



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 PM UTC

PDB ID : 8H53 / pdb_00008h53
Title : Human asparaginyl-tRNA synthetase in complex with asparagine-AMP
Authors : Park, J.S.; Han, B.W.
Deposited on : 2022-10-12
Resolution : 2.16 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

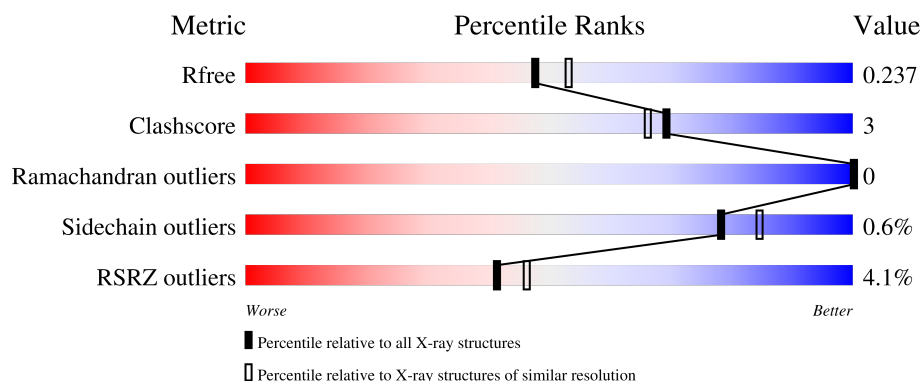
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

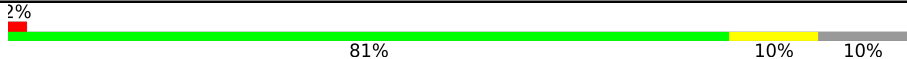
The reported resolution of this entry is 2.16 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	472	
1	B	472	
1	C	472	
1	D	472	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14571 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 Asparagine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3385	2159	581	619	26			
1	B	429	Total	C	N	O	S	0	0	0
			3395	2163	582	624	26			
1	C	428	Total	C	N	O	S	0	0	0
			3369	2146	583	614	26			
1	D	428	Total	C	N	O	S	0	0	0
			3352	2133	579	614	26			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O43776
A	78	GLY	-	expression tag	UNP O43776
A	79	SER	-	expression tag	UNP O43776
A	80	SER	-	expression tag	UNP O43776
A	81	HIS	-	expression tag	UNP O43776
A	82	HIS	-	expression tag	UNP O43776
A	83	HIS	-	expression tag	UNP O43776
A	84	HIS	-	expression tag	UNP O43776
A	85	HIS	-	expression tag	UNP O43776
A	86	HIS	-	expression tag	UNP O43776
A	87	SER	-	expression tag	UNP O43776
A	88	SER	-	expression tag	UNP O43776
A	89	GLY	-	expression tag	UNP O43776
A	90	LEU	-	expression tag	UNP O43776
A	91	VAL	-	expression tag	UNP O43776
A	92	PRO	-	expression tag	UNP O43776
A	93	ARG	-	expression tag	UNP O43776
A	94	GLY	-	expression tag	UNP O43776
A	95	SER	-	expression tag	UNP O43776
A	96	HIS	-	expression tag	UNP O43776
A	97	MET	-	expression tag	UNP O43776

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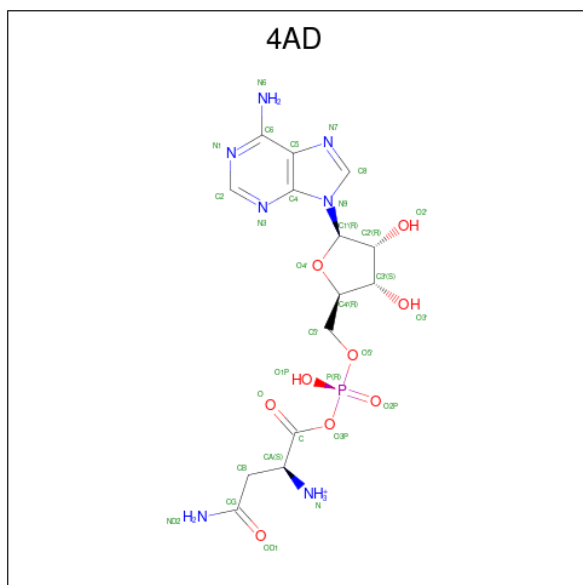
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	MET	-	initiating methionine	UNP O43776
B	78	GLY	-	expression tag	UNP O43776
B	79	SER	-	expression tag	UNP O43776
B	80	SER	-	expression tag	UNP O43776
B	81	HIS	-	expression tag	UNP O43776
B	82	HIS	-	expression tag	UNP O43776
B	83	HIS	-	expression tag	UNP O43776
B	84	HIS	-	expression tag	UNP O43776
B	85	HIS	-	expression tag	UNP O43776
B	86	HIS	-	expression tag	UNP O43776
B	87	SER	-	expression tag	UNP O43776
B	88	SER	-	expression tag	UNP O43776
B	89	GLY	-	expression tag	UNP O43776
B	90	LEU	-	expression tag	UNP O43776
B	91	VAL	-	expression tag	UNP O43776
B	92	PRO	-	expression tag	UNP O43776
B	93	ARG	-	expression tag	UNP O43776
B	94	GLY	-	expression tag	UNP O43776
B	95	SER	-	expression tag	UNP O43776
B	96	HIS	-	expression tag	UNP O43776
B	97	MET	-	expression tag	UNP O43776
C	77	MET	-	initiating methionine	UNP O43776
C	78	GLY	-	expression tag	UNP O43776
C	79	SER	-	expression tag	UNP O43776
C	80	SER	-	expression tag	UNP O43776
C	81	HIS	-	expression tag	UNP O43776
C	82	HIS	-	expression tag	UNP O43776
C	83	HIS	-	expression tag	UNP O43776
C	84	HIS	-	expression tag	UNP O43776
C	85	HIS	-	expression tag	UNP O43776
C	86	HIS	-	expression tag	UNP O43776
C	87	SER	-	expression tag	UNP O43776
C	88	SER	-	expression tag	UNP O43776
C	89	GLY	-	expression tag	UNP O43776
C	90	LEU	-	expression tag	UNP O43776
C	91	VAL	-	expression tag	UNP O43776
C	92	PRO	-	expression tag	UNP O43776
C	93	ARG	-	expression tag	UNP O43776
C	94	GLY	-	expression tag	UNP O43776
C	95	SER	-	expression tag	UNP O43776
C	96	HIS	-	expression tag	UNP O43776
C	97	MET	-	expression tag	UNP O43776

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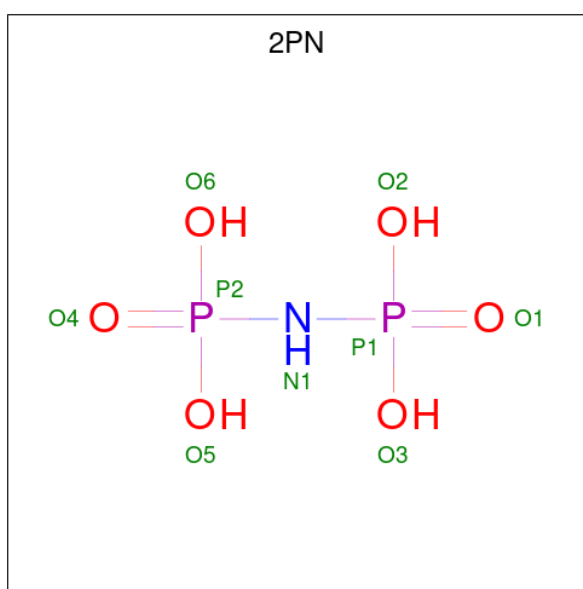
Chain	Residue	Modelled	Actual	Comment	Reference
D	77	MET	-	initiating methionine	UNP O43776
D	78	GLY	-	expression tag	UNP O43776
D	79	SER	-	expression tag	UNP O43776
D	80	SER	-	expression tag	UNP O43776
D	81	HIS	-	expression tag	UNP O43776
D	82	HIS	-	expression tag	UNP O43776
D	83	HIS	-	expression tag	UNP O43776
D	84	HIS	-	expression tag	UNP O43776
D	85	HIS	-	expression tag	UNP O43776
D	86	HIS	-	expression tag	UNP O43776
D	87	SER	-	expression tag	UNP O43776
D	88	SER	-	expression tag	UNP O43776
D	89	GLY	-	expression tag	UNP O43776
D	90	LEU	-	expression tag	UNP O43776
D	91	VAL	-	expression tag	UNP O43776
D	92	PRO	-	expression tag	UNP O43776
D	93	ARG	-	expression tag	UNP O43776
D	94	GLY	-	expression tag	UNP O43776
D	95	SER	-	expression tag	UNP O43776
D	96	HIS	-	expression tag	UNP O43776
D	97	MET	-	expression tag	UNP O43776

- Molecule 2 is 4-AMINO-1,4-DIOXOBUTAN-2-AMINIUM ADENOSINE-5'-MONOPHOSPHATE (CCD ID: 4AD) (formula: $C_{14}H_{21}N_7O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	14	7	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	14	7	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	14	7	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	14	7	9	1		

- Molecule 3 is IMIDODIPHOSPHORIC ACID (CCD ID: 2PN) (formula: $\text{H}_5\text{NO}_6\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	N	O	P	0	0
			9	1	6	2		
3	B	1	Total	N	O	P	0	0
			9	1	6	2		
3	C	1	Total	N	O	P	0	0
			9	1	6	2		
3	D	1	Total	N	O	P	0	0
			9	1	6	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	224	Total O 224 224	0	0

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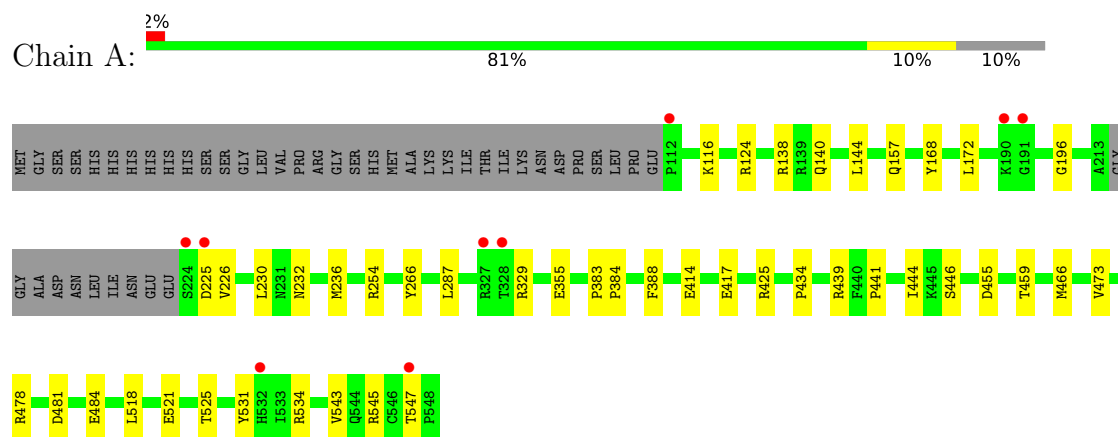
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	217	Total 217	O 217	0	0
6	C	175	Total 175	O 175	0	0
6	D	130	Total 130	O 130	0	0

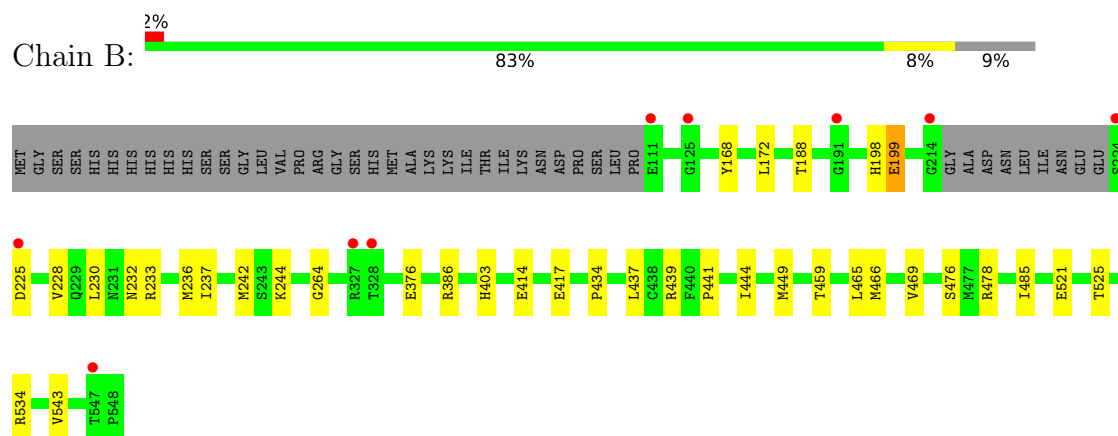
3 Residue-property plots [i](#)

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.

