



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2026 – 12:25 PM JST

PDB ID : 9WP1 / pdb\_00009wp1  
Title : Structural insights into tyrosine sulfation of CCR5 by human tyrosylprotein sulfotransferase-1  
Authors : Tanaka, S.; Asano, H.; Toyoda, K.; Nishiyori, T.; Kojo, H.; Nishimoto, E.; Teramoto, T.; Kakuta, Y.  
Deposited on : 2025-09-08  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

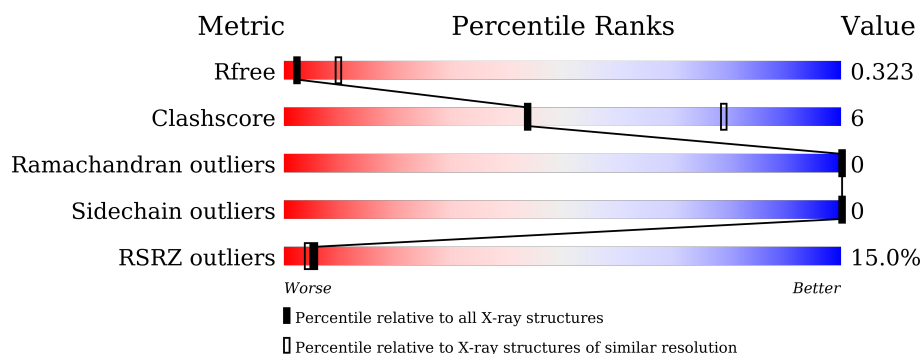
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	276	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
1	B	276	<div> <div>13%</div> <div>84%</div> <div>16%</div> </div>
1	C	276	<div> <div>16%</div> <div>86%</div> <div>14%</div> </div>
1	D	276	<div> <div>14%</div> <div>85%</div> <div>15%</div> </div>
1	E	276	<div> <div>15%</div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	276	
1	G	276	
1	H	276	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	P	6	
2	Q	6	
2	R	6	
2	S	6	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18142 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 Protein-tyrosine sulfotransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			
1	B	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			
1	C	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			
1	D	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			
1	E	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			
1	F	275	Total	C	N	O	S	1	0	0
			2187	1403	382	383	19			
1	G	275	Total	C	N	O	S	0	0	0
			2187	1403	382	383	19			
1	H	276	Total	C	N	O	S	0	0	0
			2195	1407	383	386	19			

- Molecule 2 is a protein called C-C chemokine receptor type 5.

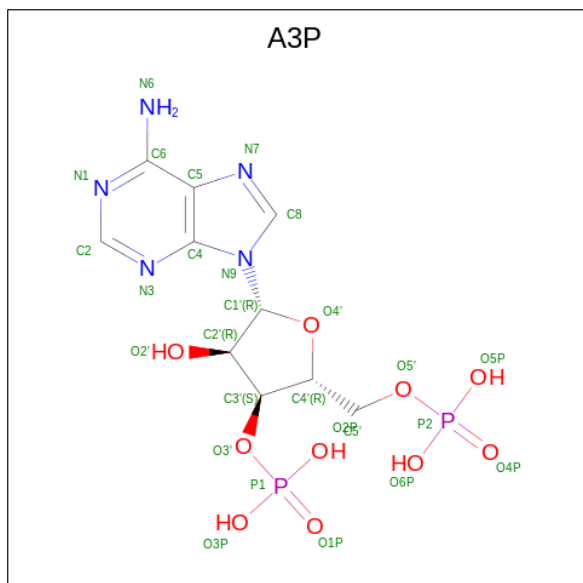
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	6	Total	C	N	O	S	0	0	0
			50	31	7	11	1			
2	M	5	Total	C	N	O	S	0	0	0
			44	28	6	9	1			
2	N	5	Total	C	N	O	S	0	0	0
			44	28	6	9	1			
2	O	5	Total	C	N	O	S	0	0	0
			44	28	6	9	1			
2	P	6	Total	C	N	O	S	0	0	0
			50	31	7	11	1			
2	Q	5	Total	C	N	O	S	0	0	0
			44	28	6	9	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	6	Total	C	N	O	S	0	0	0
			50	31	7	11	1			
2	S	5	Total	C	N	O	S	0	0	0
			44	28	6	9	1			

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

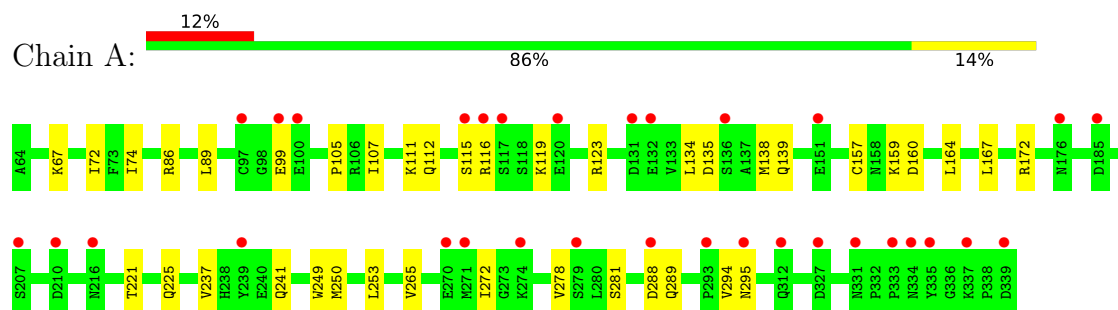
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Zn 1	0	0
5	D	1	Total 1	Zn 1	0	0
5	F	1	Total 1	Zn 1	0	0
5	H	1	Total 1	Zn 1	0	0

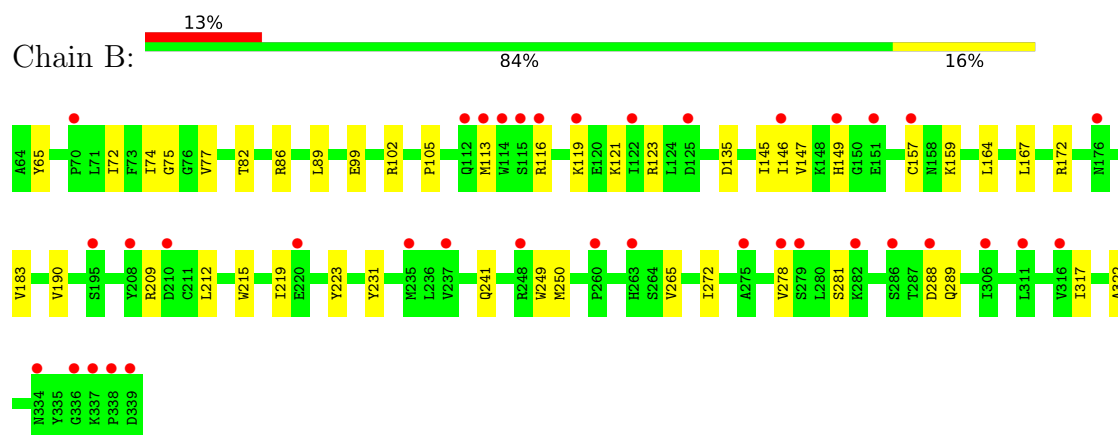
### 3 Residue-property plots [i](#)

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.

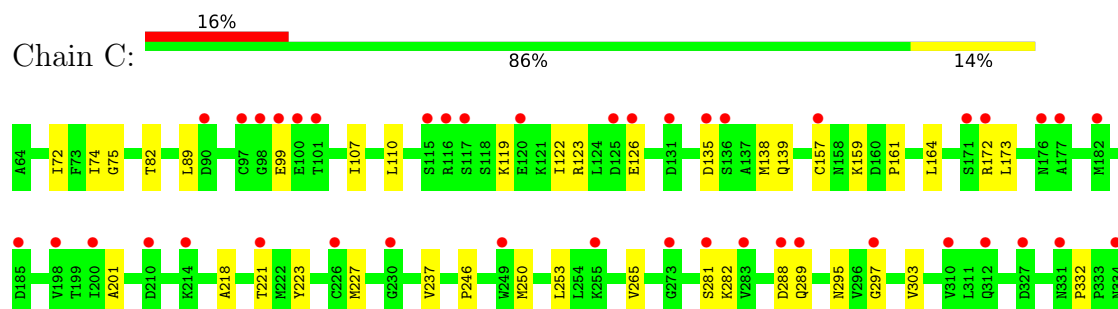
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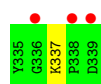


#### • Molecule 1: Protein-tyrosine sulfotransferase 1

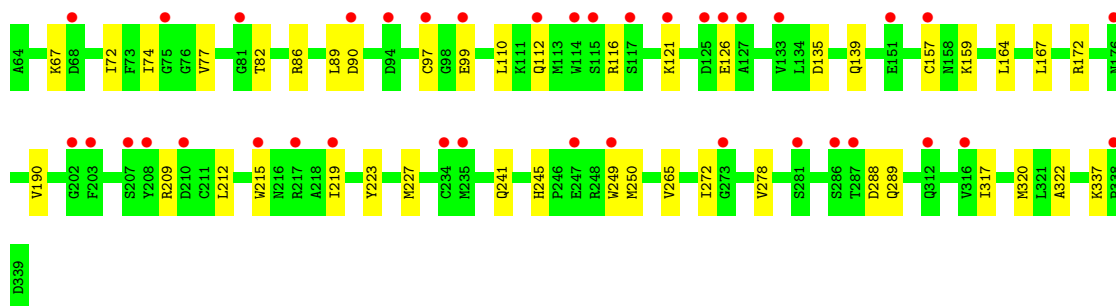
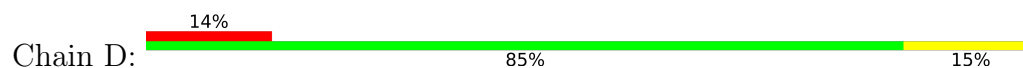


#### • Molecule 1: Protein-tyrosine sulfotransferase 1

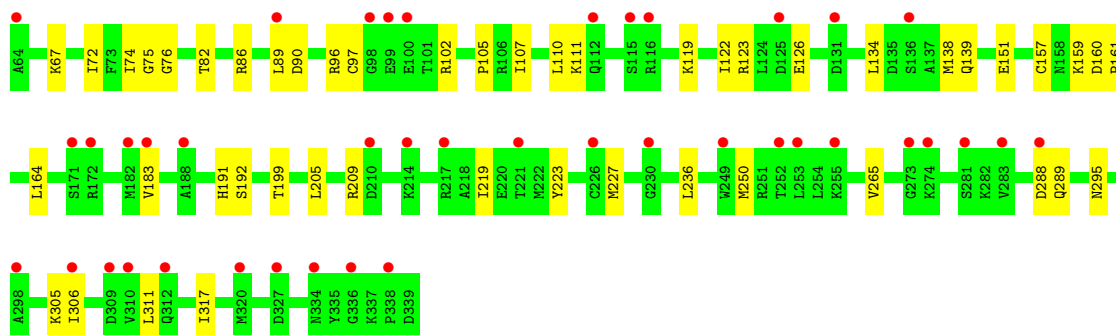
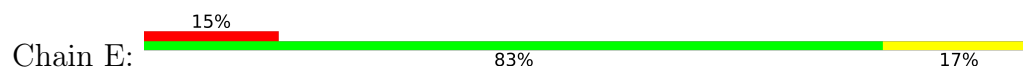




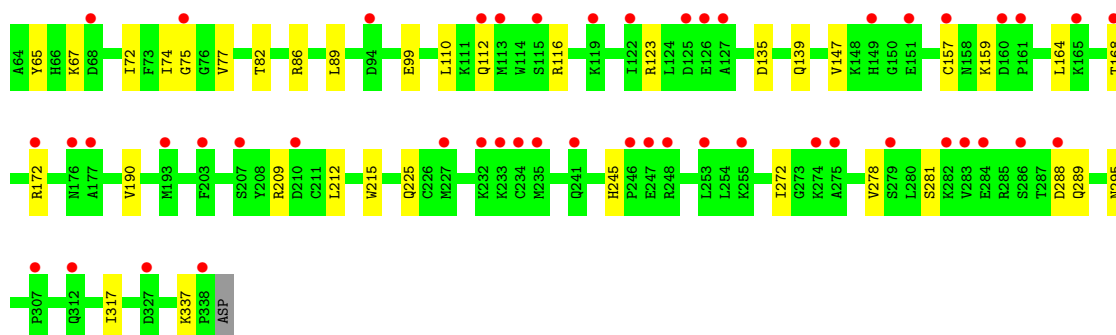
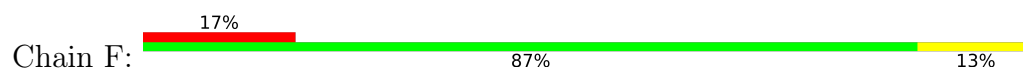
• Molecule 1: Protein-tyrosine sulfotransferase 1



