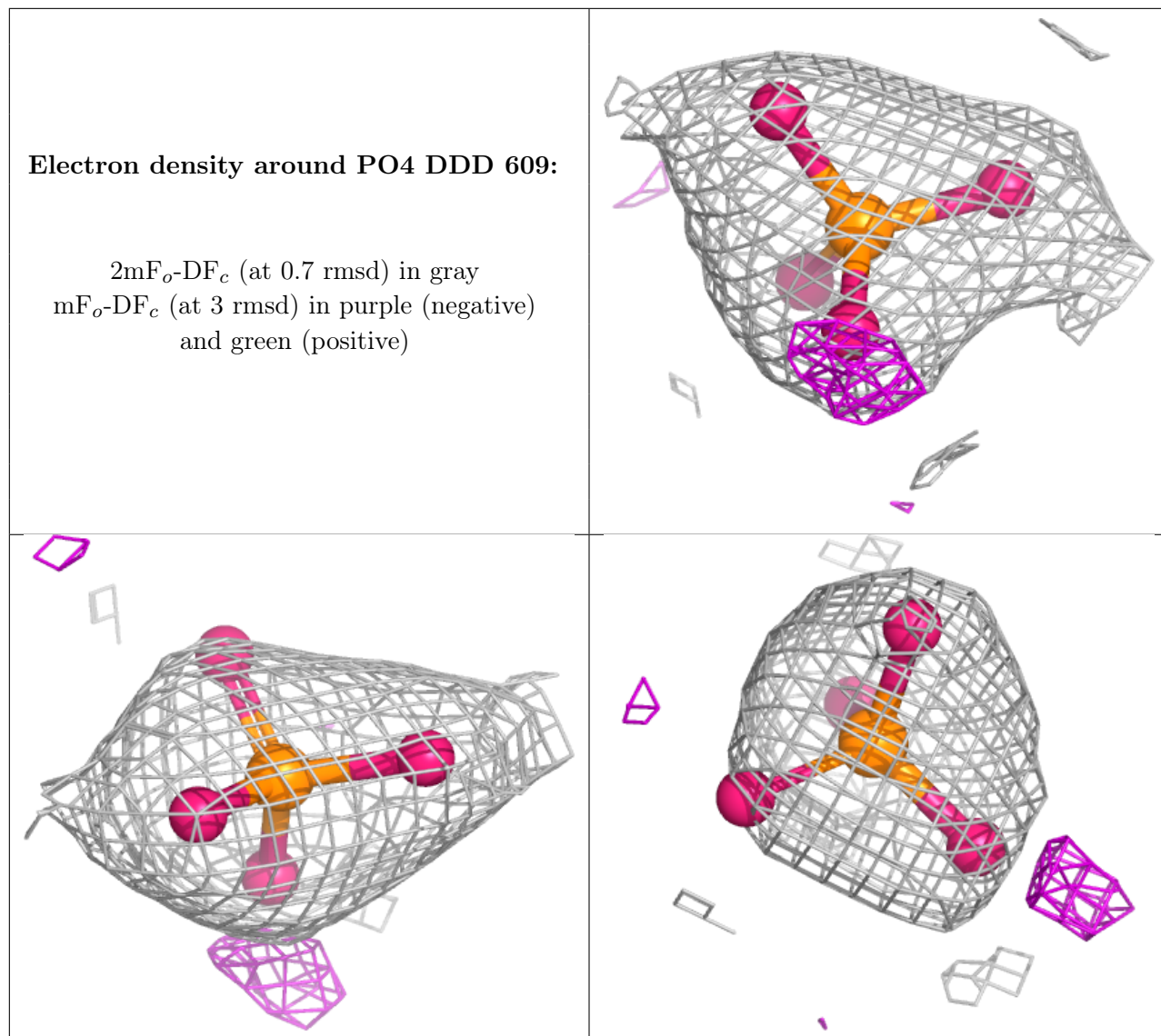
Electron density around PO4 AAA 608:

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



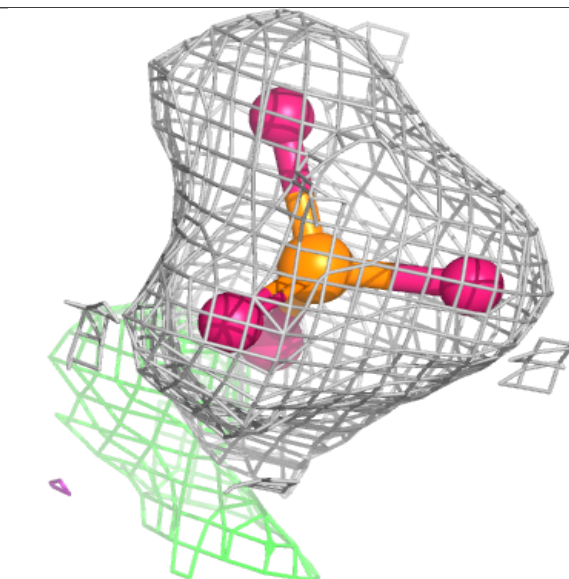
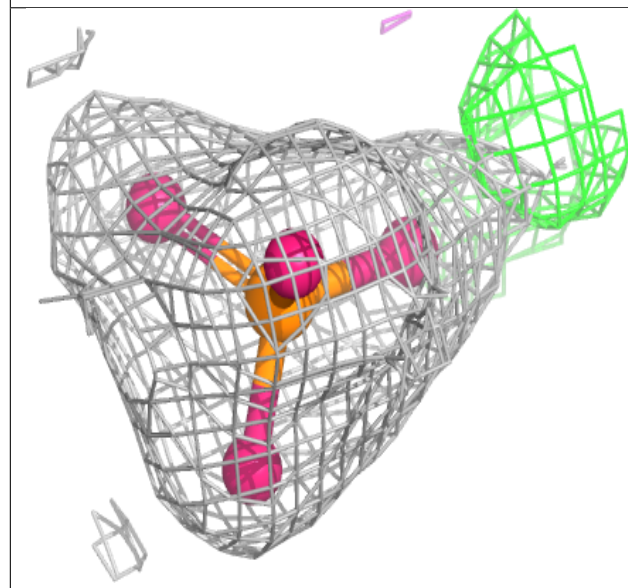
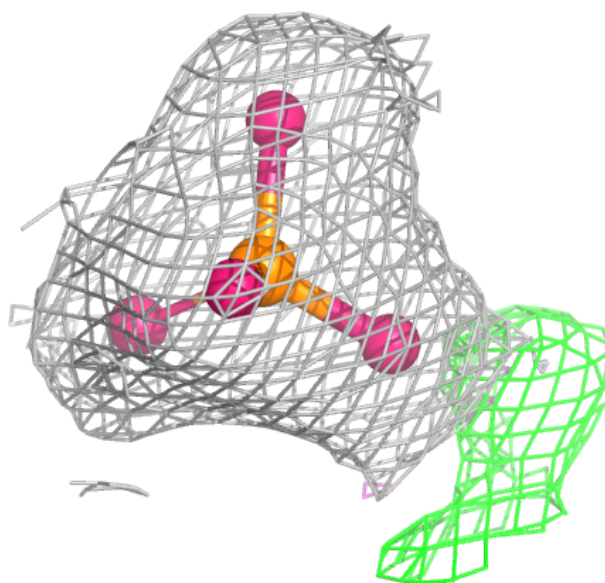
Electron density around PO4 DDD 609:

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



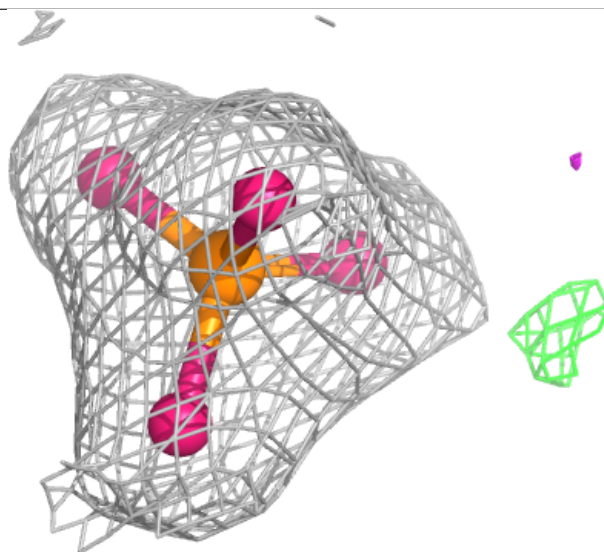
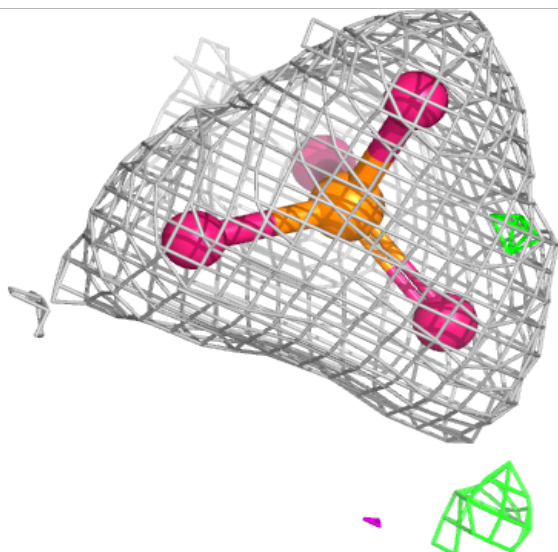
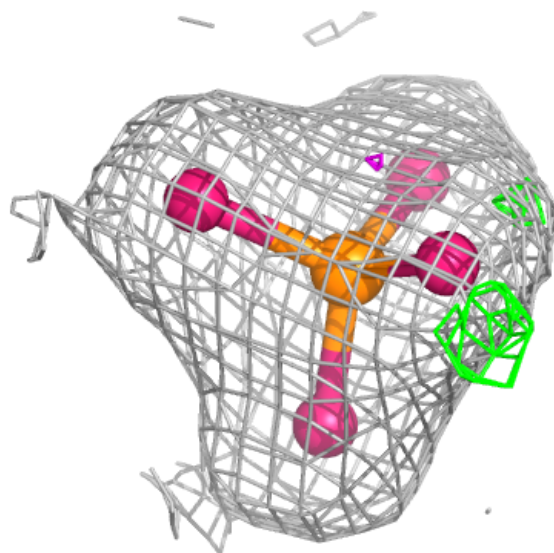
Electron density around PO4 DDD 603:

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



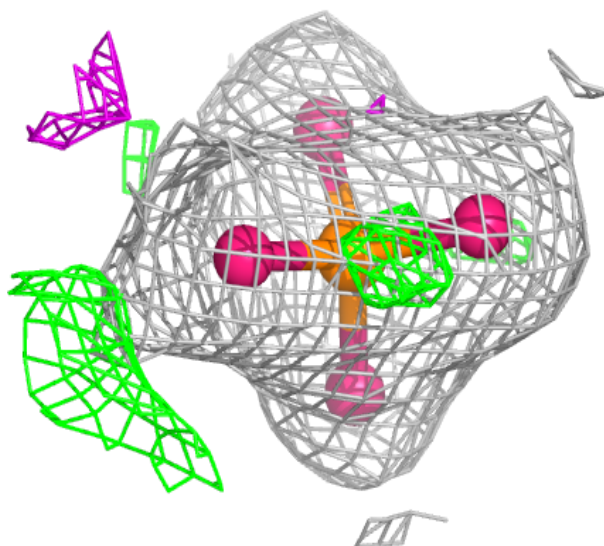
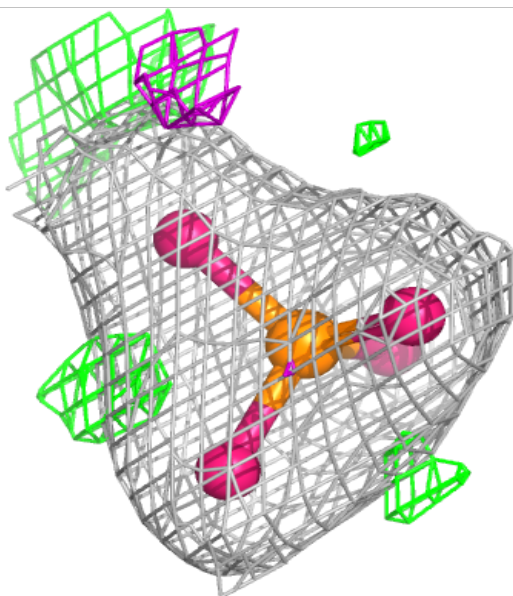
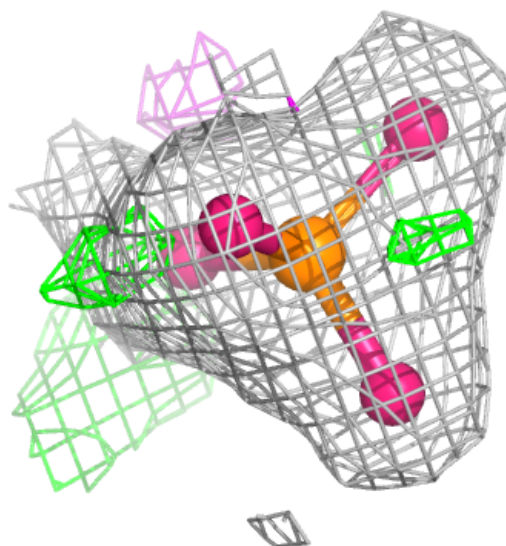
Electron density around PO4 AAA 601:

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



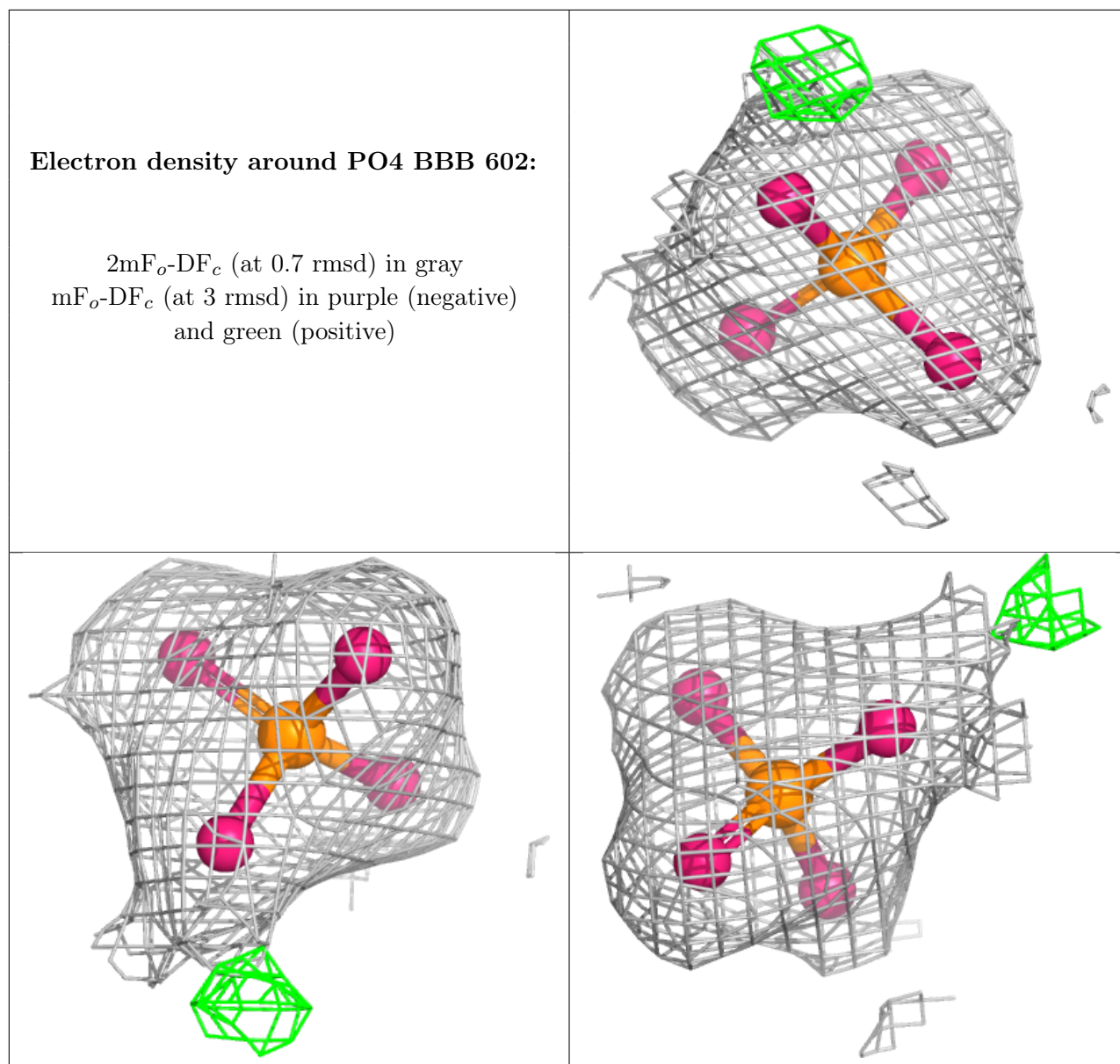
Electron density around PO4 CCC 602:

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



Electron density around PO4 BBB 602:

$2mF_o-DF_c$ (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.