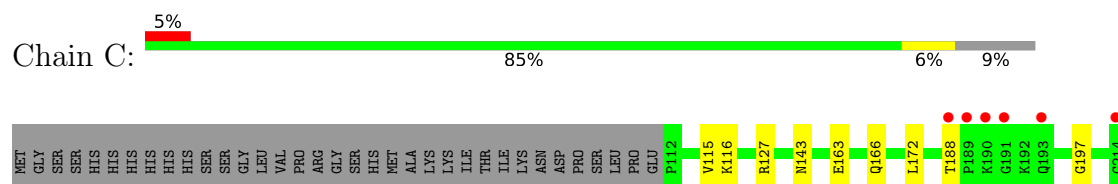
- Molecule 1: Asparagine-tRNA ligase, cytoplasmic

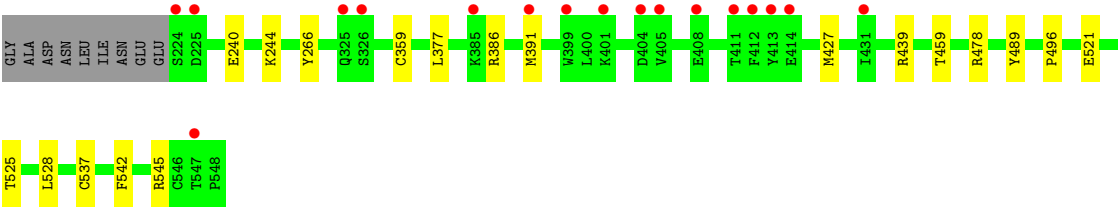


- Molecule 1: Asparagine-tRNA ligase, cytoplasmic

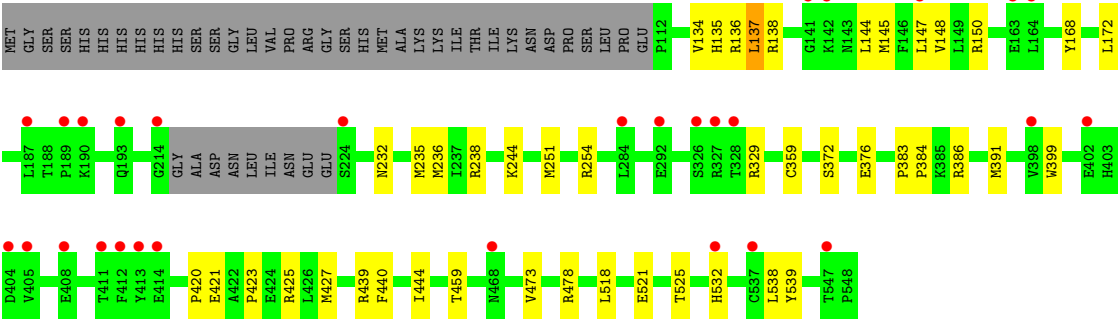
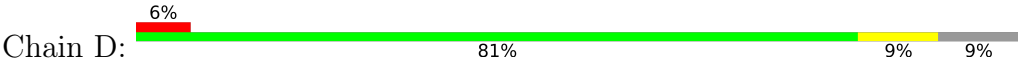


- Molecule 1: Asparagine-tRNA ligase, cytoplasmic





● Molecule 1: Asparagine–tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.42Å 125.84Å 161.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.16 49.88 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.88-2.16) 99.4 (49.88-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.237 0.205 , 0.237	Depositor DCC
R_{free} test set	6238 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5718e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, 4AD, 2PN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3469	0.32	0/4706
1	B	0.13	0/3479	0.32	0/4722
1	C	0.13	0/3452	0.31	0/4686
1	D	0.13	0/3435	0.31	0/4665
All	All	0.13	0/13835	0.31	0/18779

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3385	0	3263	26	0
1	B	3395	0	3257	19	0
1	C	3369	0	3234	19	0
1	D	3352	0	3185	30	0
2	A	31	0	20	1	0
2	B	31	0	20	1	0
2	C	31	0	20	1	0
2	D	31	0	20	1	0
3	A	9	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	1	0	0
3	C	9	0	1	0	0
3	D	9	0	1	0	0
4	A	54	0	72	5	0
4	B	36	0	48	2	0
4	C	36	0	48	5	0
4	D	30	0	40	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	224	0	0	3	0
6	B	217	0	0	0	0
6	C	175	0	0	0	0
6	D	130	0	0	0	0
All	All	14571	0	13231	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (94) 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:D:137:LEU:HD11	1:D:145:MET:HE2	1.55	0.87
1:C:478:ARG:HH22	2:C:601:4AD:HD22	1.23	0.82
1:D:478:ARG:HH22	2:D:601:4AD:HD22	1.25	0.81
1:B:478:ARG:HH22	2:B:601:4AD:HD22	1.25	0.81
1:A:478:ARG:HH22	2:A:601:4AD:HD22	1.29	0.79
1:A:455:ASP:HA	4:A:605:GOL:H2	1.71	0.73
1:A:230:LEU:HD21	1:A:534:ARG:HD2	1.77	0.67
1:A:254:ARG:HH12	4:A:611:GOL:H31	1.61	0.65
1:D:244:LYS:NZ	1:D:376:GLU:OE1	2.26	0.61
1:C:163:GLU:HA	1:C:166:GLN:HG2	1.83	0.61
1:D:421:GLU:O	1:D:425:ARG:HG3	2.01	0.61
1:D:137:LEU:HD12	1:D:138:ARG:N	2.17	0.60
1:A:116:LYS:NZ	6:A:703:HOH:O	2.34	0.59
1:D:136:ARG:HB2	1:D:148:VAL:HB	1.85	0.59
1:A:481:ASP:HB3	1:A:484:GLU:HG3	1.85	0.58
1:C:188:THR:HG22	1:C:197:GLY:C	2.29	0.57
1:A:434:PRO:HB3	1:A:466:MET:HE1	1.86	0.57
1:D:440:PHE:HB3	1:D:444:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:609:GOL:H11	1:D:254:ARG:HH12	1.70	0.57
1:D:399:TRP:CE3	1:D:427:MET:HG3	2.40	0.56
1:D:359:CYS:SG	1:D:386:ARG:HD3	2.46	0.56
1:B:441:PRO:HD2	1:B:444:ILE:HD11	1.87	0.56
1:D:521:GLU:O	1:D:525:THR:HG23	2.06	0.55
1:C:240:GLU:O	1:C:244:LYS:HG2	2.08	0.54
1:C:537:CYS:SG	4:C:606:GOL:H31	2.50	0.51
1:D:137:LEU:HD13	1:D:147:LEU:CD2	2.40	0.51
1:B:244:LYS:NZ	1:B:376:GLU:OE1	2.39	0.50
1:A:225:ASP:OD1	1:A:226:VAL:N	2.45	0.50
1:A:521:GLU:OE2	4:A:606:GOL:O1	2.30	0.50
1:C:143:ASN:ND2	1:C:166:GLN:OE1	2.45	0.50
1:B:237:ILE:HA	1:B:242:MET:HB3	1.94	0.49
1:D:372:SER:O	1:D:376:GLU:HG3	2.13	0.49
1:A:425:ARG:HD2	6:A:813:HOH:O	2.13	0.49
1:C:391:MET:HE1	1:C:427:MET:CE	2.43	0.49
1:C:359:CYS:SG	1:C:386:ARG:HD3	2.52	0.48
1:A:232:ASN:O	1:A:236:MET:HG2	2.13	0.48
1:C:266:TYR:CE1	4:C:607:GOL:H32	2.49	0.48
1:D:134:VAL:HG13	1:D:147:LEU:HD22	1.95	0.48
1:A:138:ARG:NH2	1:A:140:GLN:OE1	2.46	0.48
1:B:434:PRO:HB3	1:B:466:MET:HE1	1.96	0.48
1:B:403:HIS:HB3	4:B:606:GOL:H31	1.96	0.47
1:B:437:LEU:HD22	1:B:465:LEU:HD11	1.96	0.47
1:B:521:GLU:O	1:B:525:THR:HG23	2.14	0.47
1:C:172:LEU:O	4:C:605:GOL:O3	2.28	0.46
1:B:233:ARG:NH2	1:B:534:ARG:O	2.48	0.46
1:A:124:ARG:NH2	1:A:196:GLY:O	2.48	0.46
1:A:521:GLU:O	1:A:525:THR:HG23	2.16	0.46
1:B:168:TYR:CZ	1:B:172:LEU:HD11	2.50	0.46
1:A:545:ARG:NH1	1:A:547:THR:O	2.49	0.46
1:C:521:GLU:O	1:C:525:THR:HG23	2.16	0.46
1:D:144:LEU:HD12	1:D:144:LEU:HA	1.80	0.45
1:A:266:TYR:CE1	4:A:609:GOL:H32	2.51	0.45
1:A:441:PRO:HD2	1:A:444:ILE:HD11	1.98	0.45
1:D:168:TYR:CZ	1:D:172:LEU:HD11	2.51	0.45
1:C:127:ARG:HH22	4:C:608:GOL:C3	2.30	0.45
1:D:137:LEU:HD13	1:D:147:LEU:HD23	1.98	0.45
1:D:329:ARG:HA	1:D:532:HIS:CD2	2.52	0.45
1:D:473:VAL:HG22	1:D:518:LEU:HD12	1.98	0.44
1:A:157:GLN:NE2	6:A:701:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ARG:HE	1:B:386:ARG:HB3	1.63	0.44
1:B:225:ASP:HB3	1:B:228:VAL:HB	2.00	0.44
1:D:251:MET:HB2	1:D:251:MET:HE2	1.87	0.44
1:C:489:TYR:CD2	1:C:496:PRO:HB3	2.53	0.43
1:C:377:LEU:HD12	1:C:528:LEU:HD22	2.00	0.43
1:C:115:VAL:HG12	1:C:116:LYS:O	2.18	0.43
1:A:383:PRO:HA	1:A:384:PRO:HD3	1.92	0.43
1:A:473:VAL:HG22	1:A:518:LEU:HD12	2.00	0.43
1:A:414:GLU:O	1:A:417:GLU:HG2	2.18	0.43
1:C:127:ARG:HH22	4:C:608:GOL:H31	1.83	0.43
1:A:439:ARG:HA	1:A:459:THR:O	2.19	0.43
1:B:232:ASN:O	1:B:236:MET:HG2	2.19	0.43
1:D:135:HIS:HB2	1:D:150:ARG:HG2	2.00	0.43
1:A:329:ARG:HD2	1:A:531:TYR:CZ	2.54	0.43
1:B:264:GLY:HA2	4:B:608:GOL:H31	2.01	0.43
1:D:329:ARG:HG2	1:D:532:HIS:HD2	1.84	0.42
1:B:230:LEU:HD21	1:B:534:ARG:HD3	2.00	0.42
1:B:439:ARG:HA	1:B:459:THR:O	2.19	0.42
1:C:542:PHE:CZ	1:C:545:ARG:HD2	2.54	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.42
1:D:538:LEU:HG	1:D:539:TYR:CD2	2.55	0.42
1:D:420:PRO:HD2	1:D:423:PRO:HG2	2.01	0.42
1:A:168:TYR:CZ	1:A:172:LEU:HD11	2.55	0.41
1:B:449:MET:HG2	1:B:476:SER:OG	2.21	0.41
1:B:414:GLU:O	1:B:417:GLU:HG2	2.21	0.41
1:D:383:PRO:HA	1:D:384:PRO:HD3	1.95	0.41
1:D:235:MET:HE3	1:D:238:ARG:HD2	2.02	0.41
1:D:439:ARG:HA	1:D:459:THR:O	2.21	0.41
1:B:188:THR:CG2	1:B:199:GLU:HB3	2.51	0.41
1:D:232:ASN:O	1:D:236:MET:HG2	2.21	0.41
1:C:391:MET:HB3	1:C:391:MET:HE2	1.75	0.41
1:C:439:ARG:HA	1:C:459:THR:O	2.20	0.41
1:D:391:MET:HE2	1:D:391:MET:HB3	1.76	0.41
1:A:355:GLU:CD	1:A:388:PHE:H	2.29	0.40
1:D:137:LEU:HD12	1:D:138:ARG:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/472 (90%)	409 (97%)	14 (3%)	0	100	100
1	B	425/472 (90%)	409 (96%)	16 (4%)	0	100	100
1	C	424/472 (90%)	413 (97%)	11 (3%)	0	100	100
1	D	424/472 (90%)	411 (97%)	13 (3%)	0	100	100
All	All	1696/1888 (90%)	1642 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/415 (87%)	357 (99%)	3 (1%)	73	79
1	B	360/415 (87%)	355 (99%)	5 (1%)	59	66
1	C	355/415 (86%)	355 (100%)	0	100	100
1	D	349/415 (84%)	348 (100%)	1 (0%)	86	91
All	All	1424/1660 (86%)	1415 (99%)	9 (1%)	78	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	LEU
1	A	446	SER