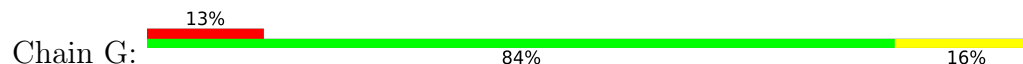
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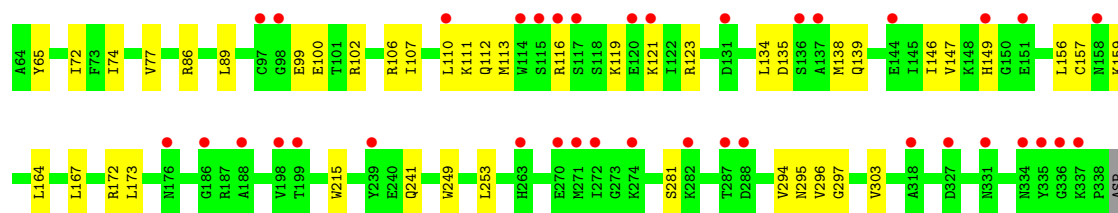
• Molecule 1: Protein-tyrosine sulfotransferase 1



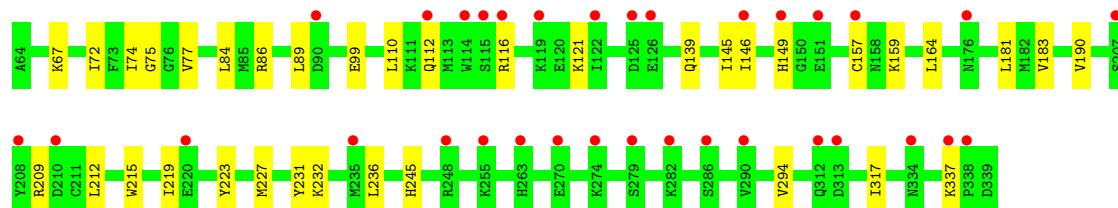
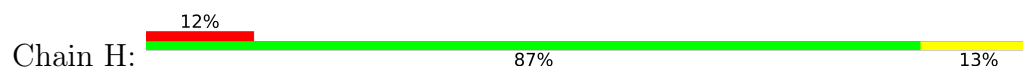
• Molecule 1: Protein-tyrosine sulfotransferase 1



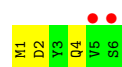




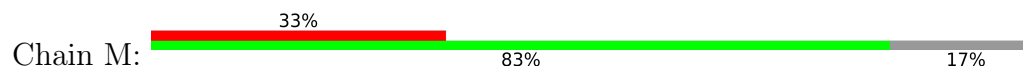
● Molecule 1: Protein-tyrosine sulfotransferase 1



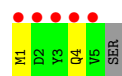
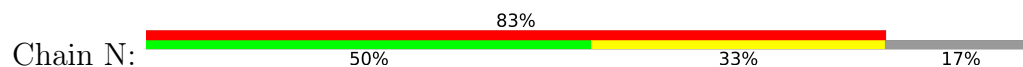
● Molecule 2: C-C chemokine receptor type 5



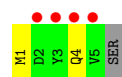
● Molecule 2: C-C chemokine receptor type 5



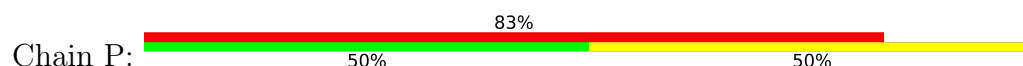
● Molecule 2: C-C chemokine receptor type 5



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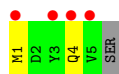


● Molecule 2: C-C chemokine receptor type 5

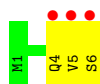




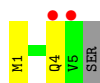
- Molecule 2: C-C chemokine receptor type 5



- Molecule 2: C-C chemokine receptor type 5



- Molecule 2: C-C chemokine receptor type 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.91Å 189.40Å 121.48Å 90.00° 125.98° 90.00°	Depositor
Resolution (Å)	49.21 – 3.20 49.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.21-3.20) 99.3 (49.21-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.273 , 0.323 0.273 , 0.323	Depositor DCC
$R_{free}$ test set	2951 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	1.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	18142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A3P, 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	0.14	0/2248	0.38	0/3042
1	B	0.17	0/2248	0.45	0/3042
1	C	0.17	0/2248	0.45	0/3042
1	D	0.18	0/2248	0.45	0/3042
1	E	0.17	0/2248	0.44	0/3042
1	F	0.18	0/2240	0.46	0/3031
1	G	0.17	0/2240	0.41	0/3031
1	H	0.17	0/2248	0.45	0/3042
2	L	0.10	0/50	0.54	0/66
2	M	0.37	0/44	0.53	0/58
2	N	0.30	0/44	0.61	0/58
2	O	0.21	0/44	0.63	0/58
2	P	0.49	0/50	1.25	0/66
2	Q	0.18	0/44	0.26	0/58
2	R	0.50	0/50	1.13	0/66
2	S	0.29	0/44	0.52	0/58
All	All	0.18	0/18338	0.45	0/24802

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

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	2195	0	2239	23	0
1	B	2195	0	2239	34	0
1	C	2195	0	2239	28	0
1	D	2195	0	2239	30	0
1	E	2195	0	2239	30	0
1	F	2187	0	2235	22	0
1	G	2187	0	2235	35	0
1	H	2195	0	2239	24	0
2	L	50	0	46	3	0
2	M	44	0	41	0	0
2	N	44	0	41	4	0
2	O	44	0	41	1	0
2	P	50	0	46	3	0
2	Q	44	0	41	1	0
2	R	50	0	46	3	0
2	S	44	0	41	1	0
3	A	27	0	11	2	0
3	B	27	0	11	0	0
3	C	27	0	11	2	0
3	D	27	0	11	1	0
3	E	27	0	11	3	0
3	F	27	0	11	1	0
3	G	27	0	11	1	0
3	H	27	0	11	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
All	All	18142	0	18335	223	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 6.