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Mol	Chain	Res	Type
1	A	543	VAL
1	B	198	HIS
1	B	199	GLU
1	B	469	VAL
1	B	485	ILE
1	B	543	VAL
1	D	137	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	186	ASN
1	A	277	GLN
1	B	229	GLN
1	B	241	ASN
1	B	277	GLN
1	C	277	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4AD	B	601	5	32,33,33	1.65	4 (12%)	46,49,49	2.03	12 (26%)
3	2PN	C	602	5	8,8,8	2.76	7 (87%)	8,13,13	1.43	1 (12%)
4	GOL	A	608	-	5,5,5	0.92	0	5,5,5	1.07	1 (20%)
4	GOL	A	611	-	5,5,5	0.91	0	5,5,5	1.11	0
4	GOL	D	605	-	5,5,5	0.95	0	5,5,5	1.08	0
4	GOL	C	603	-	5,5,5	0.97	0	5,5,5	1.07	0
4	GOL	A	604	-	5,5,5	0.90	0	5,5,5	1.05	0
4	GOL	D	607	-	5,5,5	0.92	0	5,5,5	1.08	0
4	GOL	B	603	-	5,5,5	0.94	0	5,5,5	1.11	0
2	4AD	A	601	5	32,33,33	3.05	10 (31%)	46,49,49	2.04	12 (26%)
3	2PN	D	602	5	8,8,8	2.75	6 (75%)	8,13,13	1.47	2 (25%)
4	GOL	B	608	-	5,5,5	0.83	0	5,5,5	1.15	1 (20%)
4	GOL	D	604	-	5,5,5	0.93	0	5,5,5	1.06	0
4	GOL	A	609	-	5,5,5	0.82	0	5,5,5	1.13	1 (20%)
4	GOL	B	605	-	5,5,5	1.00	0	5,5,5	0.97	0
4	GOL	A	606	-	5,5,5	0.86	0	5,5,5	1.15	1 (20%)
2	4AD	C	601	5	32,33,33	1.67	4 (12%)	46,49,49	2.01	13 (28%)
4	GOL	A	610	-	5,5,5	0.98	0	5,5,5	1.15	1 (20%)
4	GOL	D	606	-	5,5,5	0.91	0	5,5,5	1.12	0
4	GOL	B	604	-	5,5,5	0.94	0	5,5,5	1.08	0
4	GOL	A	603	-	5,5,5	0.88	0	5,5,5	1.11	1 (20%)
4	GOL	C	608	-	5,5,5	0.90	0	5,5,5	1.09	0
4	GOL	C	604	-	5,5,5	0.97	0	5,5,5	1.02	0
4	GOL	B	607	-	5,5,5	0.90	0	5,5,5	1.09	0
4	GOL	B	606	-	5,5,5	0.95	0	5,5,5	1.03	0
3	2PN	A	602	5	8,8,8	2.64	4 (50%)	8,13,13	1.45	0
2	4AD	D	601	5	32,33,33	1.68	5 (15%)	46,49,49	1.99	12 (26%)
4	GOL	C	606	-	5,5,5	0.92	0	5,5,5	1.05	0
4	GOL	C	605	-	5,5,5	0.99	0	5,5,5	1.05	0
4	GOL	D	603	-	5,5,5	0.93	0	5,5,5	1.07	0
4	GOL	A	605	-	5,5,5	0.96	0	5,5,5	1.09	0
3	2PN	B	602	5	8,8,8	2.62	4 (50%)	8,13,13	1.46	0
4	GOL	C	607	-	5,5,5	0.93	0	5,5,5	1.02	0
4	GOL	A	607	-	5,5,5	0.94	0	5,5,5	1.06	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
2	4AD	B	601	5	-	2/21/39/39	0/3/3/3
3	2PN	C	602	5	-	1/2/6/6	-
4	GOL	A	608	-	-	1/4/4/4	-
4	GOL	A	611	-	-	1/4/4/4	-
4	GOL	D	605	-	-	2/4/4/4	-
4	GOL	C	603	-	-	0/4/4/4	-
4	GOL	A	604	-	-	1/4/4/4	-
4	GOL	D	607	-	-	1/4/4/4	-
4	GOL	B	603	-	-	0/4/4/4	-
2	4AD	A	601	5	-	3/21/39/39	0/3/3/3
3	2PN	D	602	5	-	1/2/6/6	-
4	GOL	B	608	-	-	0/4/4/4	-
4	GOL	D	604	-	-	2/4/4/4	-
4	GOL	A	609	-	-	0/4/4/4	-
4	GOL	B	605	-	-	1/4/4/4	-
4	GOL	A	606	-	-	1/4/4/4	-
2	4AD	C	601	5	-	3/21/39/39	0/3/3/3
4	GOL	A	610	-	-	0/4/4/4	-
4	GOL	D	606	-	-	1/4/4/4	-
4	GOL	B	604	-	-	1/4/4/4	-
4	GOL	A	603	-	-	0/4/4/4	-
4	GOL	C	608	-	-	0/4/4/4	-
4	GOL	C	604	-	-	1/4/4/4	-
4	GOL	B	607	-	-	0/4/4/4	-
4	GOL	B	606	-	-	0/4/4/4	-
3	2PN	A	602	5	-	1/2/6/6	-
2	4AD	D	601	5	-	3/21/39/39	0/3/3/3
4	GOL	C	606	-	-	2/4/4/4	-
4	GOL	C	605	-	-	0/4/4/4	-
4	GOL	D	603	-	-	0/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-
3	2PN	B	602	5	-	1/2/6/6	-
4	GOL	C	607	-	-	1/4/4/4	-
4	GOL	A	607	-	-	0/4/4/4	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	4AD	C2'-C3'	-8.34	1.30	1.53
2	A	601	4AD	O4'-C4'	-7.26	1.28	1.45
2	A	601	4AD	O4'-C1'	6.04	1.56	1.42
2	A	601	4AD	C6-N6	5.92	1.49	1.34
2	C	601	4AD	C6-N6	5.91	1.49	1.34
2	D	601	4AD	C6-N6	5.88	1.49	1.34
2	B	601	4AD	C6-N6	5.87	1.49	1.34
2	A	601	4AD	C1'-N9	-4.17	1.34	1.46
2	A	601	4AD	C3'-C4'	4.01	1.63	1.53
2	D	601	4AD	CG-ND2	3.89	1.45	1.32
2	A	601	4AD	CG-ND2	3.82	1.45	1.32
2	B	601	4AD	CG-ND2	3.81	1.45	1.32
2	A	601	4AD	O2'-C2'	3.81	1.52	1.43
2	C	601	4AD	CG-ND2	3.79	1.45	1.32
3	D	602	2PN	P1-O1	3.60	1.51	1.46
3	D	602	2PN	P2-O4	3.58	1.51	1.46
3	C	602	2PN	P2-O4	3.57	1.51	1.46
3	C	602	2PN	P1-O1	3.56	1.51	1.46
3	B	602	2PN	P1-O1	3.50	1.51	1.46
3	A	602	2PN	P1-O1	3.49	1.51	1.46
3	B	602	2PN	P2-O4	3.48	1.51	1.46
3	A	602	2PN	P2-O4	3.48	1.51	1.46
3	C	602	2PN	P2-N1	3.12	1.71	1.63
3	C	602	2PN	P1-N1	3.11	1.71	1.63
3	D	602	2PN	P2-N1	3.06	1.71	1.63
3	D	602	2PN	P1-N1	3.05	1.71	1.63
3	A	602	2PN	P2-N1	2.89	1.70	1.63
2	B	601	4AD	C5-C4	-2.88	1.33	1.39
2	D	601	4AD	C5-C4	-2.82	1.34	1.39
3	B	602	2PN	P2-N1	2.79	1.70	1.63
2	A	601	4AD	C5-C4	-2.79	1.34	1.39
2	C	601	4AD	C5-C4	-2.76	1.34	1.39
3	A	602	2PN	P1-N1	2.76	1.70	1.63
3	B	602	2PN	P1-N1	2.74	1.70	1.63
2	C	601	4AD	C5-N7	-2.48	1.34	1.39
2	D	601	4AD	C5-N7	-2.44	1.34	1.39
2	A	601	4AD	C5-N7	-2.37	1.34	1.39
2	B	601	4AD	C5-N7	-2.35	1.34	1.39
3	C	602	2PN	P2-O5	-2.04	1.51	1.56
3	C	602	2PN	P1-O3	-2.03	1.51	1.56
2	D	601	4AD	OD1-CG	-2.03	1.17	1.23
3	D	602	2PN	P2-O6	-2.01	1.51	1.56
3	C	602	2PN	P1-O2	-2.01	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	2PN	P2-O5	-2.00	1.51	1.56

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	4AD	N1-C2-N3	-5.75	119.87	128.58
2	D	601	4AD	N1-C2-N3	-5.64	120.05	128.58
2	C	601	4AD	N1-C2-N3	-5.60	120.11	128.58
2	A	601	4AD	N1-C2-N3	-5.51	120.23	128.58
2	A	601	4AD	C5-C4-N3	-5.23	119.51	126.72
2	B	601	4AD	C5-C4-N3	-5.18	119.58	126.72
2	C	601	4AD	C5-C4-N3	-5.07	119.73	126.72
2	D	601	4AD	C5-C4-N3	-4.89	119.99	126.72
2	C	601	4AD	N6-C6-N1	-4.87	107.52	118.38
2	A	601	4AD	N6-C6-N1	-4.66	108.00	118.38
2	B	601	4AD	N6-C6-N1	-4.62	108.09	118.38
2	D	601	4AD	N6-C6-N1	-4.60	108.13	118.38
2	B	601	4AD	N9-C8-N7	-4.44	107.64	113.94
2	D	601	4AD	N9-C8-N7	-4.37	107.74	113.94
2	A	601	4AD	N9-C8-N7	-4.29	107.85	113.94
2	C	601	4AD	N9-C8-N7	-4.26	107.90	113.94
2	C	601	4AD	C5-C6-N6	3.75	132.56	123.29
2	B	601	4AD	C2-N3-C4	3.60	120.62	111.83
2	D	601	4AD	C5-C6-N6	3.52	132.00	123.29
2	A	601	4AD	C2-N3-C4	3.49	120.36	111.83
2	C	601	4AD	C2-N3-C4	3.44	120.23	111.83
2	A	601	4AD	C5-C6-N6	3.44	131.81	123.29
2	D	601	4AD	C2-N3-C4	3.35	120.02	111.83
2	B	601	4AD	C5-C6-N6	3.32	131.52	123.29
2	A	601	4AD	N3-C4-N9	3.32	132.81	127.17
2	B	601	4AD	N3-C4-N9	3.30	132.78	127.17
2	D	601	4AD	N3-C4-N9	3.05	132.35	127.17
2	B	601	4AD	C5-N7-C8	3.01	108.19	103.45
2	C	601	4AD	C5-N7-C8	3.00	108.17	103.45
2	C	601	4AD	N3-C4-N9	2.99	132.25	127.17
2	A	601	4AD	C5-N7-C8	2.97	108.12	103.45
2	D	601	4AD	C5-N7-C8	2.96	108.10	103.45
2	A	601	4AD	O3P-P-O5'	2.95	111.87	103.00
2	D	601	4AD	C4-N9-C8	2.49	108.36	105.74
2	B	601	4AD	C4-N9-C1'	-2.49	120.81	126.63
2	B	601	4AD	C4-N9-C8	2.48	108.35	105.74
2	B	601	4AD	O3P-P-O5'	2.48	110.45	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	4AD	O3P-P-O5'	2.47	110.44	103.00
2	D	601	4AD	C4-N9-C1'	-2.35	121.13	126.63
2	C	601	4AD	O3P-P-O5'	2.32	109.99	103.00
2	C	601	4AD	C4-C5-N7	-2.29	107.97	110.58
2	A	601	4AD	C4-N9-C8	2.28	108.13	105.74
2	C	601	4AD	C4-N9-C1'	-2.20	121.49	126.63
2	D	601	4AD	C4-C5-N7	-2.13	108.14	110.58
2	C	601	4AD	C4-N9-C8	2.11	107.95	105.74
2	A	601	4AD	C4-N9-C1'	-2.11	121.70	126.63
4	A	609	GOL	C3-C2-C1	-2.09	104.14	111.80
2	B	601	4AD	C4-C5-N7	-2.09	108.20	110.58
4	A	608	GOL	C3-C2-C1	-2.08	104.16	111.80
4	A	603	GOL	C3-C2-C1	-2.07	104.19	111.80
2	A	601	4AD	C4-C5-N7	-2.07	108.22	110.58
4	B	608	GOL	C3-C2-C1	-2.06	104.24	111.80
4	A	606	GOL	C3-C2-C1	-2.03	104.34	111.80
2	C	601	4AD	C5-C4-N9	2.02	108.01	105.81
4	A	610	GOL	C3-C2-C1	-2.02	104.40	111.80
3	D	602	2PN	O6-P2-O4	-2.01	108.41	113.45
3	D	602	2PN	O2-P1-O1	-2.00	108.43	113.45
3	C	602	2PN	O5-P2-O4	-2.00	108.43	113.45

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	2PN	P1-N1-P2-O4
3	B	602	2PN	P1-N1-P2-O4
3	C	602	2PN	P2-N1-P1-O1
3	D	602	2PN	P1-N1-P2-O4
4	A	605	GOL	O1-C1-C2-C3
4	D	604	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-C3
4	A	604	GOL	O1-C1-C2-C3
4	A	611	GOL	C1-C2-C3-O3
4	B	605	GOL	C1-C2-C3-O3
4	C	606	GOL	C1-C2-C3-O3
4	D	605	GOL	O1-C1-C2-O2
2	A	601	4AD	CA-CB-CG-ND2
2	B	601	4AD	CA-CB-CG-ND2
4	A	605	GOL	O1-C1-C2-O2
2	A	601	4AD	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	B	601	4AD	CA-CB-CG-OD1
2	C	601	4AD	CA-CB-CG-ND2
4	B	604	GOL	O1-C1-C2-O2
4	C	606	GOL	O2-C2-C3-O3
2	C	601	4AD	CA-CB-CG-OD1
4	A	606	GOL	O1-C1-C2-O2
4	D	604	GOL	O1-C1-C2-O2
4	D	607	GOL	O1-C1-C2-O2
2	D	601	4AD	CA-CB-CG-ND2
4	D	606	GOL	O2-C2-C3-O3
4	C	607	GOL	O1-C1-C2-C3
2	A	601	4AD	C-O3P-P-O5'
2	C	601	4AD	C-O3P-P-O5'
2	D	601	4AD	C-O3P-P-O5'
2	D	601	4AD	CA-CB-CG-OD1
4	A	608	GOL	O1-C1-C2-O2
4	C	604	GOL	O2-C2-C3-O3

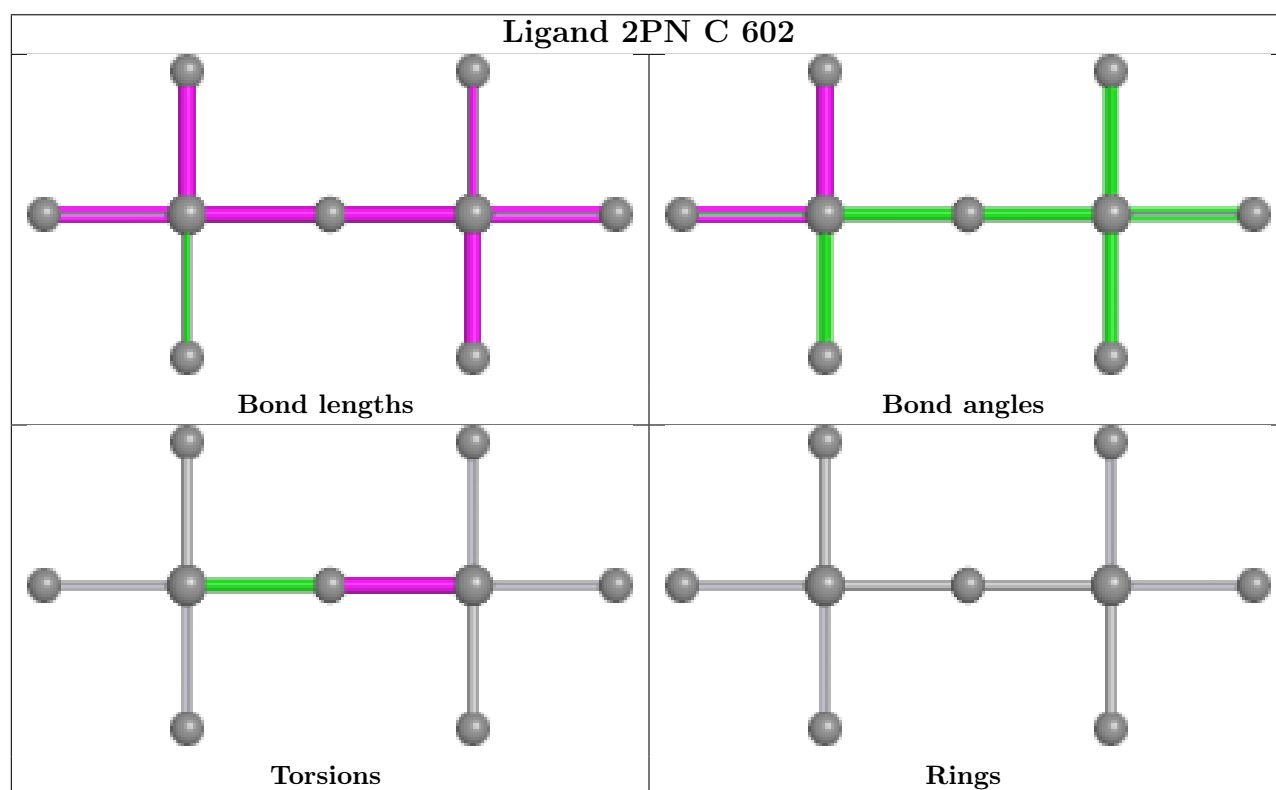
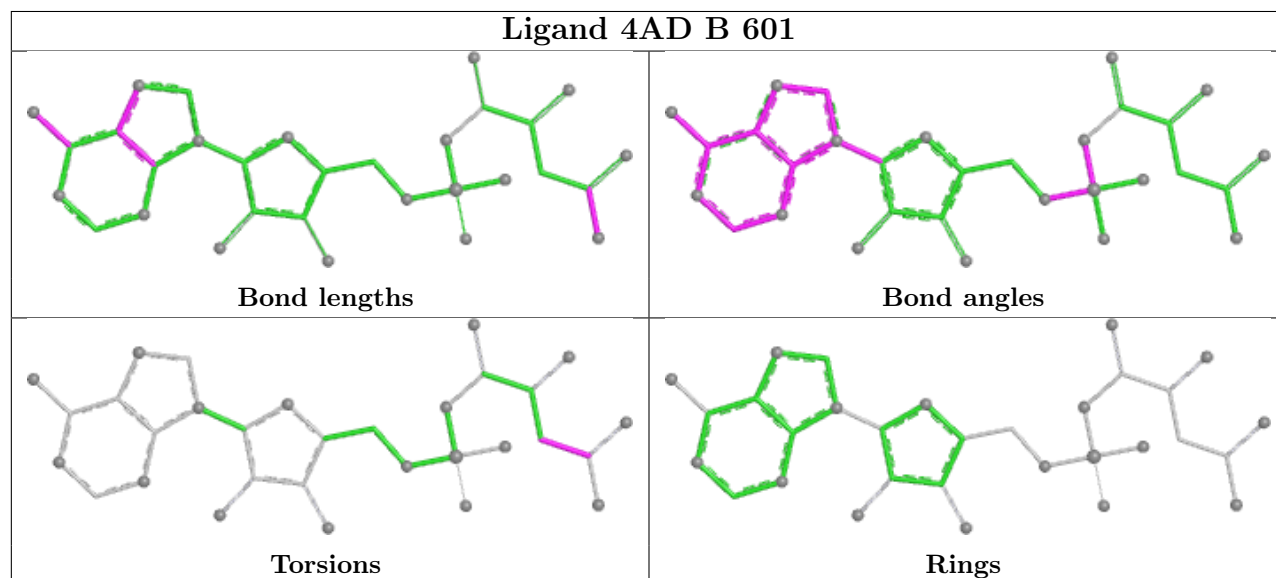
There are no ring outliers.

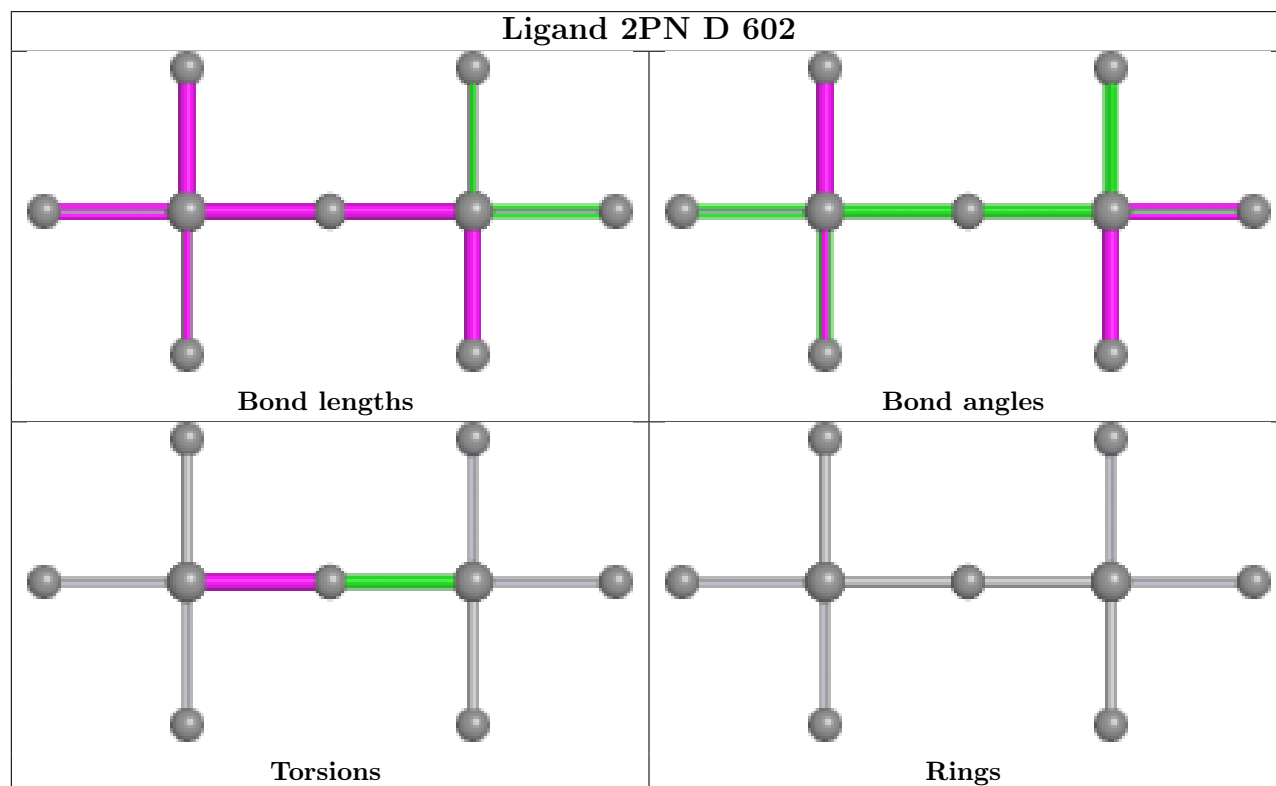
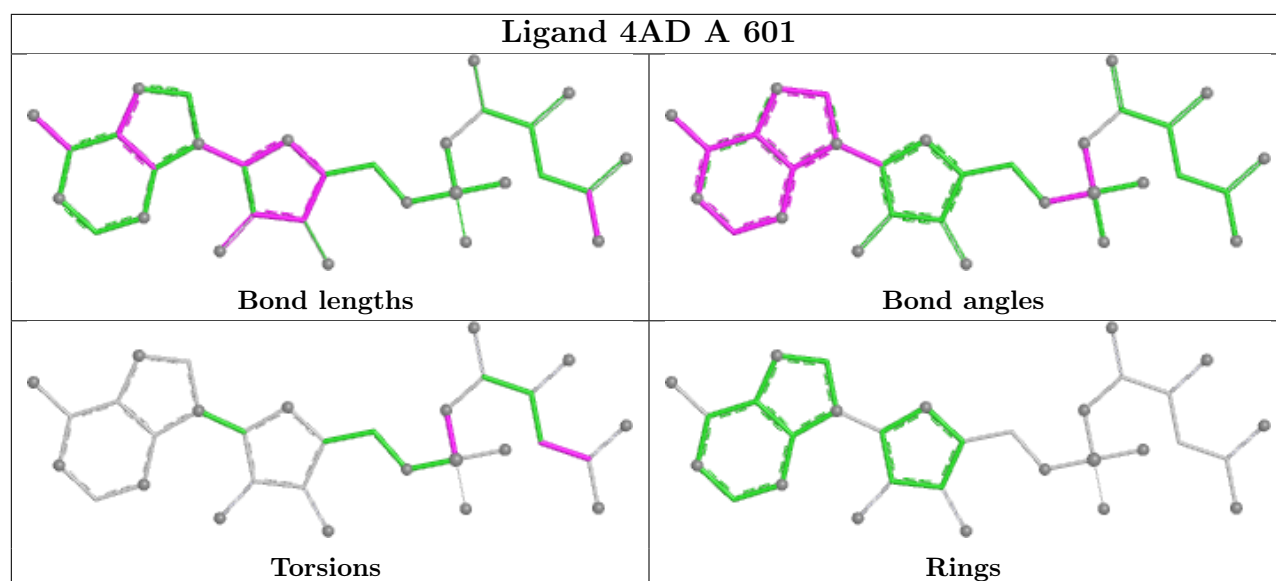
14 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	4AD	1	0
4	A	611	GOL	1	0
2	A	601	4AD	1	0
4	B	608	GOL	1	0
4	A	609	GOL	2	0
4	A	606	GOL	1	0
2	C	601	4AD	1	0
4	C	608	GOL	2	0
4	B	606	GOL	1	0
2	D	601	4AD	1	0
4	C	606	GOL	1	0
4	C	605	GOL	1	0
4	A	605	GOL	1	0
4	C	607	GOL	1	0

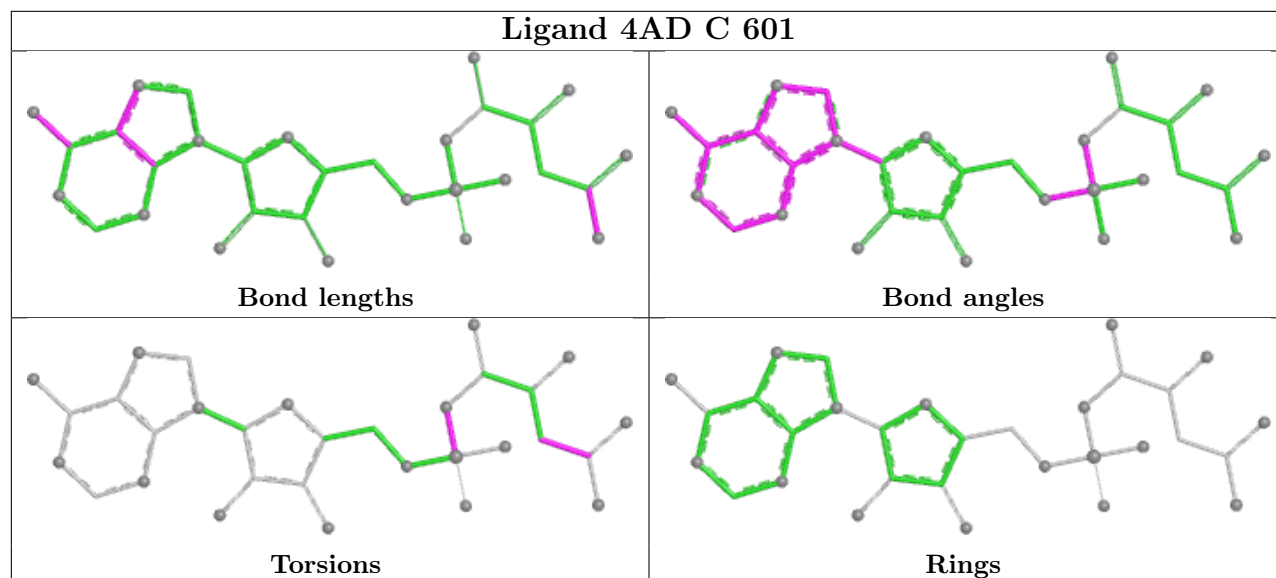
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