All (223) 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)
2:N:1:MET:HB2	2:N:4:GLN:HG2	1.53	0.90
1:G:110:LEU:HD12	1:H:110:LEU:HD22	1.52	0.89
2:L:1:MET:HB2	2:L:4:GLN:HG2	1.65	0.77
1:D:245:HIS:NE2	1:D:337:LYS:O	2.19	0.75
1:C:72:ILE:HB	1:C:157:CYS:HB3	1.71	0.73
1:E:72:ILE:HB	1:E:157:CYS:HB3	1.71	0.73
1:D:288:ASP:OD1	1:D:289:GLN:NE2	2.21	0.72
1:A:72:ILE:HB	1:A:157:CYS:HB3	1.71	0.72
1:H:245:HIS:NE2	1:H:337:LYS:O	2.23	0.72
2:Q:1:MET:HB2	2:Q:4:GLN:HG2	1.71	0.70
1:F:288:ASP:OD1	1:F:289:GLN:NE2	2.24	0.70
1:G:72:ILE:HB	1:G:157:CYS:HB3	1.73	0.70
1:F:86:ARG:HG2	1:F:159:LYS:HD3	1.75	0.68
1:D:227:MET:HE2	1:G:296:VAL:H	1.57	0.67
1:B:86:ARG:HG2	1:B:159:LYS:HD3	1.75	0.66
1:G:241:GLN:HG3	1:G:249:TRP:NE1	2.11	0.66
1:H:72:ILE:HB	1:H:157:CYS:HB3	1.78	0.65
1:F:72:ILE:HB	1:F:157:CYS:HB3	1.78	0.64
1:B:72:ILE:HB	1:B:157:CYS:HB3	1.80	0.64
1:D:74:ILE:HD11	1:D:89:LEU:HD12	1.79	0.64
1:A:288:ASP:OD1	1:A:289:GLN:NE2	2.30	0.64
1:D:86:ARG:HG2	1:D:159:LYS:HD3	1.79	0.64
1:A:86:ARG:HG2	1:A:159:LYS:HD3	1.80	0.63
2:O:1:MET:HB2	2:O:4:GLN:HG2	1.81	0.62
1:G:65:TYR:CG	1:G:147:VAL:HG21	2.33	0.62
1:G:106:ARG:HH21	2:R:4:GLN:HG3	1.64	0.62
1:F:135:ASP:OD2	1:F:172:ARG:NH1	2.28	0.62
1:H:183:VAL:HG22	1:H:219:ILE:HD11	1.81	0.61
1:C:288:ASP:OD1	1:C:289:GLN:NE2	2.34	0.60
1:G:74:ILE:HD11	1:G:89:LEU:HD12	1.83	0.60
1:B:288:ASP:OD1	1:B:289:GLN:NE2	2.34	0.60
1:D:135:ASP:OD2	1:D:172:ARG:NH1	2.30	0.60
1:E:223:TYR:O	1:E:227:MET:HG2	2.01	0.60
1:G:86:ARG:HG2	1:G:159:LYS:HD2	1.84	0.60
1:D:72:ILE:HB	1:D:157:CYS:HB3	1.83	0.59
1:C:74:ILE:HD11	1:C:89:LEU:HD12	1.85	0.59
1:E:74:ILE:HD11	1:E:89:LEU:HD12	1.84	0.59
1:B:322:ALA:HB1	1:C:303:VAL:HG11	1.85	0.59
1:F:74:ILE:HD11	1:F:89:LEU:HD12	1.84	0.59
1:E:105:PRO:HG3	1:E:160:ASP:HB3	1.85	0.58
1:B:113:MET:HA	1:B:116:ARG:HG2	1.84	0.58
1:F:245:HIS:NE2	1:F:337:LYS:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:ILE:O	1:H:149:HIS:CD2	2.57	0.58
1:C:159:LYS:HE2	1:C:161:PRO:HD3	1.86	0.57
1:D:77:VAL:HG11	1:D:215:TRP:HD1	1.69	0.57
1:F:123:ARG:HH12	2:P:2:ASP:HA	1.70	0.57
1:E:86:ARG:HG2	1:E:159:LYS:HD3	1.87	0.56
1:G:112:GLN:HG2	1:G:116:ARG:HE	1.70	0.56
1:H:86:ARG:HG2	1:H:159:LYS:HD3	1.87	0.56
1:H:74:ILE:HD11	1:H:89:LEU:HD12	1.87	0.56
1:B:65:TYR:CG	1:B:147:VAL:HG21	2.41	0.55
1:G:146:ILE:HA	1:G:149:HIS:CD2	2.42	0.55
1:F:99:GLU:HG2	1:F:281:SER:HB2	1.89	0.55
1:G:294:VAL:HA	3:G:401:A3P:HN62	1.72	0.55
1:G:112:GLN:O	1:G:116:ARG:HG3	2.08	0.54
1:B:99:GLU:HG2	1:B:281:SER:HB2	1.90	0.54
1:B:183:VAL:HG22	1:B:219:ILE:HD11	1.90	0.53
1:A:99:GLU:HG2	1:A:281:SER:HB2	1.91	0.53
1:B:250:MET:HE2	1:B:265:VAL:HB	1.91	0.53
1:A:241:GLN:HB3	1:A:249:TRP:NE1	2.24	0.52
1:D:322:ALA:HB1	1:G:303:VAL:HG11	1.90	0.52
1:G:111:LYS:HE2	1:G:134:LEU:HD13	1.91	0.52
1:D:190:VAL:HG21	1:D:212:LEU:HG	1.91	0.52
1:E:192:SER:OG	3:E:401:A3P:O2P	2.26	0.52
1:H:72:ILE:O	1:H:157:CYS:HA	2.10	0.52
1:D:223:TYR:OH	1:G:297:GLY:HA2	2.11	0.51
1:G:106:ARG:HH21	2:R:4:GLN:CG	2.22	0.51
1:B:241:GLN:HB3	1:B:249:TRP:HE1	1.76	0.51
1:G:135:ASP:OD2	1:G:172:ARG:NH1	2.37	0.51
1:C:201:ALA:HA	2:N:1:MET:HE1	1.93	0.51
1:G:100:GLU:OE2	1:G:159:LYS:NZ	2.31	0.51
1:C:110:LEU:HD22	1:D:110:LEU:HD22	1.93	0.50
1:F:72:ILE:O	1:F:157:CYS:HA	2.11	0.50
1:G:139:GLN:NE2	1:G:173:LEU:O	2.43	0.50
1:H:145:ILE:O	1:H:149:HIS:HD2	1.94	0.50
1:B:74:ILE:HD11	1:B:89:LEU:HD12	1.93	0.49
1:H:146:ILE:O	1:H:149:HIS:CD2	2.65	0.49
1:E:288:ASP:OD1	1:E:289:GLN:NE2	2.45	0.49
1:B:65:TYR:CD2	1:B:147:VAL:HG21	2.47	0.49
1:F:168:THR:HG23	1:F:225:GLN:HB3	1.93	0.49
1:H:77:VAL:HG11	1:H:215:TRP:HD1	1.78	0.49
1:C:237:VAL:HG21	1:C:253:LEU:HD21	1.95	0.49
1:F:77:VAL:HG11	1:F:215:TRP:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:HG2	1:C:281:SER:HB2	1.94	0.48
1:A:107:ILE:HG23	1:A:138:MET:HE1	1.94	0.48
1:G:110:LEU:HA	1:G:113:MET:HE3	1.94	0.48
1:H:190:VAL:HG21	1:H:212:LEU:HG	1.96	0.48
1:E:183:VAL:HG22	1:E:219:ILE:HD11	1.94	0.48
1:A:105:PRO:HG3	1:A:160:ASP:HB3	1.95	0.48
1:F:112:GLN:O	1:F:116:ARG:HG3	2.14	0.48
1:B:146:ILE:HA	1:B:149:HIS:CD2	2.49	0.47
1:B:322:ALA:HB1	1:C:303:VAL:CG1	2.44	0.47
1:E:102:ARG:O	1:E:105:PRO:HD2	2.14	0.47
1:H:99:GLU:N	1:H:99:GLU:OE1	2.47	0.47
1:F:67:LYS:HD2	1:F:139:GLN:NE2	2.29	0.47
1:F:245:HIS:CE1	1:F:337:LYS:O	2.67	0.47
1:C:250:MET:HE2	1:C:265:VAL:HB	1.96	0.47
1:D:72:ILE:O	1:D:157:CYS:HA	2.14	0.47
1:E:110:LEU:HD22	1:F:110:LEU:HD22	1.96	0.47
1:A:119:LYS:O	1:A:123:ARG:HG3	2.14	0.47
1:B:99:GLU:OE1	1:B:99:GLU:N	2.46	0.47
1:E:199:THR:HA	1:E:205:LEU:HD11	1.97	0.47
1:F:272:ILE:HD13	1:F:278:VAL:HB	1.97	0.46
1:H:75:GLY:HA3	1:H:164:LEU:HD13	1.98	0.46
1:B:102:ARG:O	1:B:105:PRO:HD2	2.15	0.46
1:C:135:ASP:OD2	1:C:172:ARG:NH1	2.44	0.46
1:D:164:LEU:O	1:D:167:LEU:HB2	2.16	0.46
1:E:288:ASP:OD1	1:E:288:ASP:N	2.44	0.46
1:F:295:ASN:O	3:F:401:A3P:H2	2.15	0.46
2:P:5:VAL:O	2:P:6:SER:C	2.57	0.46
1:A:72:ILE:O	1:A:157:CYS:HA	2.16	0.46
1:C:223:TYR:O	1:C:227:MET:HG2	2.16	0.46
1:E:250:MET:HE2	1:E:265:VAL:HB	1.97	0.46
2:R:5:VAL:O	2:R:6:SER:C	2.58	0.46
1:D:112:GLN:O	1:D:116:ARG:HG3	2.16	0.46
1:D:241:GLN:HB3	1:D:249:TRP:NE1	2.31	0.46
1:E:119:LYS:O	1:E:123:ARG:HG3	2.17	0.45
1:D:272:ILE:HD13	1:D:278:VAL:HB	1.98	0.45
1:D:227:MET:CE	1:G:296:VAL:H	2.27	0.45
1:B:77:VAL:HG11	1:B:215:TRP:HD1	1.82	0.45
1:E:96:ARG:NE	1:E:151:GLU:O	2.26	0.45
1:A:250:MET:HE2	1:A:265:VAL:HB	1.98	0.45
1:A:294:VAL:HA	3:A:401:A3P:HN62	1.82	0.45
1:E:306:ILE:HB	1:E:311:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:TYR:CE1	1:H:227:MET:HE3	2.52	0.45
1:A:67:LYS:HD2	1:A:139:GLN:NE2	2.32	0.45
1:A:74:ILE:HD11	1:A:89:LEU:HD12	1.99	0.45
3:D:401:A3P:O3P	3:D:401:A3P:O2'	2.32	0.45
1:G:146:ILE:HG22	1:G:156:LEU:HD13	1.98	0.45
1:D:82:THR:C	1:D:159:LYS:HD2	2.42	0.45
1:D:227:MET:HE3	1:D:227:MET:HA	1.98	0.45
1:G:65:TYR:CD2	1:G:147:VAL:HG21	2.52	0.45
1:A:111:LYS:HE2	1:A:134:LEU:HD13	1.99	0.44
1:F:65:TYR:CG	1:F:147:VAL:HG21	2.51	0.44
1:B:123:ARG:HH22	2:L:2:ASP:HA	1.82	0.44
1:A:237:VAL:HG21	1:A:253:LEU:HD21	1.98	0.44
1:A:272:ILE:HD13	1:A:278:VAL:HB	1.99	0.44
1:C:119:LYS:O	1:C:123:ARG:HG3	2.18	0.44
1:E:75:GLY:HA3	1:E:164:LEU:HD13	2.00	0.44
1:E:111:LYS:HE2	1:E:134:LEU:HD13	1.99	0.44
1:E:82:THR:HB	1:E:159:LYS:HD2	2.00	0.44
1:B:119:LYS:O	1:B:123:ARG:HG3	2.18	0.44
1:B:223:TYR:OH	1:C:297:GLY:HA2	2.18	0.44
1:E:76:GLY:O	1:E:161:PRO:HB3	2.16	0.44
3:E:401:A3P:O3P	3:E:401:A3P:O2'	2.34	0.44
1:C:201:ALA:HB2	2:N:1:MET:SD	2.57	0.44
1:A:164:LEU:O	1:A:167:LEU:HB2	2.18	0.44
1:E:67:LYS:HD2	1:E:139:GLN:NE2	2.33	0.44
1:B:272:ILE:HD13	1:B:278:VAL:HB	2.00	0.44
1:E:90:ASP:OD2	1:E:97:CYS:HB2	2.17	0.44
1:H:121:LYS:HD2	1:H:121:LYS:HA	1.53	0.44
1:B:209:ARG:NH1	1:B:317:ILE:HD11	2.33	0.43
1:C:82:THR:OG1	1:C:159:LYS:HE3	2.18	0.43
1:D:67:LYS:HD2	1:D:139:GLN:NE2	2.33	0.43
1:D:250:MET:HE2	1:D:265:VAL:HB	1.98	0.43
1:A:295:ASN:O	3:A:401:A3P:H2	2.18	0.43
1:H:112:GLN:O	1:H:116:ARG:HG3	2.18	0.43
1:B:72:ILE:O	1:B:157:CYS:HA	2.19	0.43
1:G:110:LEU:HA	1:G:110:LEU:HD23	1.90	0.43
1:H:231:TYR:OH	1:H:232:LYS:HE3	2.19	0.43
1:B:231:TYR:CE2	1:C:246:PRO:HG2	2.53	0.43
1:E:295:ASN:O	3:E:401:A3P:H2	2.19	0.43
1:G:164:LEU:O	1:G:167:LEU:HB2	2.18	0.43
1:B:121:LYS:HD2	1:B:121:LYS:HA	1.57	0.43
1:B:145:ILE:O	1:B:149:HIS:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLN:HB3	1:B:249:TRP:NE1	2.34	0.43
1:D:227:MET:CE	1:G:296:VAL:HG22	2.48	0.43
1:G:102:ARG:HB3	1:G:106:ARG:HH12	1.83	0.43
2:S:1:MET:HB3	2:S:4:GLN:HB3	2.00	0.42
1:A:135:ASP:OD2	1:A:172:ARG:NH1	2.44	0.42
1:H:84:LEU:HD11	1:H:294:VAL:HG22	2.01	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.52	0.42
1:B:288:ASP:OD1	1:B:288:ASP:N	2.50	0.42
1:D:219:ILE:HG23	1:D:320:MET:HG3	2.00	0.42
1:E:72:ILE:O	1:E:157:CYS:HA	2.20	0.42
1:F:82:THR:C	1:F:159:LYS:HD2	2.43	0.42
1:H:146:ILE:O	1:H:149:HIS:HD2	2.01	0.42
1:C:107:ILE:HG23	1:C:138:MET:HE1	2.01	0.42
1:H:67:LYS:HD2	1:H:139:GLN:NE2	2.33	0.42
1:G:107:ILE:HG23	1:G:138:MET:HE1	2.00	0.42
1:C:72:ILE:O	1:C:157:CYS:HA	2.20	0.42
1:C:218:ALA:O	1:C:221:THR:HG22	2.18	0.42
1:D:227:MET:HE3	1:G:295:ASN:HB2	2.02	0.42
1:F:190:VAL:HG21	1:F:212:LEU:HG	2.02	0.42
1:D:121:LYS:HD2	1:D:121:LYS:HA	1.67	0.42
1:C:75:GLY:HA3	1:C:164:LEU:HD13	2.02	0.42
1:C:139:GLN:NE2	1:C:173:LEU:O	2.51	0.42
1:G:121:LYS:HD2	1:G:121:LYS:HA	1.84	0.42
1:H:146:ILE:HA	1:H:149:HIS:CD2	2.54	0.42
1:B:190:VAL:HG21	1:B:212:LEU:HG	2.02	0.42
1:C:337:LYS:HA	1:C:337:LYS:HD3	1.91	0.42
1:A:221:THR:HG22	1:A:225:GLN:HE21	1.83	0.42
1:E:191:HIS:CE1	1:E:305:LYS:HG3	2.54	0.42
1:F:209:ARG:NH1	1:F:317:ILE:HD11	2.35	0.42
1:B:123:ARG:NH2	2:L:2:ASP:HA	2.34	0.41
1:E:107:ILE:HG23	1:E:138:MET:HE1	2.02	0.41
1:B:164:LEU:O	1:B:167:LEU:HB2	2.19	0.41
3:C:401:A3P:O1P	3:C:401:A3P:O2'	2.36	0.41
1:D:99:GLU:OE1	1:D:99:GLU:N	2.50	0.41
1:F:75:GLY:HA3	1:F:164:LEU:HD13	2.03	0.41
1:G:119:LYS:O	1:G:123:ARG:HG3	2.21	0.41
1:C:295:ASN:O	3:C:401:A3P:H2	2.21	0.41
1:G:99:GLU:HG2	1:G:281:SER:HB2	2.01	0.41
1:H:181:LEU:HD23	1:H:236:LEU:HD11	2.03	0.41
1:H:209:ARG:NH1	1:H:317:ILE:HD11	2.35	0.41
1:G:77:VAL:HG11	1:G:215:TRP:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:NH1	1:D:317:ILE:HD11	2.36	0.41
1:E:236:LEU:HD12	1:E:236:LEU:HA	1.85	0.41
1:A:111:LYS:NZ	1:A:115:SER:OG	2.41	0.41
1:B:75:GLY:HA3	1:B:164:LEU:HD13	2.02	0.41
1:B:82:THR:C	1:B:159:LYS:HD2	2.45	0.41
1:E:199:THR:O	2:P:2:ASP:HB2	2.20	0.41
1:A:112:GLN:O	1:A:116:ARG:HG3	2.20	0.41
1:B:135:ASP:OD2	1:B:172:ARG:NH1	2.45	0.41
1:C:303:VAL:CG2	1:C:332:PRO:HB3	2.51	0.41
1:C:122:ILE:O	1:C:126:GLU:HG2	2.20	0.40
2:N:1:MET:CB	2:N:4:GLN:HG2	2.36	0.40
1:G:72:ILE:O	1:G:157:CYS:HA	2.21	0.40
1:E:209:ARG:NH1	1:E:317:ILE:HD11	2.36	0.40
1:C:282:LYS:NZ	1:D:126:GLU:OE2	2.32	0.40
1:D:90:ASP:OD2	1:D:97:CYS:HB2	2.21	0.40
1:E:122:ILE:O	1:E:126:GLU:HG2	2.21	0.40
1:G:249:TRP:O	1:G:253:LEU:HD13	2.22	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	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	B	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	C	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	D	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	E	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	F	273/276 (99%)	269 (98%)	4 (2%)	0	100	100
1	G	273/276 (99%)	268 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
2	M	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	N	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	O	3/6 (50%)	3 (100%)	0	0	100	100
2	P	4/6 (67%)	4 (100%)	0	0	100	100
2	Q	3/6 (50%)	3 (100%)	0	0	100	100
2	R	4/6 (67%)	4 (100%)	0	0	100	100
2	S	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	2217/2256 (98%)	2174 (98%)	43 (2%)	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	241/241 (100%)	241 (100%)	0	100	100
1	B	241/241 (100%)	241 (100%)	0	100	100
1	C	241/241 (100%)	241 (100%)	0	100	100
1	D	241/241 (100%)	241 (100%)	0	100	100
1	E	241/241 (100%)	241 (100%)	0	100	100
1	F	240/241 (100%)	240 (100%)	0	100	100
1	G	240/241 (100%)	240 (100%)	0	100	100
1	H	241/241 (100%)	241 (100%)	0	100	100
2	L	6/6 (100%)	6 (100%)	0	100	100
2	M	5/6 (83%)	5 (100%)	0	100	100
2	N	5/6 (83%)	5 (100%)	0	100	100
2	O	5/6 (83%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	6/6 (100%)	6 (100%)	0	100	100
2	Q	5/6 (83%)	5 (100%)	0	100	100
2	R	6/6 (100%)	6 (100%)	0	100	100
2	S	5/6 (83%)	5 (100%)	0	100	100
All	All	1969/1976 (100%)	1969 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	267	HIS
1	A	331	ASN
1	B	149	HIS
1	B	267	HIS
1	B	331	ASN
1	C	112	GLN
1	C	331	ASN
1	D	149	HIS
1	D	267	HIS
1	E	267	HIS
1	F	241	GLN
1	F	267	HIS
1	G	149	HIS
1	H	149	HIS
1	H	267	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	$\# Z  > 2$
3	A3P	G	401	-	29,29,29	0.71	0	44,45,45	0.65	1 (2%)
3	A3P	C	401	-	29,29,29	0.72	0	44,45,45	0.67	1 (2%)
3	A3P	E	401	-	29,29,29	0.72	0	44,45,45	0.71	1 (2%)
3	A3P	F	401	-	29,29,29	0.74	0	44,45,45	0.67	1 (2%)
3	A3P	A	401	-	29,29,29	0.73	0	44,45,45	0.68	1 (2%)
3	A3P	B	401	-	29,29,29	0.72	0	44,45,45	0.69	1 (2%)
3	A3P	H	401	-	29,29,29	0.71	0	44,45,45	0.73	1 (2%)
3	A3P	D	401	-	29,29,29	0.72	0	44,45,45	0.75	1 (2%)