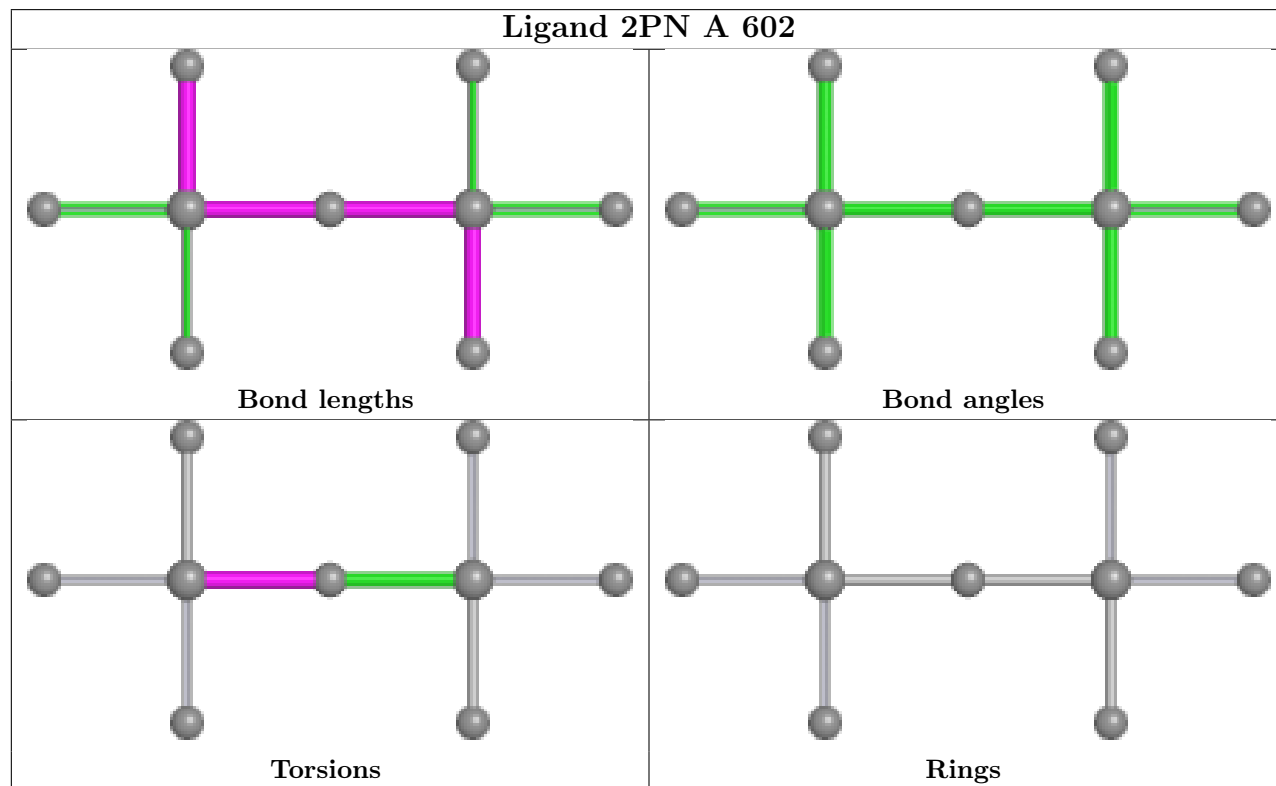


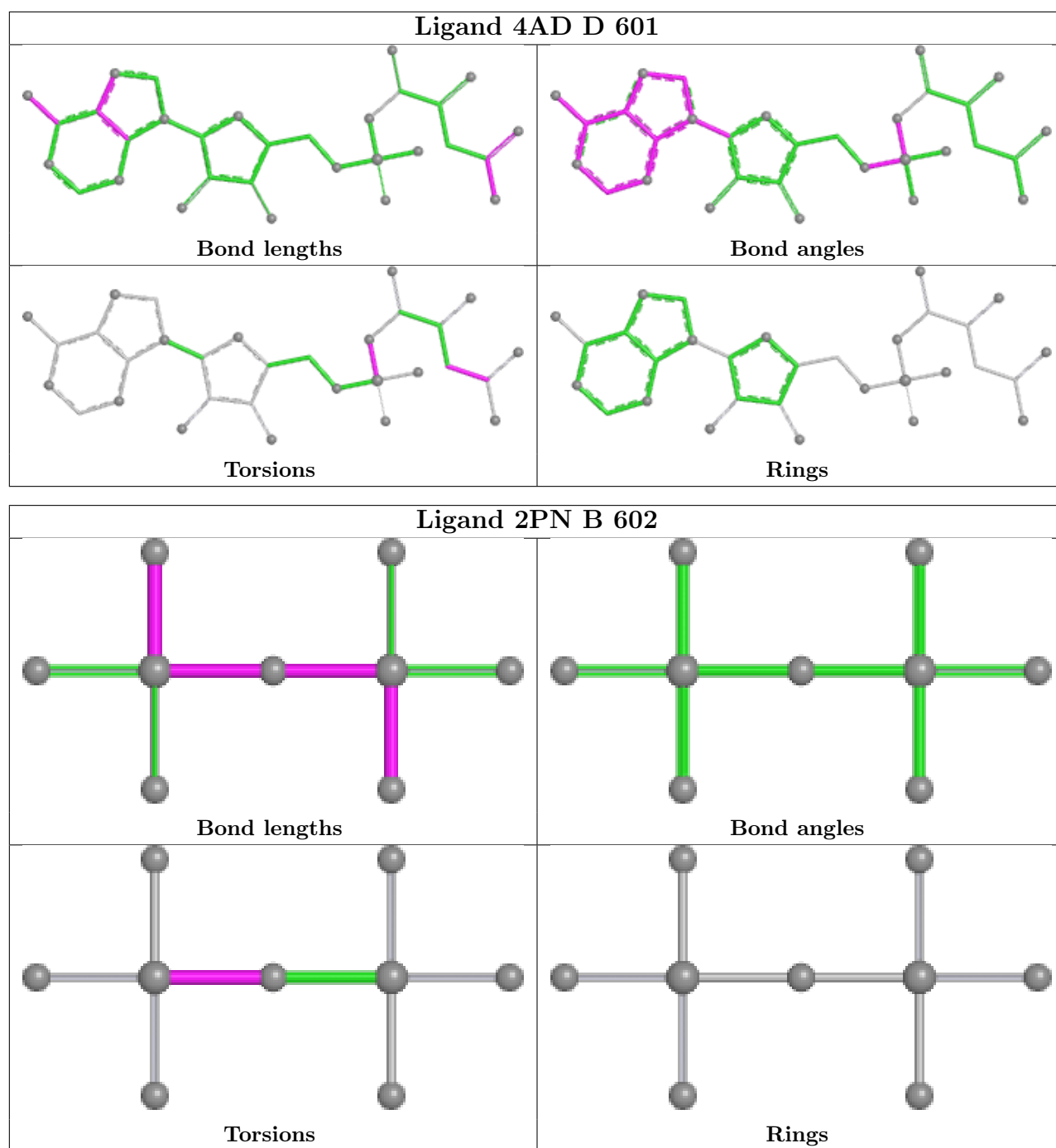


Ligand 4AD C 601



Ligand 2PN A 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/472 (90%)	0.17	9 (2%) 63 67	22, 35, 53, 73	0
1	B	429/472 (90%)	0.14	9 (2%) 63 67	21, 35, 53, 66	0
1	C	428/472 (90%)	0.22	23 (5%) 31 35	22, 38, 62, 87	0
1	D	428/472 (90%)	0.58	29 (6%) 23 26	24, 46, 76, 96	0
All	All	1712/1888 (90%)	0.28	70 (4%) 41 46	21, 38, 63, 96	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	412	PHE	5.7
1	B	224	SER	4.9
1	A	224	SER	4.3
1	A	191	GLY	4.3
1	C	214	GLY	4.1
1	D	214	GLY	4.1
1	C	191	GLY	4.0
1	C	189	PRO	3.9
1	D	189	PRO	3.8
1	D	414	GLU	3.5
1	D	224	SER	3.4
1	C	412	PHE	3.4
1	C	326	SER	3.4
1	A	190	LYS	3.3
1	A	225	ASP	3.3
1	B	547	THR	3.1
1	D	411	THR	3.1
1	D	404	ASP	3.1
1	D	408	GLU	3.0
1	B	111	GLU	3.0
1	D	405	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	402	GLU	3.0
1	B	214	GLY	3.0
1	D	163	GLU	2.9
1	C	404	ASP	2.9
1	C	224	SER	2.9
1	C	391	MET	2.8
1	B	225	ASP	2.8
1	D	398	VAL	2.8
1	D	413	TYR	2.8
1	D	190	LYS	2.8
1	D	147	LEU	2.7
1	C	408	GLU	2.6
1	C	411	THR	2.6
1	C	188	THR	2.5
1	D	326	SER	2.4
1	D	328	THR	2.4
1	B	327	ARG	2.4
1	C	193	GLN	2.4
1	A	112	PRO	2.4
1	C	325	GLN	2.3
1	D	193	GLN	2.3
1	D	468	ASN	2.3
1	D	141	GLY	2.3
1	C	401	LYS	2.3
1	D	532	HIS	2.3
1	B	191	GLY	2.3
1	C	413	TYR	2.3
1	C	547	THR	2.3
1	D	547	THR	2.3
1	C	414	GLU	2.2
1	D	187	LEU	2.2
1	D	284	LEU	2.2
1	C	190	LYS	2.2
1	D	164	LEU	2.2
1	A	328	THR	2.2
1	D	537	CYS	2.2
1	A	547	THR	2.2
1	D	292	GLU	2.1
1	D	327	ARG	2.1
1	B	328	THR	2.1
1	C	385	LYS	2.1
1	B	125	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	142	LYS	2.1
1	C	405	VAL	2.1
1	C	225	ASP	2.0
1	A	327	ARG	2.0
1	C	431	ILE	2.0
1	C	399	TRP	2.0
1	A	532	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
4	GOL	B	608	6/6	0.70	0.20	42,43,48,50	0
4	GOL	D	606	6/6	0.75	0.19	50,52,57,61	0
4	GOL	A	607	6/6	0.79	0.16	46,51,53,53	0
3	2PN	D	602	9/9	0.80	0.11	55,62,67,68	0
4	GOL	D	607	6/6	0.80	0.22	47,50,54,56	0
4	GOL	B	604	6/6	0.82	0.16	40,46,48,48	0
4	GOL	A	603	6/6	0.82	0.14	38,44,49,55	0
4	GOL	C	605	6/6	0.83	0.18	37,40,43,45	0
4	GOL	C	608	6/6	0.83	0.14	45,49,56,58	0
4	GOL	B	605	6/6	0.85	0.21	37,42,46,47	0
4	GOL	A	609	6/6	0.85	0.13	42,44,54,55	0
3	2PN	A	602	9/9	0.85	0.11	49,53,67,68	0
4	GOL	D	604	6/6	0.86	0.19	42,47,54,55	0
3	2PN	C	602	9/9	0.86	0.10	48,59,63,65	0
4	GOL	C	603	6/6	0.86	0.10	39,45,48,52	0
4	GOL	A	610	6/6	0.87	0.18	39,44,48,50	0