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
3	A3P	G	401	-	-	6/15/31/31	0/3/3/3
3	A3P	C	401	-	-	2/15/31/31	0/3/3/3
3	A3P	E	401	-	-	3/15/31/31	0/3/3/3
3	A3P	F	401	-	-	3/15/31/31	0/3/3/3
3	A3P	A	401	-	-	2/15/31/31	0/3/3/3
3	A3P	B	401	-	-	3/15/31/31	0/3/3/3
3	A3P	H	401	-	-	4/15/31/31	0/3/3/3
3	A3P	D	401	-	-	3/15/31/31	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	A3P	P2-O5'-C5'	-3.94	107.44	118.30
3	H	401	A3P	P2-O5'-C5'	-3.91	107.53	118.30
3	E	401	A3P	P2-O5'-C5'	-3.81	107.80	118.30
3	B	401	A3P	P2-O5'-C5'	-3.63	108.30	118.30
3	F	401	A3P	P2-O5'-C5'	-3.47	108.74	118.30
3	A	401	A3P	P2-O5'-C5'	-3.47	108.75	118.30
3	C	401	A3P	P2-O5'-C5'	-3.31	109.16	118.30
3	G	401	A3P	P2-O5'-C5'	-3.28	109.26	118.30

There are no chirality outliers.

All (26) torsion outliers are listed below:

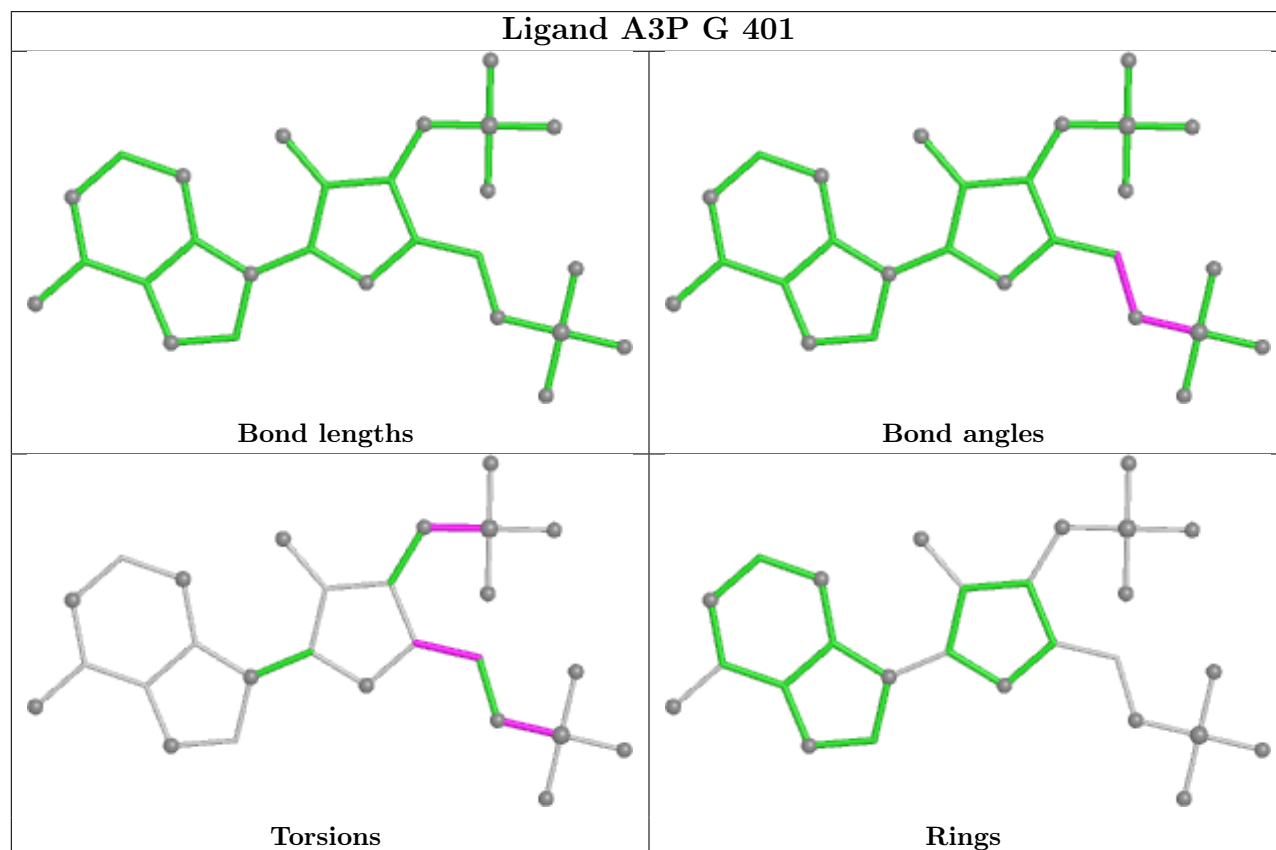
Mol	Chain	Res	Type	Atoms
3	A	401	A3P	C3'-C4'-C5'-O5'
3	B	401	A3P	C3'-O3'-P1-O2P
3	C	401	A3P	C3'-C4'-C5'-O5'
3	D	401	A3P	C3'-O3'-P1-O3P
3	E	401	A3P	C3'-C4'-C5'-O5'
3	F	401	A3P	C3'-C4'-C5'-O5'
3	G	401	A3P	C5'-O5'-P2-O4P
3	G	401	A3P	C5'-O5'-P2-O6P
3	G	401	A3P	C3'-C4'-C5'-O5'
3	D	401	A3P	C3'-C4'-C5'-O5'
3	G	401	A3P	O4'-C4'-C5'-O5'
3	H	401	A3P	C3'-C4'-C5'-O5'
3	B	401	A3P	C3'-C4'-C5'-O5'
3	A	401	A3P	O4'-C4'-C5'-O5'
3	C	401	A3P	O4'-C4'-C5'-O5'
3	E	401	A3P	O4'-C4'-C5'-O5'
3	F	401	A3P	O4'-C4'-C5'-O5'
3	D	401	A3P	O4'-C4'-C5'-O5'
3	E	401	A3P	C3'-O3'-P1-O3P
3	F	401	A3P	C3'-O3'-P1-O2P
3	G	401	A3P	C3'-O3'-P1-O2P
3	H	401	A3P	C3'-O3'-P1-O2P
3	H	401	A3P	C3'-O3'-P1-O3P
3	H	401	A3P	O4'-C4'-C5'-O5'
3	B	401	A3P	O4'-C4'-C5'-O5'
3	G	401	A3P	C5'-O5'-P2-O5P

There are no ring outliers.

6 monomers are involved in 10 short contacts:

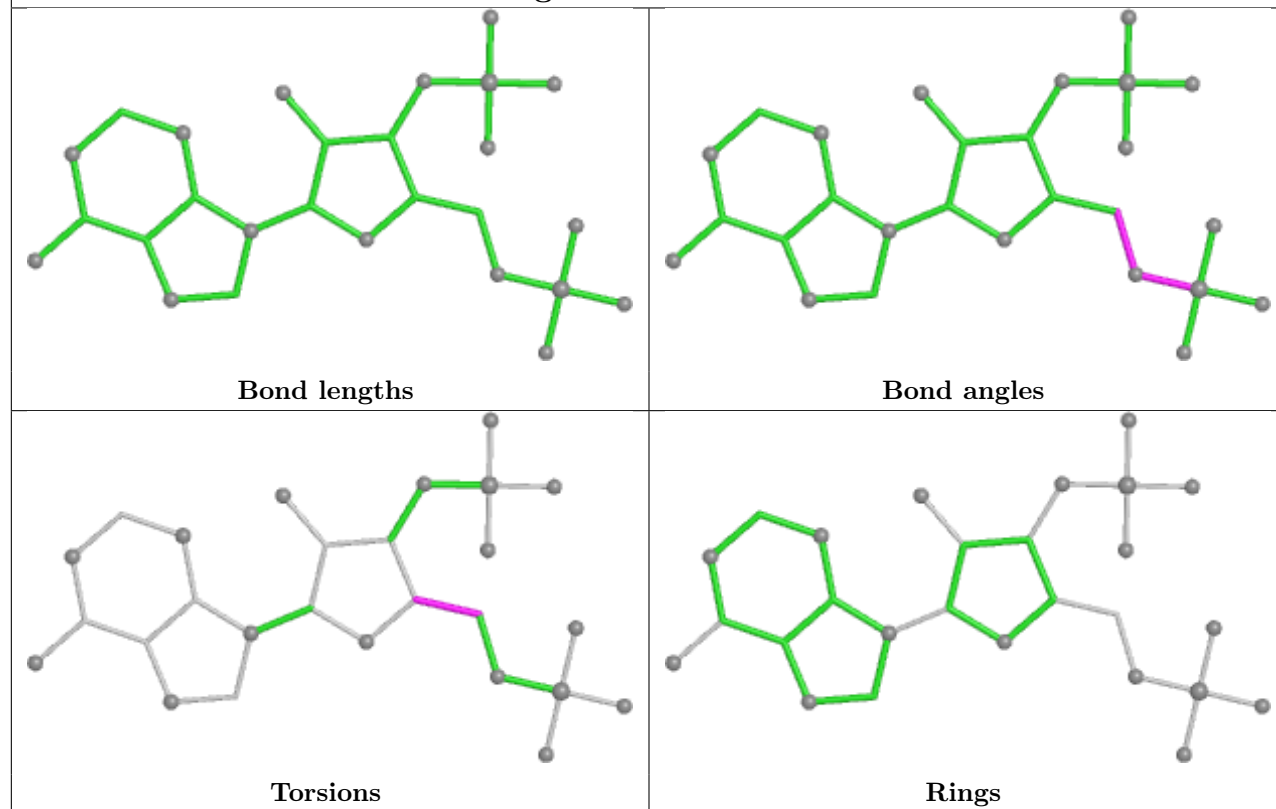
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	A3P	1	0
3	C	401	A3P	2	0
3	E	401	A3P	3	0
3	F	401	A3P	1	0
3	A	401	A3P	2	0
3	D	401	A3P	1	0

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.