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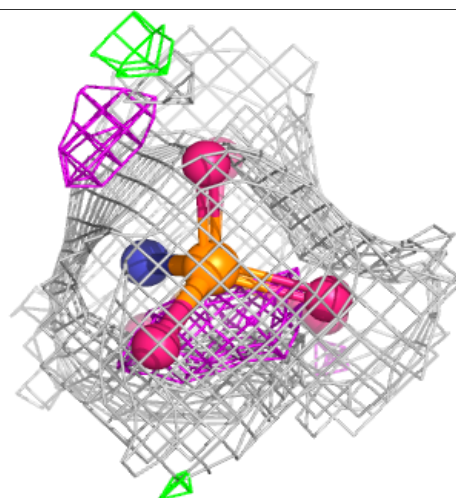
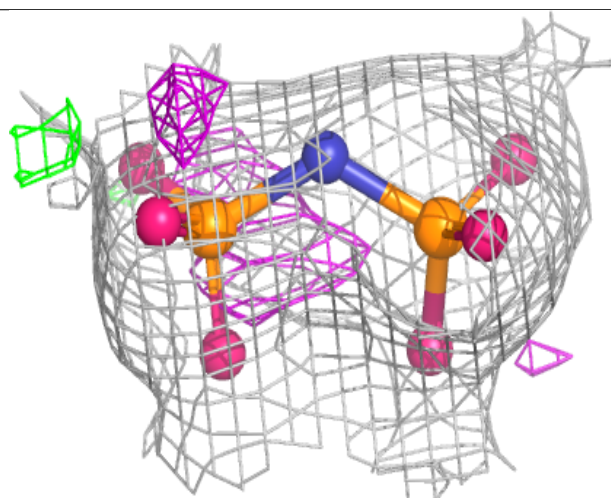
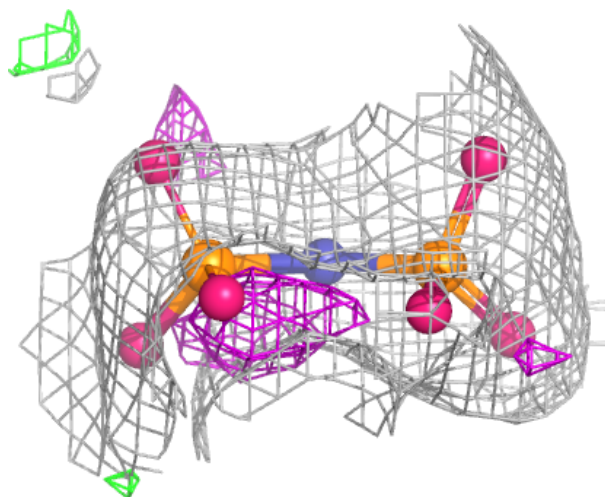
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	611	6/6	0.87	0.23	42,46,50,55	0
3	2PN	B	602	9/9	0.87	0.10	51,52,62,65	0
4	GOL	A	608	6/6	0.87	0.15	46,52,57,57	0
4	GOL	B	606	6/6	0.87	0.12	48,53,58,59	0
4	GOL	A	604	6/6	0.87	0.17	41,47,48,55	0
5	MG	A	613	1/1	0.87	0.10	52,52,52,52	0
4	GOL	D	605	6/6	0.88	0.13	34,39,43,43	0
4	GOL	C	604	6/6	0.88	0.14	39,42,45,46	0
4	GOL	D	603	6/6	0.88	0.10	40,46,47,50	0
4	GOL	C	607	6/6	0.88	0.14	33,41,44,46	0
4	GOL	C	606	6/6	0.91	0.12	30,35,39,41	0
2	4AD	A	601	31/31	0.91	0.10	21,31,39,44	0
4	GOL	A	606	6/6	0.91	0.14	29,38,39,41	0
4	GOL	B	607	6/6	0.93	0.15	33,35,40,47	0
2	4AD	D	601	31/31	0.93	0.09	26,37,42,44	0
5	MG	B	610	1/1	0.93	0.11	48,48,48,48	0
2	4AD	C	601	31/31	0.94	0.08	20,32,35,37	0
2	4AD	B	601	31/31	0.94	0.08	19,32,38,41	0
4	GOL	B	603	6/6	0.95	0.06	35,35,38,41	0
5	MG	C	610	1/1	0.95	0.05	49,49,49,49	0
4	GOL	A	605	6/6	0.96	0.08	33,34,37,45	0
5	MG	D	608	1/1	0.96	0.07	56,56,56,56	0
5	MG	D	609	1/1	0.96	0.05	52,52,52,52	0
5	MG	B	609	1/1	0.98	0.03	49,49,49,49	0
5	MG	C	609	1/1	0.99	0.04	53,53,53,53	0
5	MG	A	612	1/1	0.99	0.02	48,48,48,48	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.

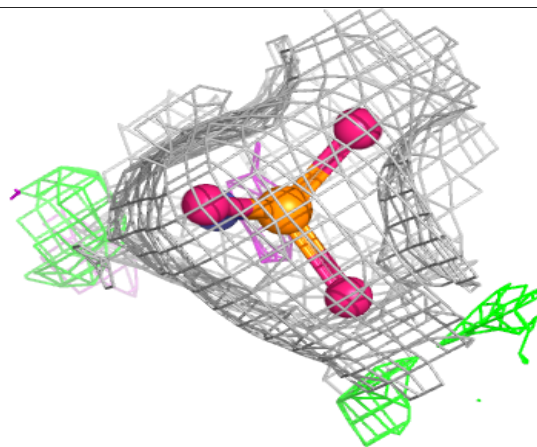
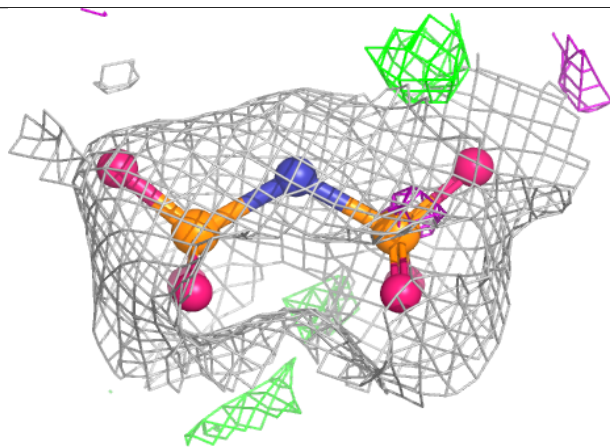
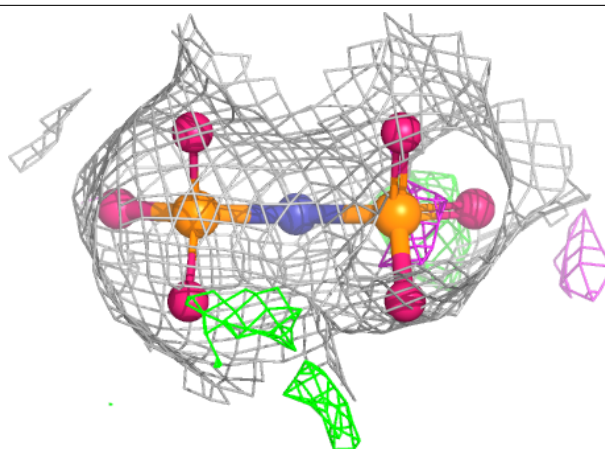
Electron density around 2PN D 602:

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



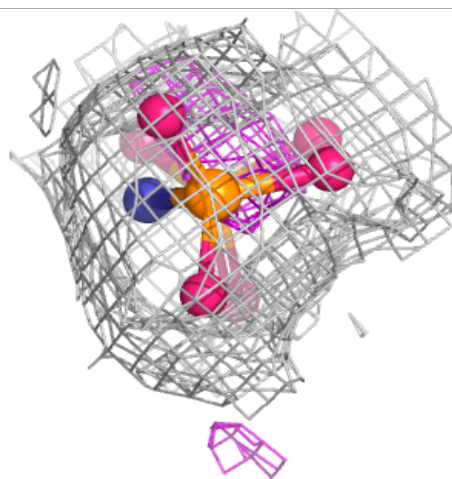
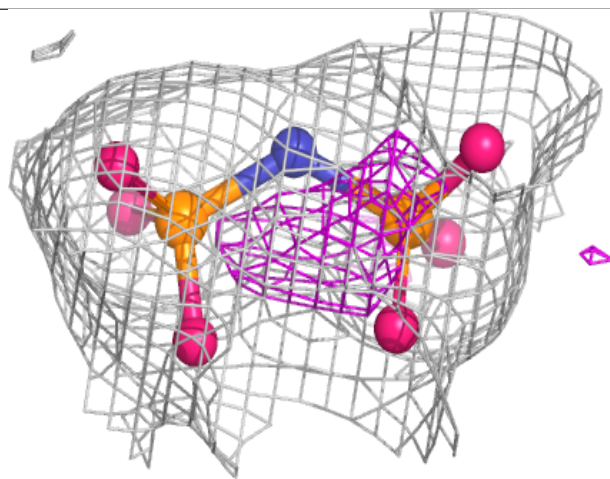
Electron density around 2PN A 602:

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



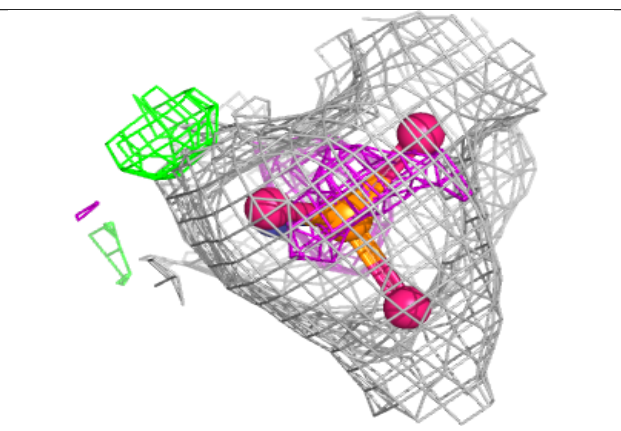
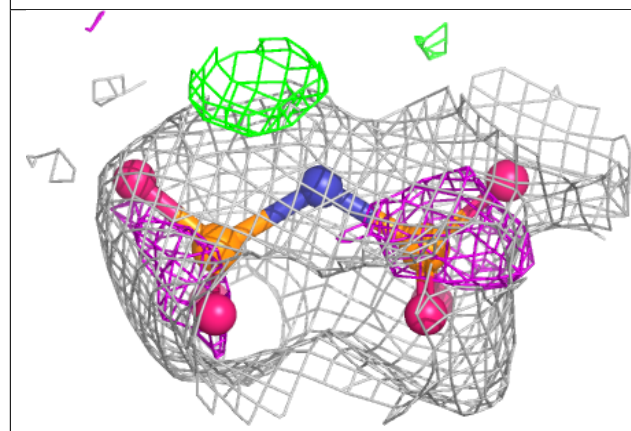
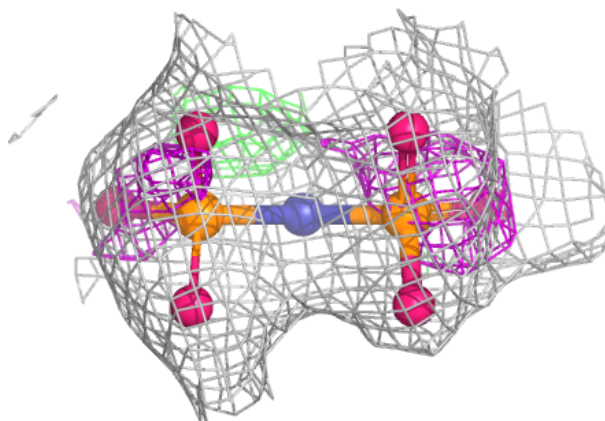
Electron density around 2PN C 602:

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



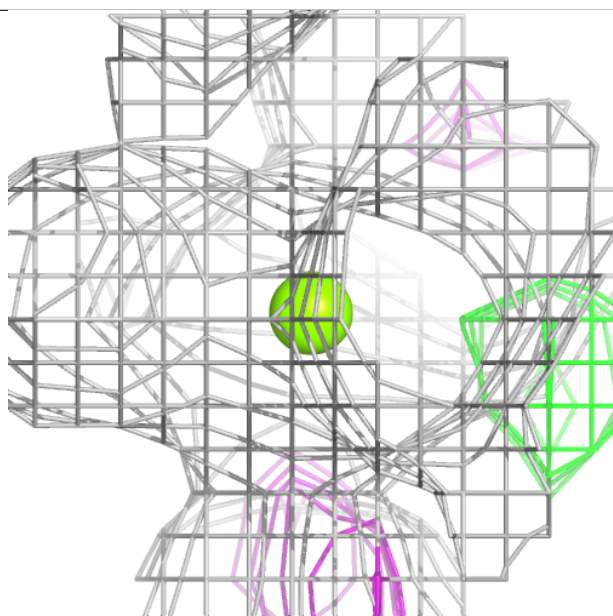
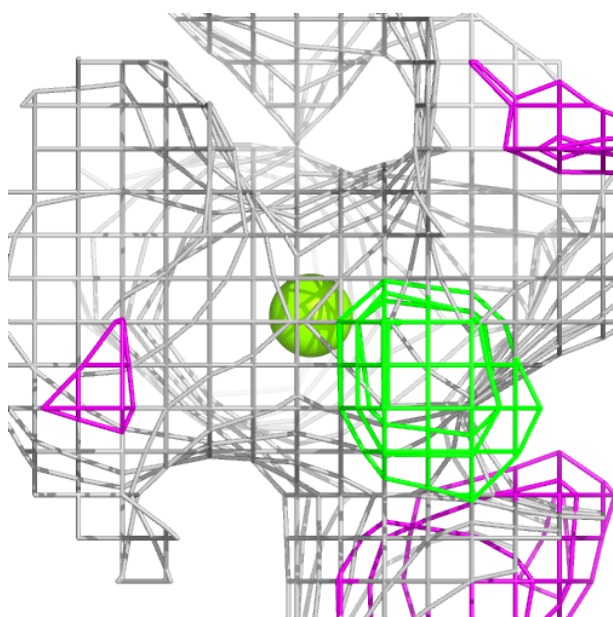
Electron density around 2PN B 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



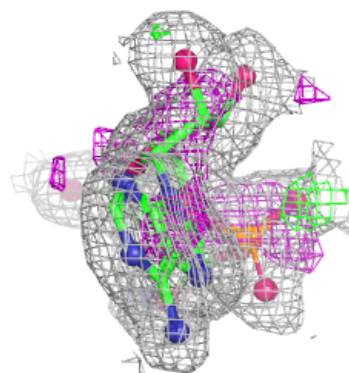
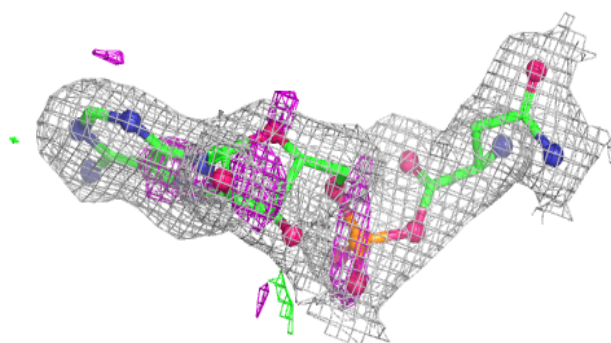
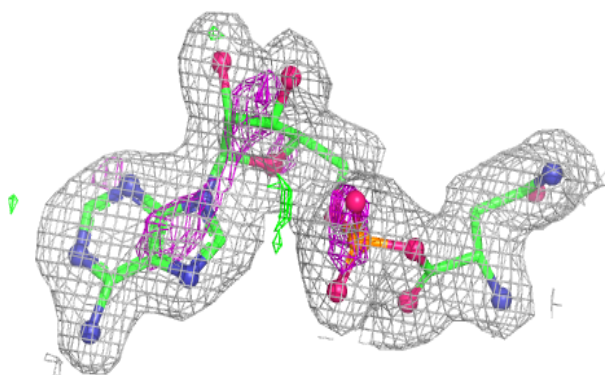
Electron density around MG A 613:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