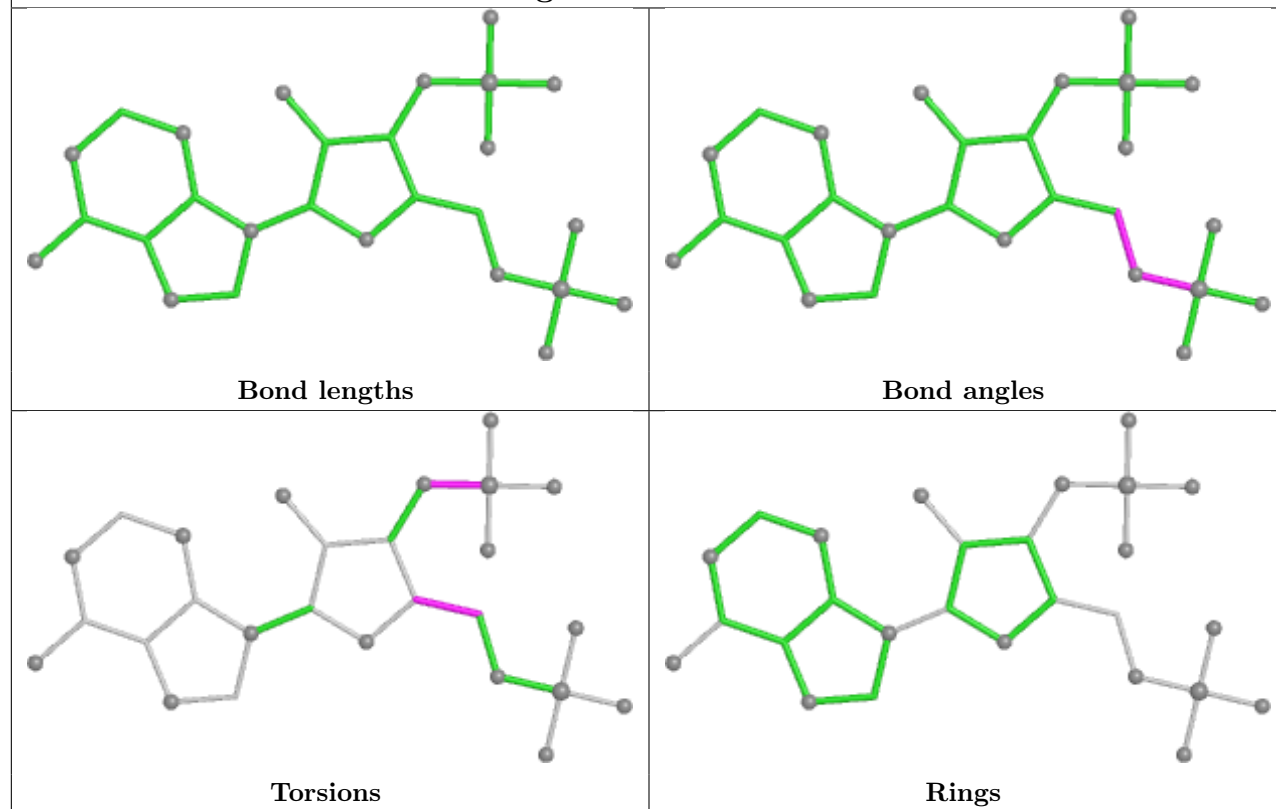




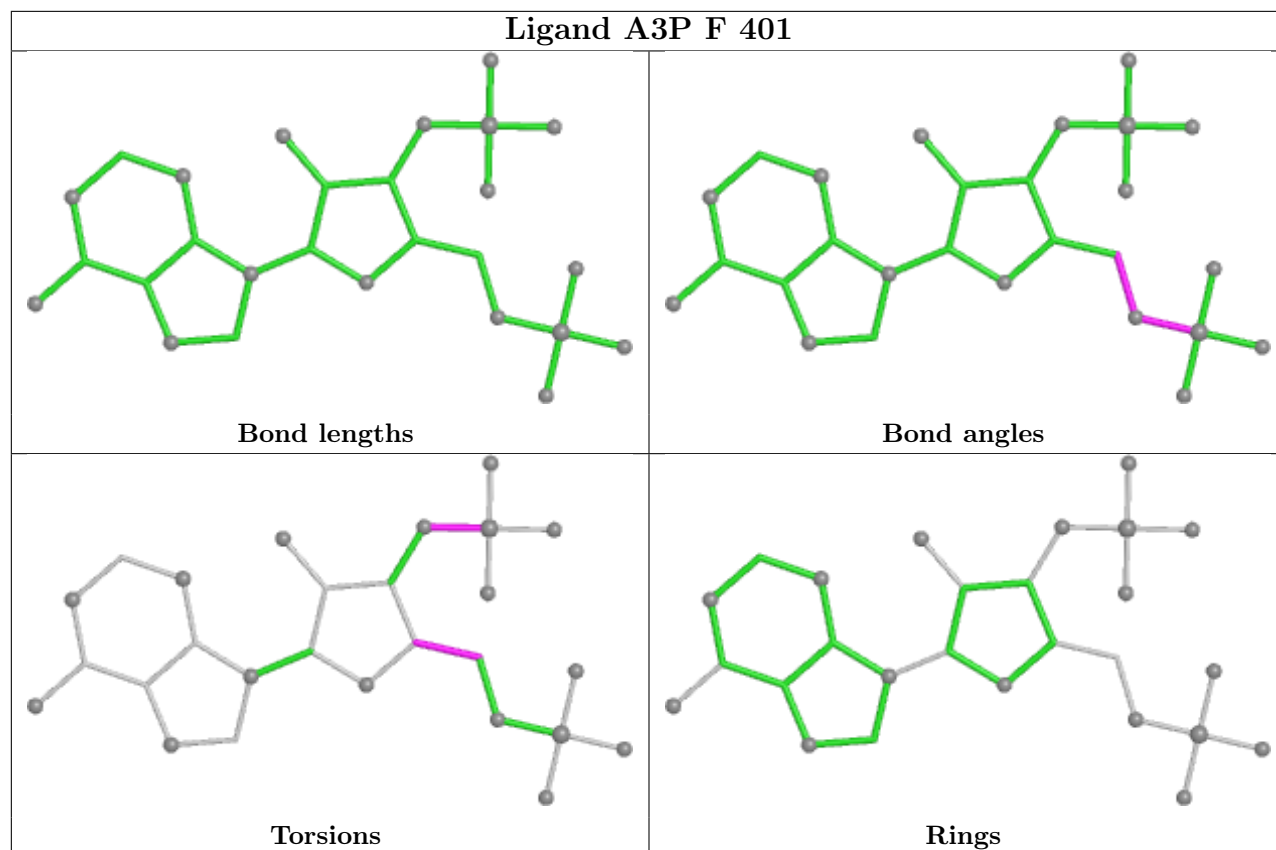
## Ligand A3P C 401



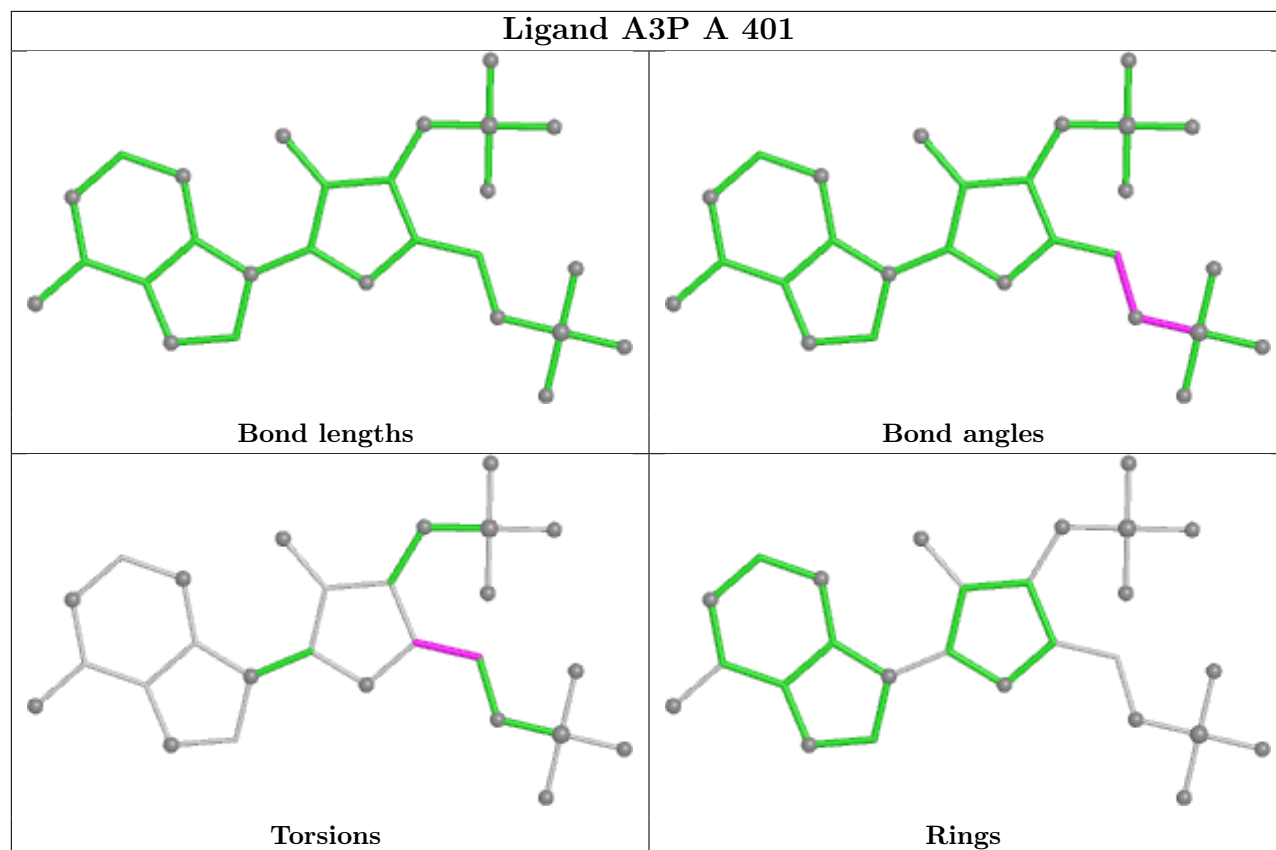
## Ligand A3P E 401



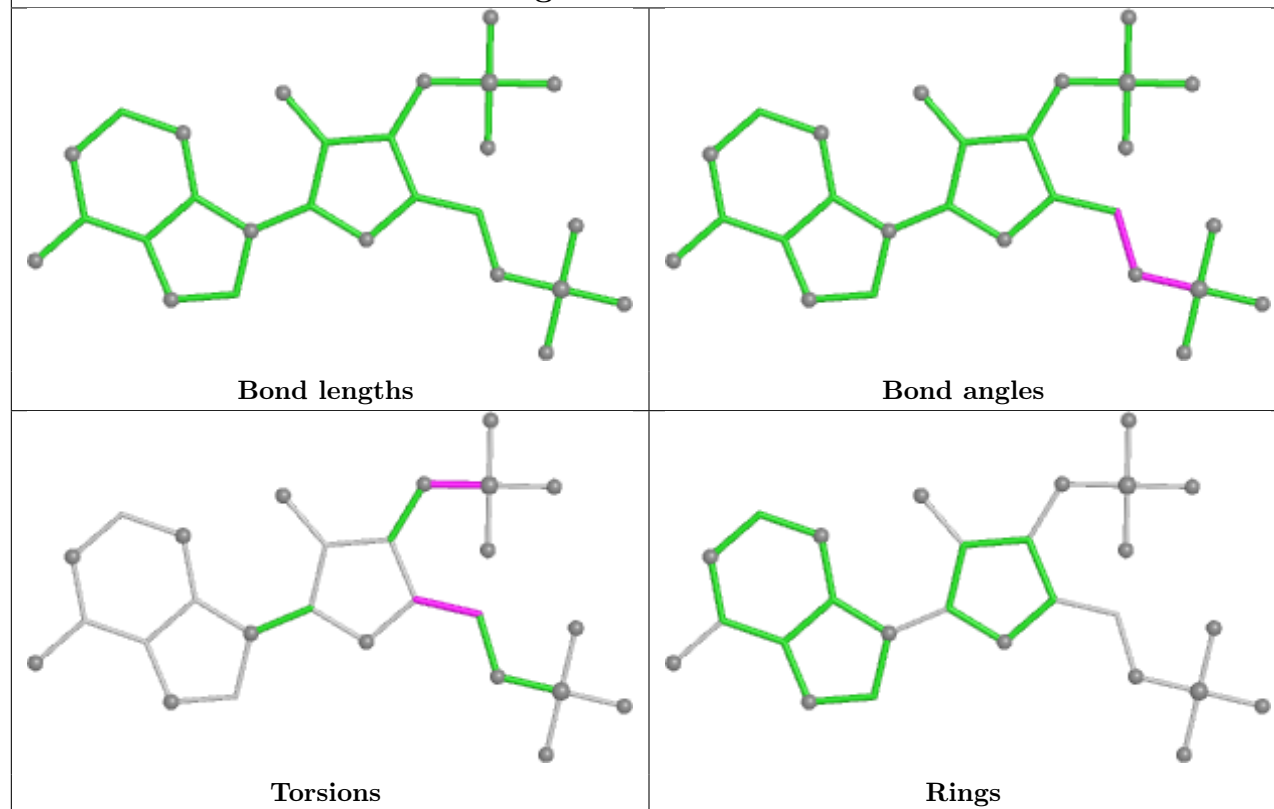
## Ligand A3P F 401



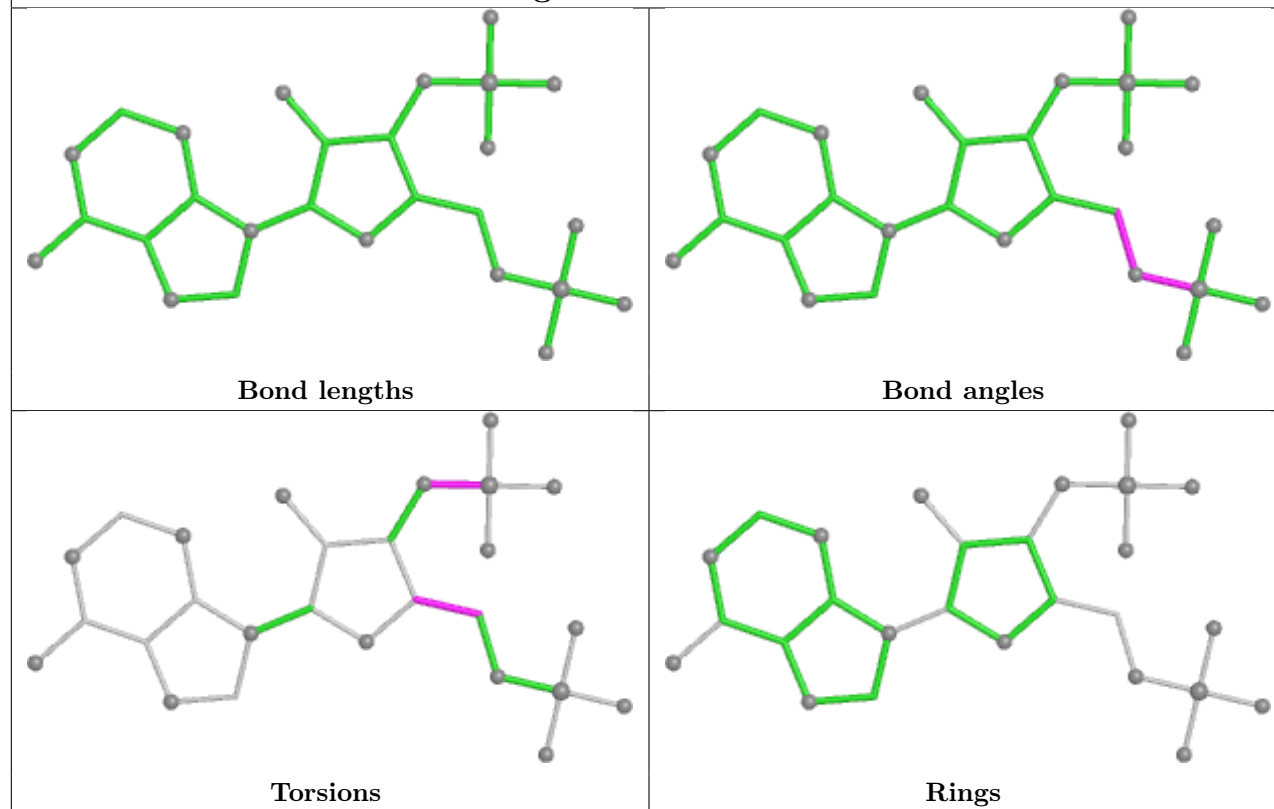
## Ligand A3P A 401

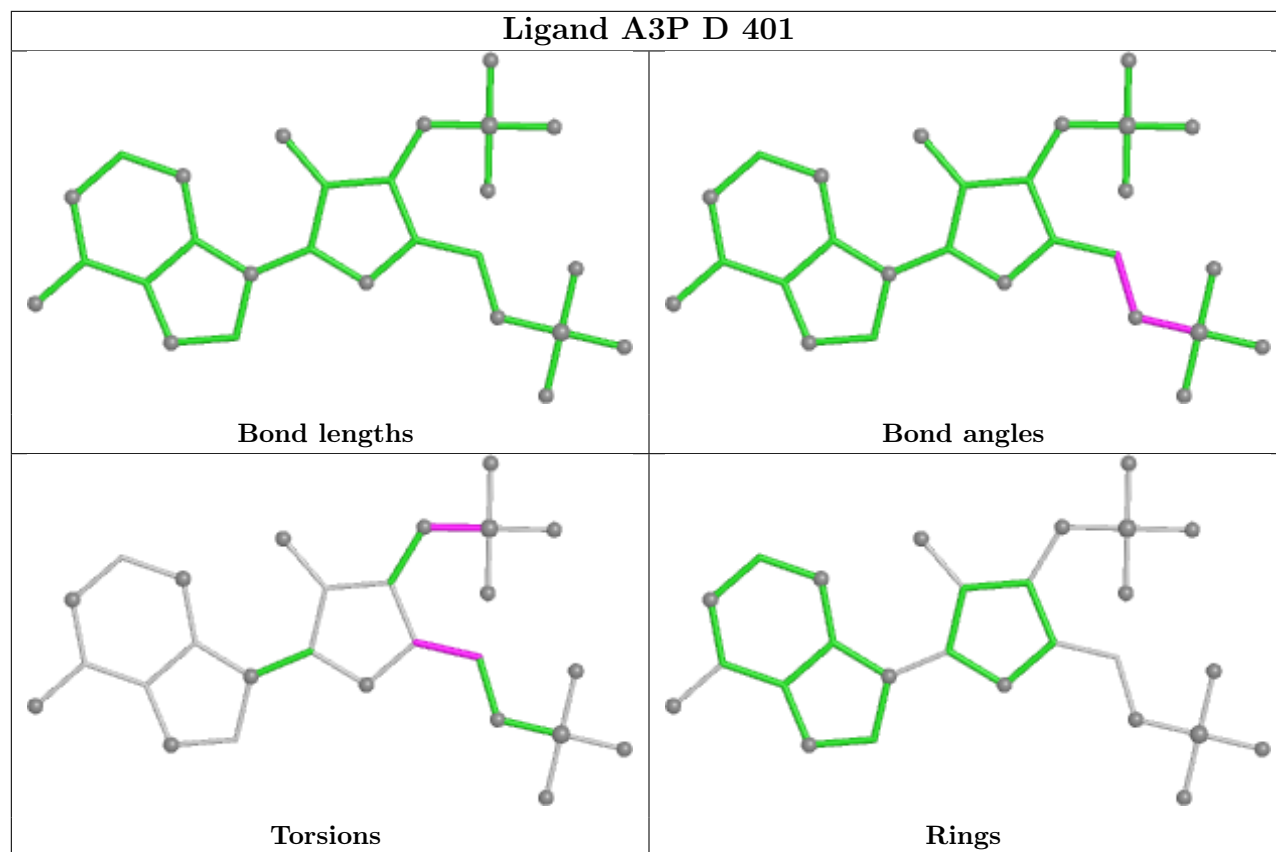


## Ligand A3P B 401



## Ligand A3P H 401





## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	276/276 (100%)	1.05	32 (11%) 9 7	4, 19, 47, 62	0
1	B	276/276 (100%)	1.11	37 (13%) 7 6	5, 20, 48, 69	0
1	C	276/276 (100%)	1.29	45 (16%) 4 3	7, 21, 44, 61	0
1	D	276/276 (100%)	1.23	38 (13%) 6 5	4, 20, 44, 71	0