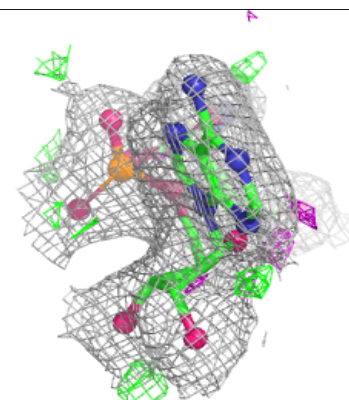
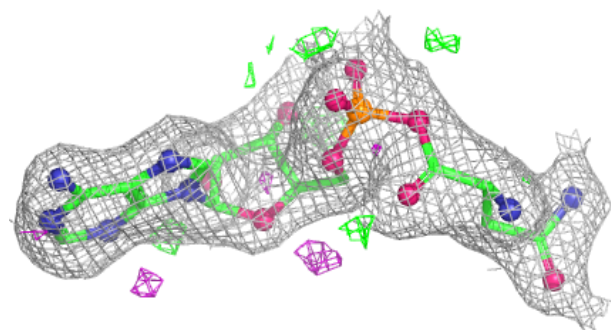
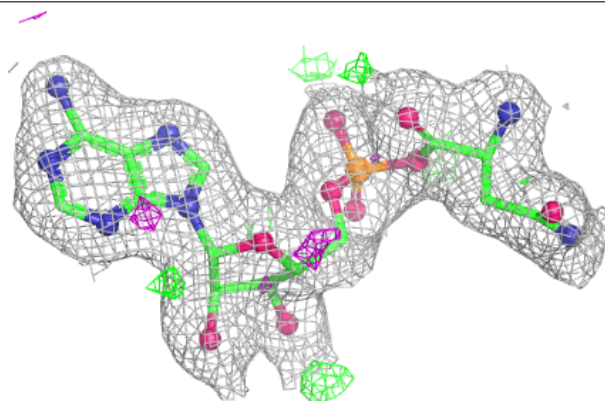


Electron density around 4AD A 601:

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

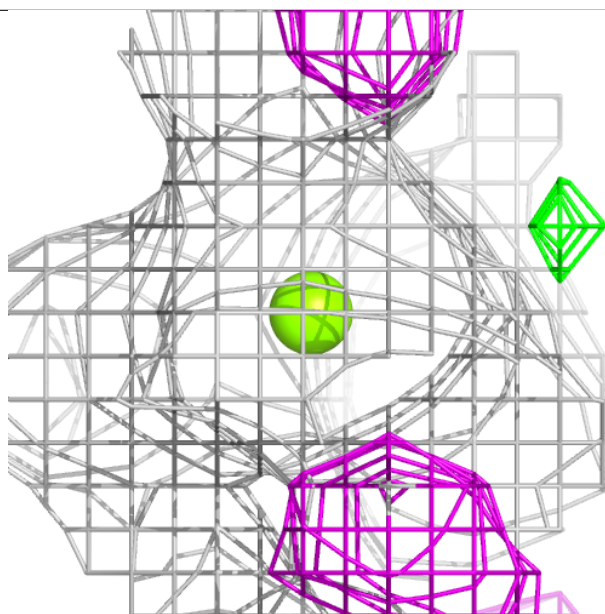
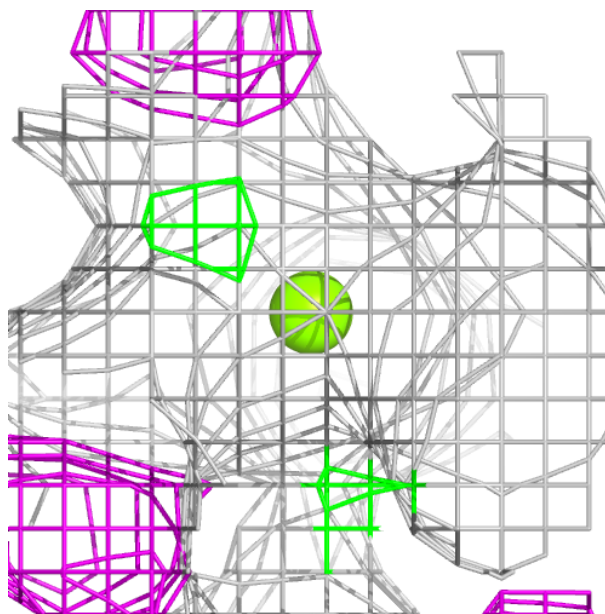
**Electron density around 4AD D 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



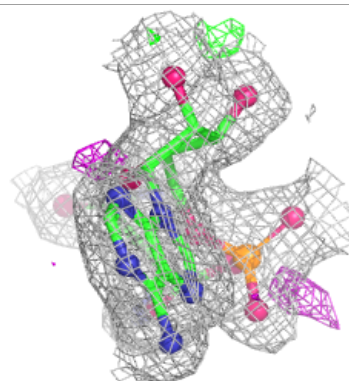
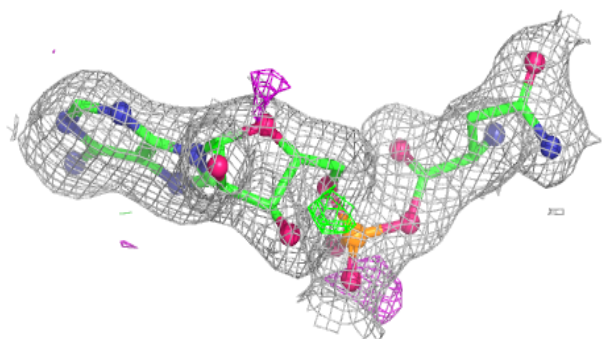
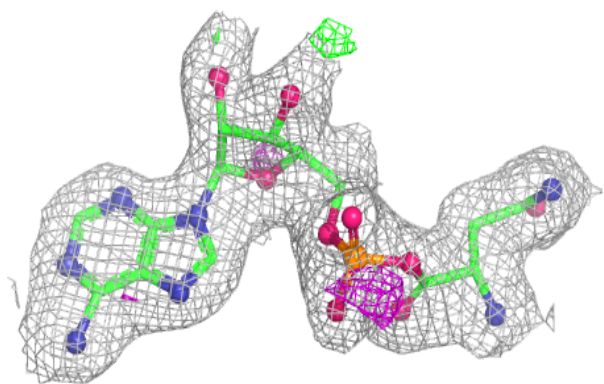
Electron density around MG B 610:

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and green (positive)

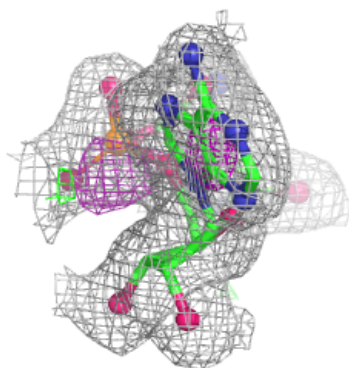
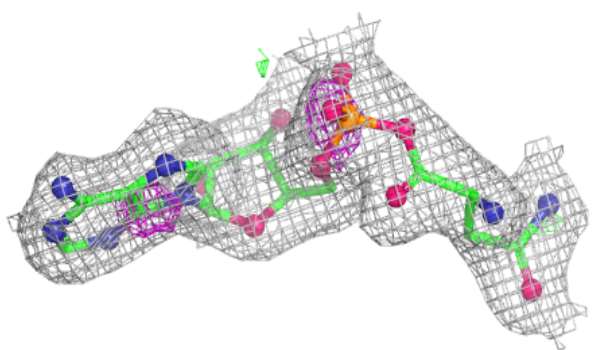
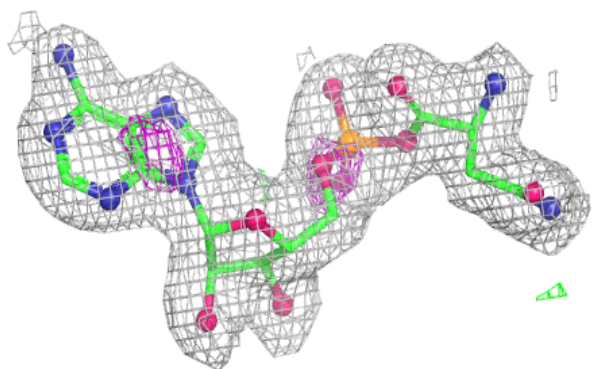


Electron density around 4AD C 601:

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and green (positive)

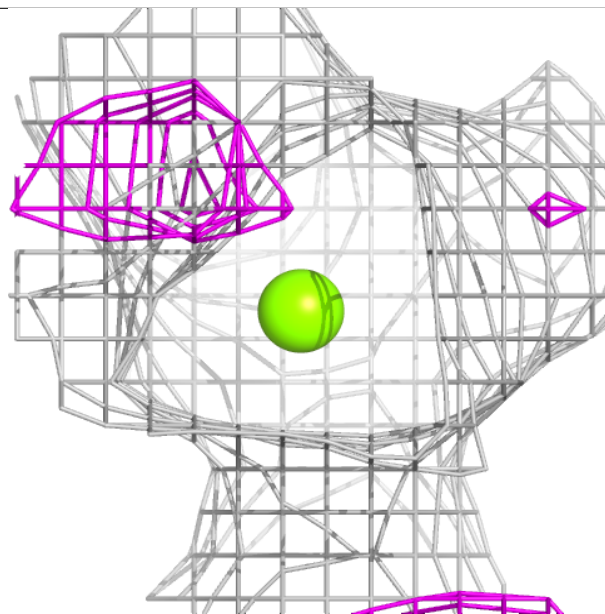
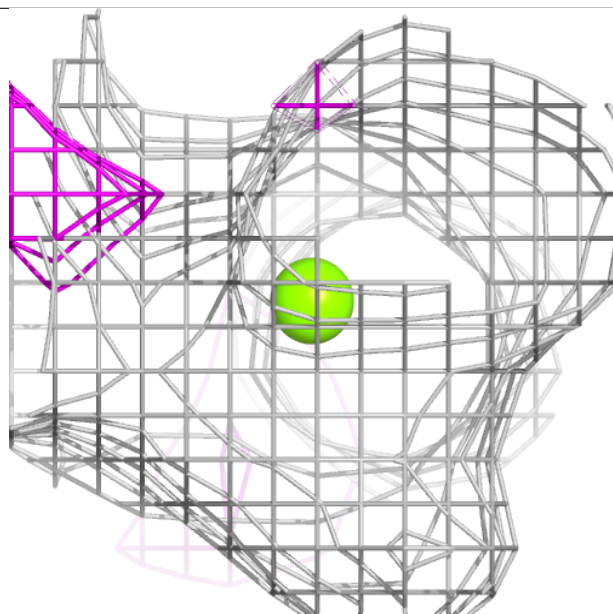
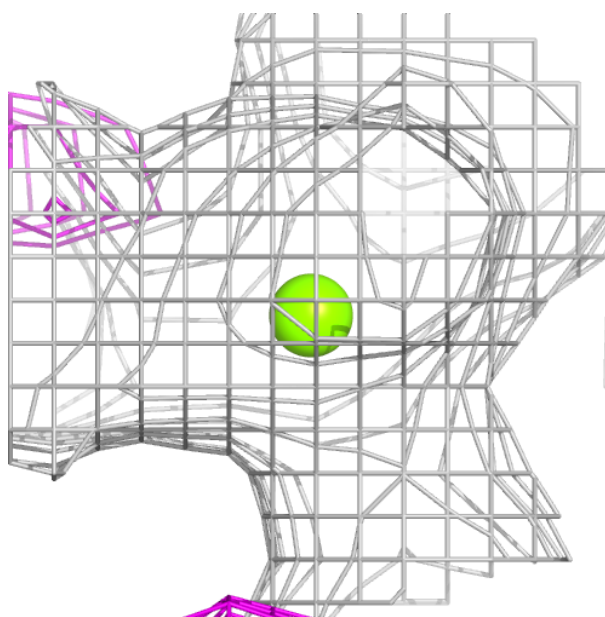
**Electron density around 4AD B 601:**

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



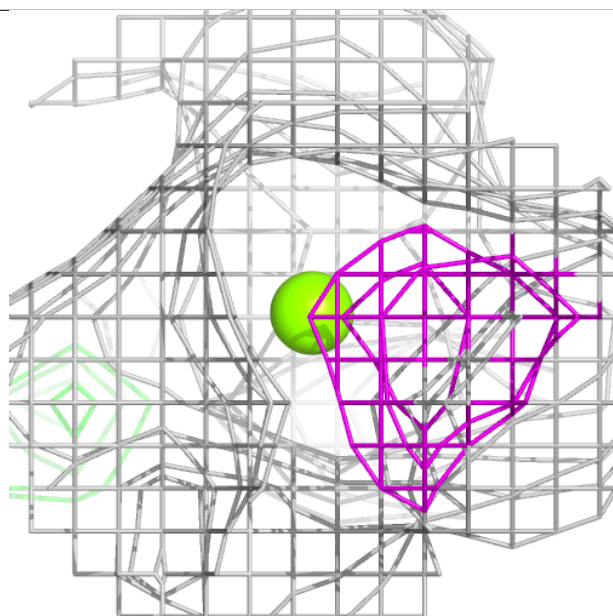
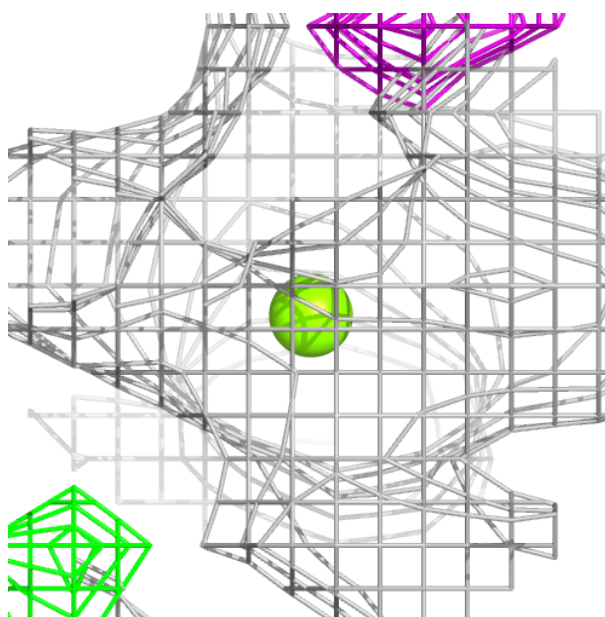
Electron density around MG C 610:

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



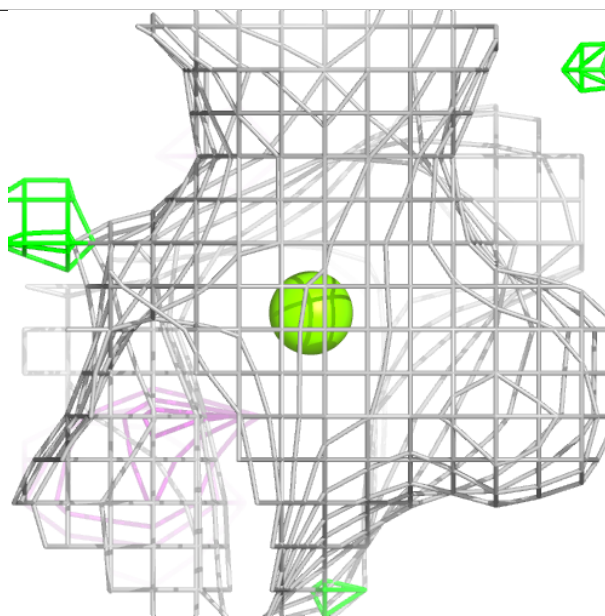
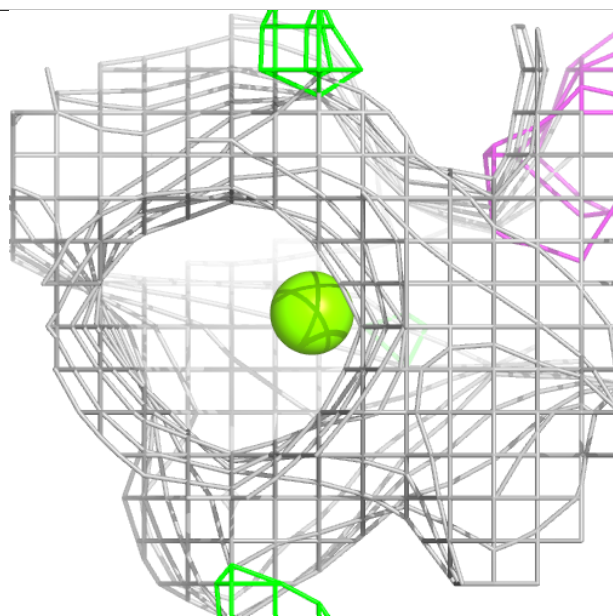
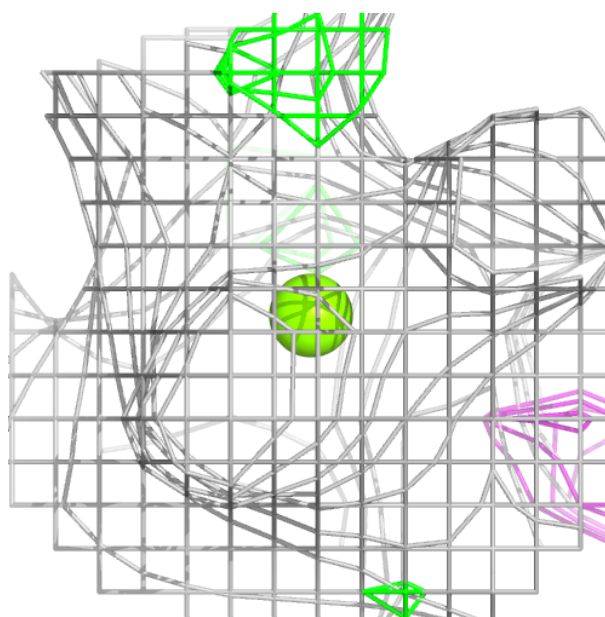
Electron density around MG D 608:

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



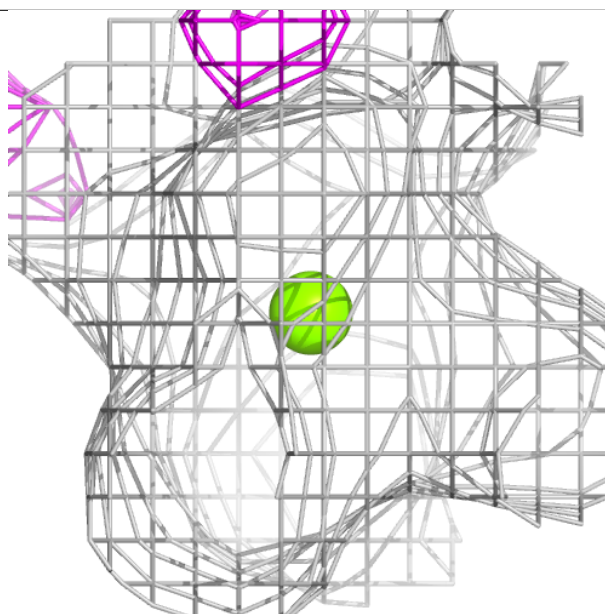
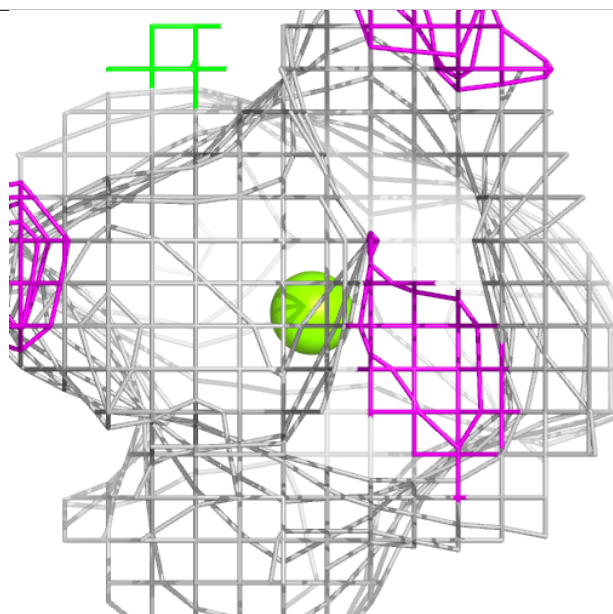
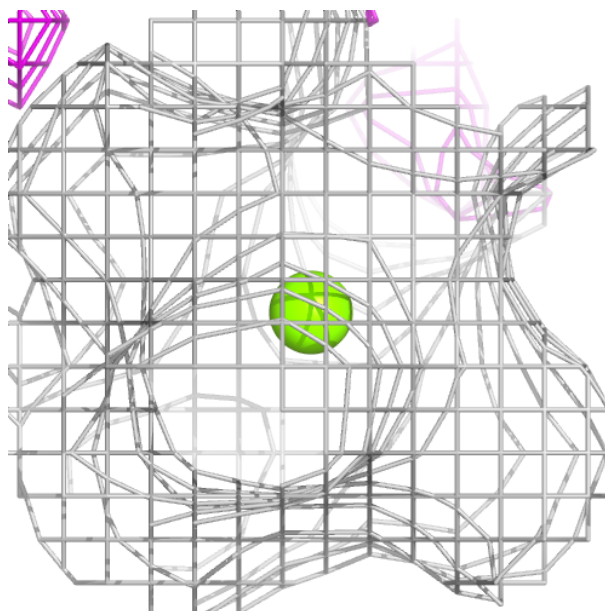
Electron density around MG D 609:

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



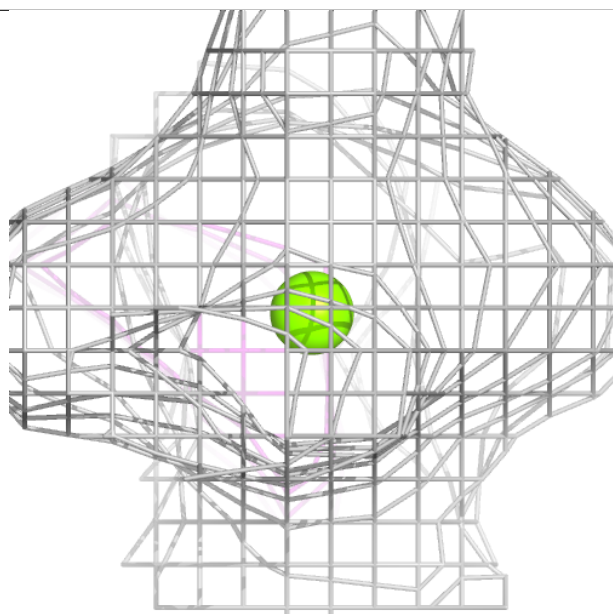
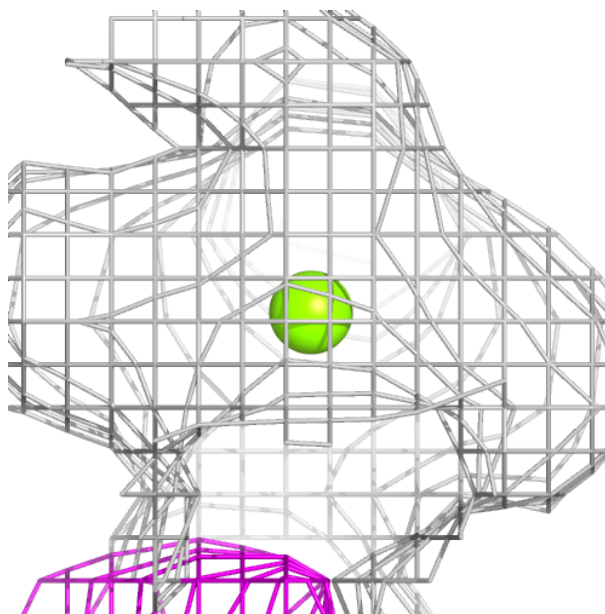
Electron density around MG B 609:

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



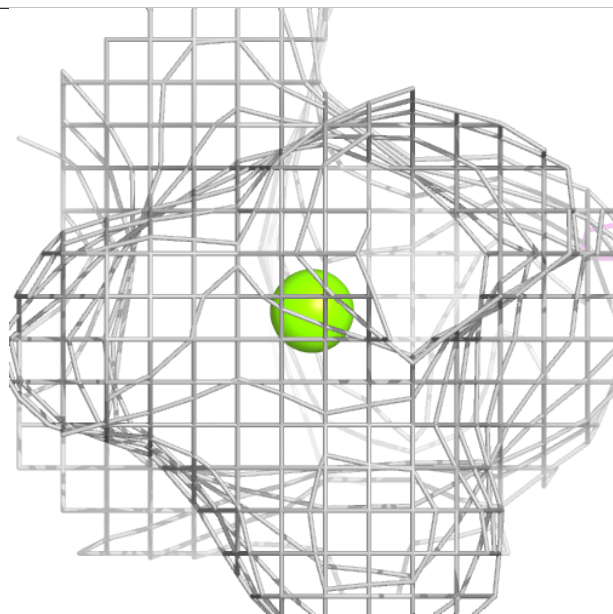
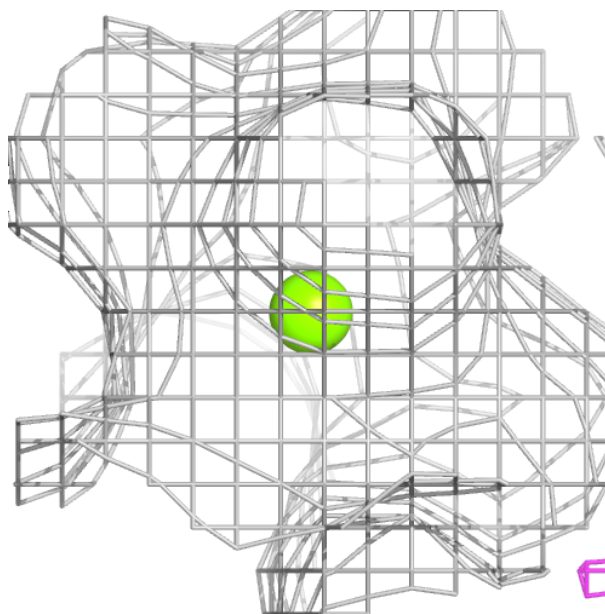
Electron density around MG C 609:

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



Electron density around MG A 612:

$2mF_o-DF_c$ (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.