1	E	276/276 (100%)	1.22	41 (14%) 5 4	5, 19, 42, 65	0
1	F	275/276 (99%)	1.27	48 (17%) 4 3	6, 23, 49, 65	1 (0%)
1	G	275/276 (99%)	1.05	37 (13%) 7 5	4, 21, 45, 70	0
1	H	276/276 (100%)	1.11	33 (11%) 9 6	4, 23, 47, 81	0
2	L	6/6 (100%)	2.13	2 (33%) 1 1	29, 42, 46, 55	1 (16%)
2	M	5/6 (83%)	2.02	2 (40%) 1 1	41, 43, 53, 60	0
2	N	5/6 (83%)	3.15	5 (100%) 0 0	38, 43, 52, 56	0
2	O	5/6 (83%)	2.54	4 (80%) 0 0	38, 41, 48, 56	0
2	P	6/6 (100%)	3.24	5 (83%) 0 0	29, 44, 55, 55	1 (16%)
2	Q	5/6 (83%)	2.16	4 (80%) 0 0	36, 40, 51, 59	0
2	R	6/6 (100%)	2.17	3 (50%) 0 1	31, 40, 47, 59	1 (16%)
2	S	5/6 (83%)	1.93	2 (40%) 1 1	41, 43, 54, 64	0
All	All	2249/2256 (99%)	1.19	338 (15%) 5 4	4, 21, 47, 81	4 (0%)

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	115	SER	6.6
1	F	115	SER	6.5
2	P	6	SER	6.5
1	E	131	ASP	6.2
1	B	115	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	G	117	SER	5.8
1	D	176	ASN	5.7
1	F	176	ASN	5.3
1	G	239	TYR	5.2
1	B	338	PRO	4.7
1	A	239	TYR	4.7
1	H	286	SER	4.6
2	L	6	SER	4.6
1	C	131	ASP	4.6
1	C	327	ASP	4.6
2	R	6	SER	4.6
1	D	338	PRO	4.5
1	B	122	ILE	4.4
1	C	99	GLU	4.4
1	B	176	ASN	4.3
1	E	334	ASN	4.3
1	F	327	ASP	4.2
1	G	115	SER	4.2
1	B	286	SER	4.2
2	N	5	VAL	4.1
1	H	338	PRO	4.1
1	F	210	ASP	4.0
1	C	214	LYS	3.9
1	D	125	ASP	3.9
1	B	339	ASP	3.9
2	N	2	ASP	3.9
1	B	149	HIS	3.9
2	S	5	VAL	3.9
1	A	131	ASP	3.8
1	D	210	ASP	3.8
2	P	5	VAL	3.8
1	H	116	ARG	3.8
1	F	275	ALA	3.8
1	C	115	SER	3.7
1	G	288	ASP	3.7
1	C	336	GLY	3.7
1	A	116	ARG	3.7
1	F	234	CYS	3.7
2	M	5	VAL	3.7
1	H	122	ILE	3.7
1	A	97	CYS	3.7
1	C	98	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	90	ASP	3.6
1	A	151	GLU	3.6
1	H	282	LYS	3.5
1	B	334	ASN	3.5
1	D	115	SER	3.5
1	F	125	ASP	3.5
1	E	98	GLY	3.4
1	H	270	GLU	3.4
1	A	115	SER	3.4
1	C	100	GLU	3.3
1	E	116	ARG	3.3
1	G	282	LYS	3.3
1	B	151	GLU	3.3
1	A	136	SER	3.3
1	A	339	ASP	3.3
1	B	278	VAL	3.3
2	O	5	VAL	3.3
1	B	288	ASP	3.3
1	C	338	PRO	3.2
1	E	99	GLU	3.2
1	E	255	LYS	3.2
1	H	149	HIS	3.2
1	C	116	ARG	3.2
1	A	120	GLU	3.2
1	E	115	SER	3.2
1	D	157	CYS	3.2
1	A	334	ASN	3.2
1	D	235	MET	3.2
1	E	188	ALA	3.2
1	E	288	ASP	3.1
1	C	230	GLY	3.1
2	L	5	VAL	3.1
1	H	334	ASN	3.1
1	D	312	GLN	3.1
1	E	125	ASP	3.1
1	G	98	GLY	3.1
1	C	171	SER	3.1
1	F	274	LYS	3.1
1	G	274	LYS	3.1
1	E	182	MET	3.1
1	E	273	GLY	3.1
1	B	112	GLN	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	126	GLU	3.0
1	C	210	ASP	3.0
1	G	263	HIS	3.0
1	E	283	VAL	3.0
1	B	220	GLU	3.0
1	C	182	MET	3.0
1	C	339	ASP	3.0
1	B	235	MET	3.0
1	F	193	MET	3.0
1	C	125	ASP	3.0
1	E	327	ASP	3.0
1	E	214	LYS	3.0
2	O	4	GLN	3.0
2	P	4	GLN	3.0
1	H	176	ASN	3.0
1	D	114	TRP	3.0
1	B	210	ASP	3.0
2	N	4	GLN	3.0
1	D	287	THR	3.0
1	A	274	LYS	2.9
1	C	135	ASP	2.9
1	E	172	ARG	2.9
1	F	255	LYS	2.9
1	G	121	LYS	2.9
1	G	331	ASN	2.9
1	G	188	ALA	2.9
1	D	207	SER	2.9
1	A	312	GLN	2.9
2	Q	4	GLN	2.9
1	H	90	ASP	2.9
1	C	198	VAL	2.9
1	G	327	ASP	2.9
1	G	116	ARG	2.9
1	C	283	VAL	2.8
1	B	195	SER	2.8
1	A	176	ASN	2.8
1	F	282	LYS	2.8
1	F	127	ALA	2.8
1	G	337	LYS	2.8
1	H	114	TRP	2.8
1	E	171	SER	2.8
1	H	337	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	327	ASP	2.8
1	B	125	ASP	2.8
1	D	249	TRP	2.8
1	G	186	GLY	2.8
2	N	3	TYR	2.8
1	E	210	ASP	2.7
1	B	263	HIS	2.7
1	H	248	ARG	2.7
1	B	157	CYS	2.7
1	D	126	GLU	2.7
1	H	151	GLU	2.7
1	F	75	GLY	2.7
1	E	309	ASP	2.7
1	B	237	VAL	2.7
2	R	4	GLN	2.7
2	S	4	GLN	2.7
1	C	172	ARG	2.7
1	C	136	SER	2.7
1	C	334	ASN	2.7
1	F	279	SER	2.7
1	H	210	ASP	2.7
1	D	273	GLY	2.6
1	G	151	GLU	2.6
1	F	338	PRO	2.6
1	G	334	ASN	2.6
1	H	279	SER	2.6
1	A	132	GLU	2.6
1	E	100	GLU	2.6
1	F	119	LYS	2.6
1	F	165	LYS	2.6
1	D	203	PHE	2.6
1	G	271	MET	2.6
1	F	307	PRO	2.6
1	E	312	GLN	2.6
1	B	336	GLY	2.6
1	D	81	GLY	2.6
1	D	99	GLU	2.6
1	D	234	CYS	2.6
1	B	279	SER	2.6
1	H	312	GLN	2.6
1	A	295	ASN	2.5
1	C	288	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	177	ALA	2.5
1	D	215	TRP	2.5
1	F	168	THR	2.5
1	G	287	THR	2.5
1	B	208	TYR	2.5
1	B	282	LYS	2.5
1	D	151	GLU	2.5
1	B	114	TRP	2.5
1	C	117	SER	2.5
1	D	281	SER	2.5
1	D	286	SER	2.5
1	H	290	VAL	2.5
1	G	131	ASP	2.5
1	F	227	MET	2.5
1	F	172	ARG	2.5
1	E	226	CYS	2.5
1	G	158	ASN	2.5
1	E	221	THR	2.5
1	G	114	TRP	2.5
1	E	274	LYS	2.5
1	C	273	GLY	2.5
1	C	297	GLY	2.5
1	C	200	ILE	2.4
1	F	113	MET	2.4
1	H	235	MET	2.4
1	A	331	ASN	2.4
1	E	310	VAL	2.4
1	D	112	GLN	2.4
1	B	306	ILE	2.4
1	C	226	CYS	2.4
1	F	286	SER	2.4
1	H	119	LYS	2.4
1	C	331	ASN	2.4
1	A	185	ASP	2.4
1	D	90	ASP	2.4
1	B	337	LYS	2.4
1	A	207	SER	2.4
1	H	313	ASP	2.4
2	Q	3	TYR	2.4
1	C	255	LYS	2.4
1	D	121	LYS	2.4
1	G	136	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	157	CYS	2.4
1	C	310	VAL	2.4
1	D	133	VAL	2.4
1	E	252	THR	2.4
1	D	68	ASP	2.4
1	D	202	GLY	2.4
1	F	235	MET	2.4
1	E	136	SER	2.4
1	B	70	PRO	2.4
1	C	97	CYS	2.4
1	H	157	CYS	2.4
1	E	336	GLY	2.3
1	C	185	ASP	2.3
1	D	208	TYR	2.3
1	E	217	ARG	2.3
1	B	113	MET	2.3
1	G	120	GLU	2.3
1	A	333	PRO	2.3
1	B	116	ARG	2.3
1	C	176	ASN	2.3
1	G	110	LEU	2.3
1	G	176	ASN	2.3
1	F	112	GLN	2.3
1	F	149	HIS	2.3
2	O	2	ASP	2.3
1	B	260	PRO	2.3
1	C	221	THR	2.3
1	G	199	THR	2.3
1	H	255	LYS	2.3
1	E	183	VAL	2.3
1	G	270	GLU	2.2
1	C	177	ALA	2.2
1	D	127	ALA	2.2
2	P	1	MET	2.2
1	A	117	SER	2.2
1	F	157	CYS	2.2
1	A	270	GLU	2.2
1	F	151	GLU	2.2
1	G	144	GLU	2.2
1	A	335	TYR	2.2
1	H	112	GLN	2.2
1	A	210	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	68	ASP	2.2
1	F	160	ASP	2.2
2	P	2	ASP	2.2
1	A	293	PRO	2.2
1	F	246	PRO	2.2
1	B	119	LYS	2.2
1	A	279	SER	2.2
1	E	112	GLN	2.2
1	E	89	LEU	2.2
1	F	126	GLU	2.2
1	G	97	CYS	2.2
1	G	336	GLY	2.2
1	D	94	ASP	2.2
1	H	274	LYS	2.2
1	E	281	SER	2.2
1	D	247	GLU	2.2
1	D	75	GLY	2.2
1	E	338	PRO	2.2
1	F	161	PRO	2.2
1	D	217	ARG	2.2
1	H	125	ASP	2.2
1	D	316	VAL	2.1
1	H	208	TYR	2.1
2	O	3	TYR	2.1
1	H	146	ILE	2.1
1	F	312	GLN	2.1
1	F	233	LYS	2.1
1	C	120	GLU	2.1
1	A	288	ASP	2.1
1	B	316	VAL	2.1
1	C	249	TRP	2.1
1	F	232	LYS	2.1
1	B	248	ARG	2.1
1	C	289	GLN	2.1
1	F	241	GLN	2.1
1	D	117	SER	2.1
1	F	247	GLU	2.1
1	A	216	ASN	2.1
1	D	97	CYS	2.1
1	F	288	ASP	2.1
2	R	5	VAL	2.1
1	A	337	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	335	TYR	2.1
1	A	271	MET	2.1
1	H	220	GLU	2.1
1	F	283	VAL	2.1
1	G	198	VAL	2.1
1	C	101	THR	2.1
1	E	320	MET	2.1
2	M	1	MET	2.1
1	G	137	ALA	2.1
1	A	100	GLU	2.1
1	F	207	SER	2.1
1	E	249	TRP	2.1
1	E	253	LEU	2.1
1	E	306	ILE	2.1
1	G	272	ILE	2.1
1	C	126	GLU	2.1
2	Q	5	VAL	2.0
1	F	248	ARG	2.0
1	F	253	LEU	2.0
2	N	1	MET	2.0
1	B	275	ALA	2.0
1	F	94	ASP	2.0
1	G	318	ALA	2.0
1	F	284	GLU	2.0
1	B	311	LEU	2.0
1	B	146	ILE	2.0
1	C	281	SER	2.0
1	H	207	SER	2.0
1	G	149	HIS	2.0
1	H	263	HIS	2.0
2	Q	1	MET	2.0
1	E	64	ALA	2.0
1	E	298	ALA	2.0
1	E	230	GLY	2.0
1	F	203	PHE	2.0
1	C	312	GLN	2.0
1	A	99	GLU	2.0
1	D	219	ILE	2.0
1	F	122	ILE	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](#)

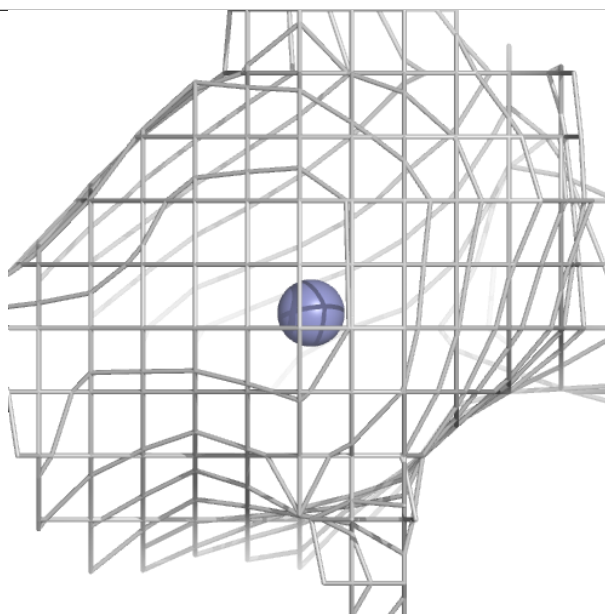
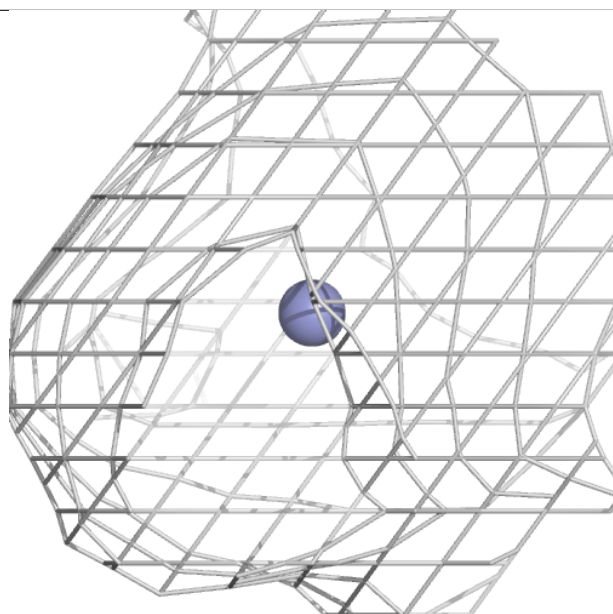
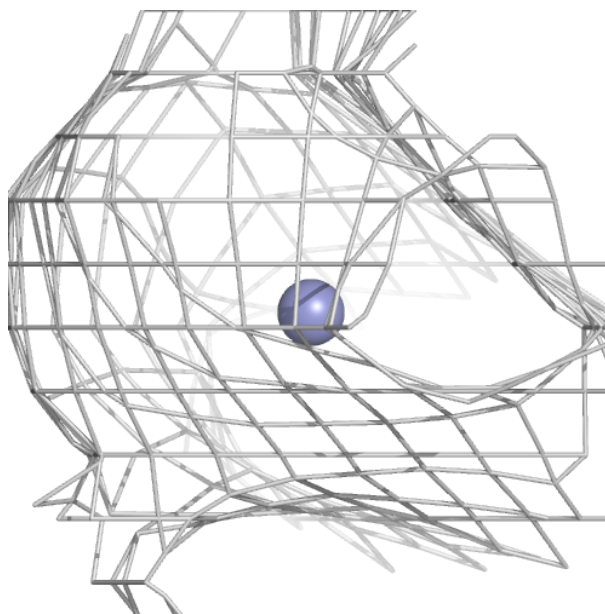
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	D	403	1/1	0.67	0.17	100,100,100,100	0
5	ZN	F	403	1/1	0.75	0.15	100,100,100,100	0
5	ZN	B	403	1/1	0.81	0.11	60,60,60,60	0
4	MG	C	402	1/1	0.90	0.10	10,10,10,10	0
4	MG	B	402	1/1	0.91	0.07	17,17,17,17	0
4	MG	G	402	1/1	0.92	0.10	9,9,9,9	0
3	A3P	B	401	27/27	0.92	0.13	9,18,31,36	0
3	A3P	F	401	27/27	0.92	0.12	9,19,26,28	0
4	MG	D	402	1/1	0.92	0.08	21,21,21,21	0
5	ZN	H	403	1/1	0.92	0.07	52,52,52,52	0
3	A3P	D	401	27/27	0.93	0.11	3,15,25,27	0
3	A3P	A	401	27/27	0.93	0.12	3,6,11,18	0
3	A3P	H	401	27/27	0.94	0.11	7,12,25,33	0
3	A3P	C	401	27/27	0.94	0.10	0,10,17,18	0
3	A3P	G	401	27/27	0.94	0.12	4,7,16,27	0
3	A3P	E	401	27/27	0.95	0.11	5,9,18,23	0
4	MG	E	402	1/1	0.95	0.05	8,8,8,8	0
4	MG	A	402	1/1	0.95	0.12	4,4,4,4	0
4	MG	H	402	1/1	0.95	0.05	18,18,18,18	0
4	MG	F	402	1/1	0.99	0.04	13,13,13,13	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.

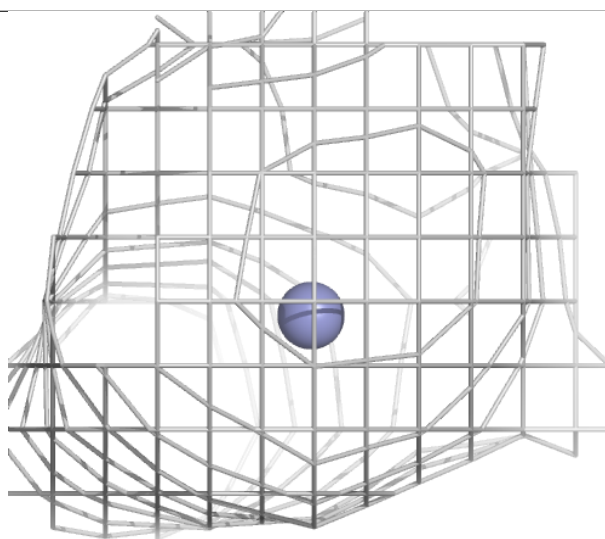
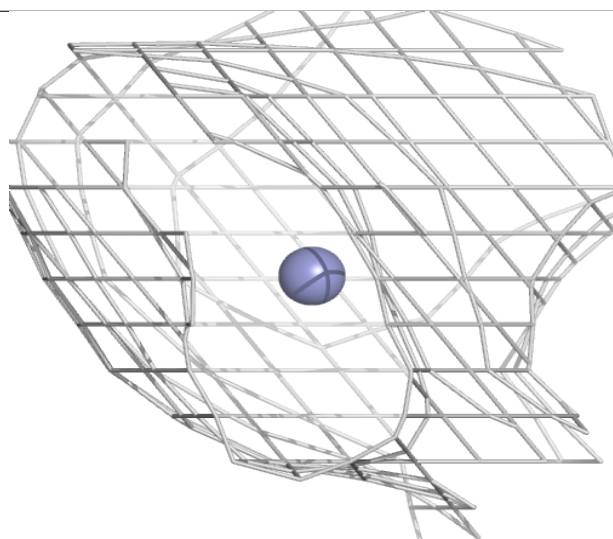
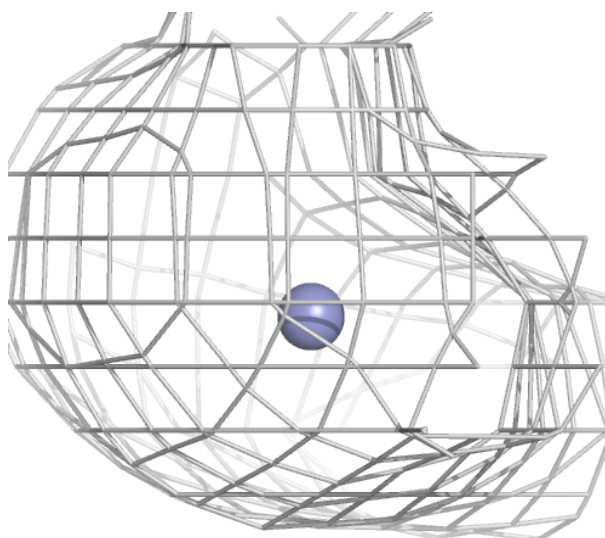
**Electron density around ZN D 403:**

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



**Electron density around ZN F 403:**

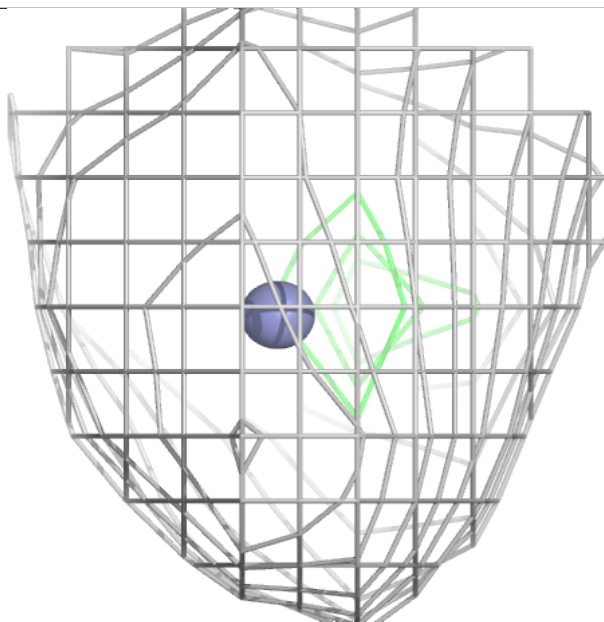
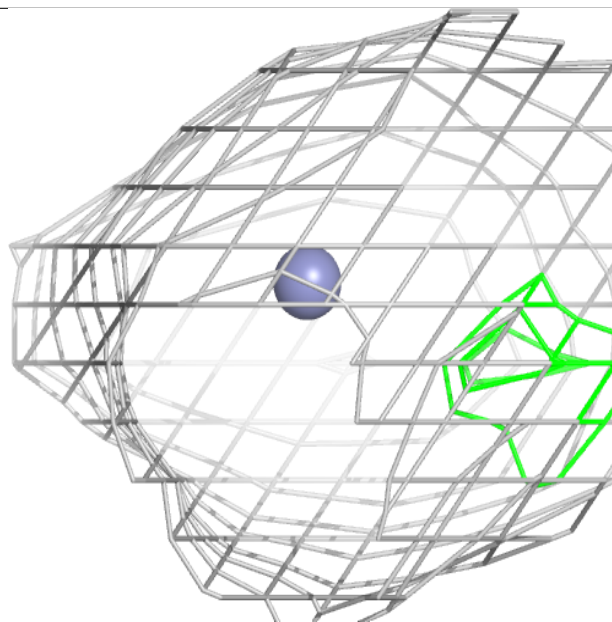
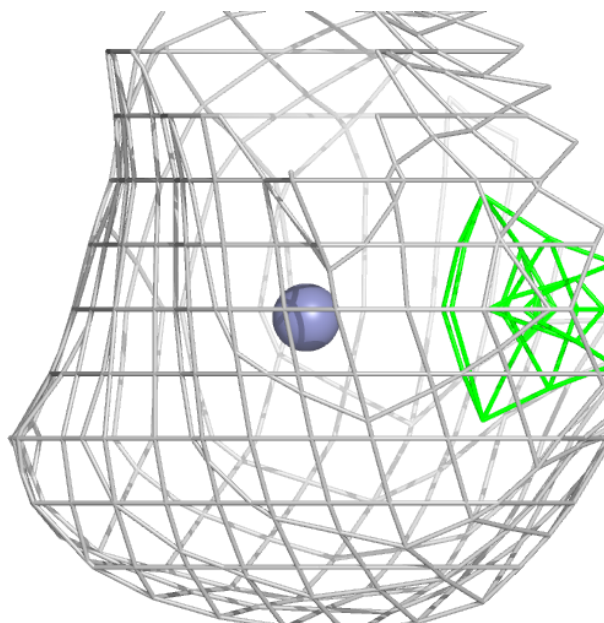
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





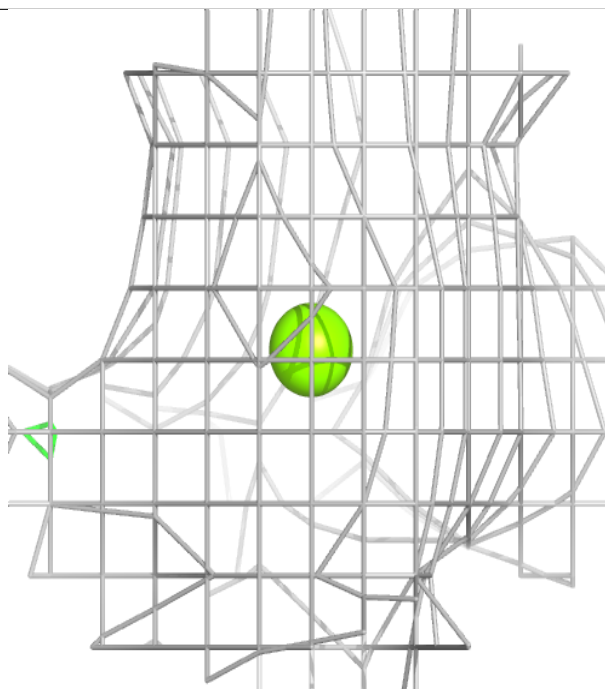
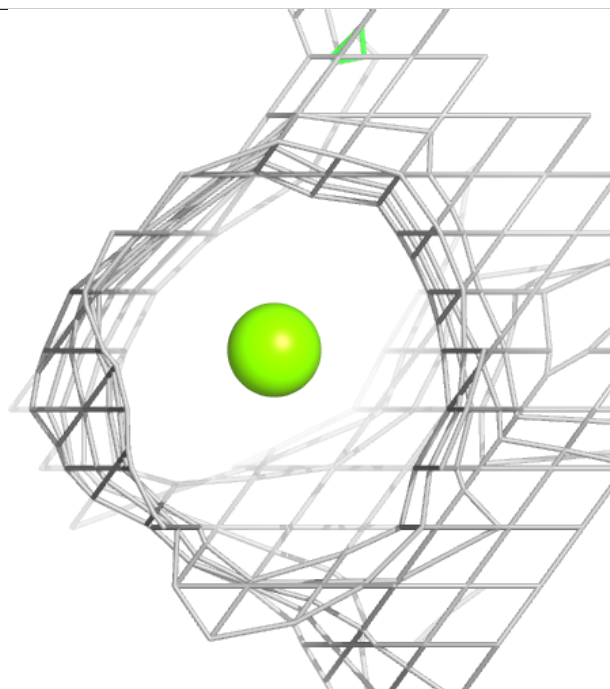
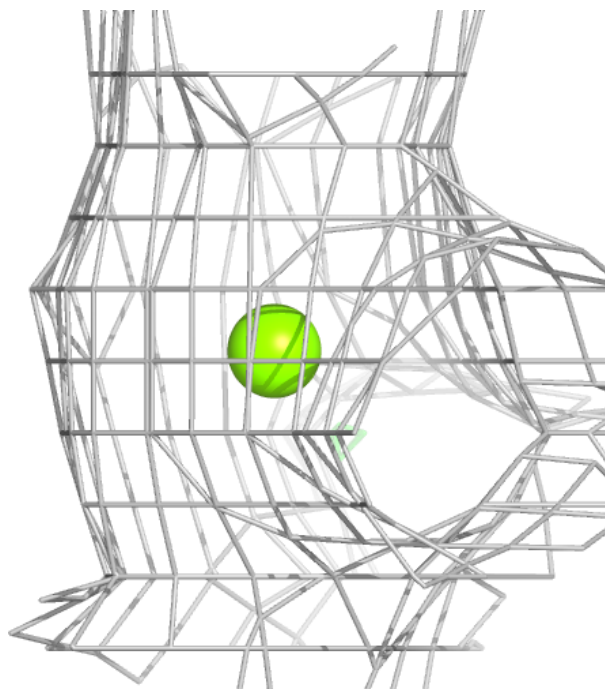
**Electron density around ZN B 403:**

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



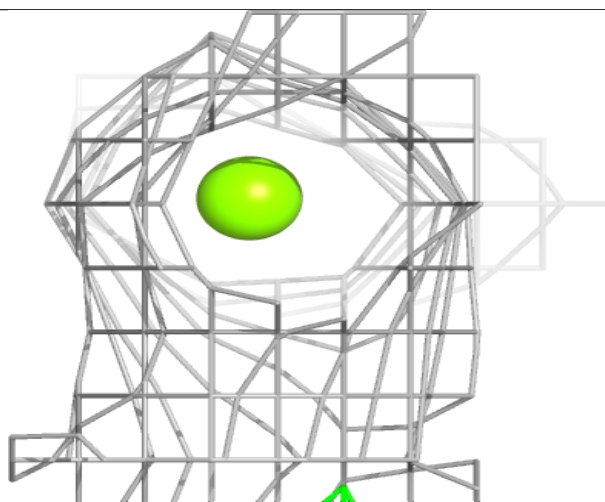
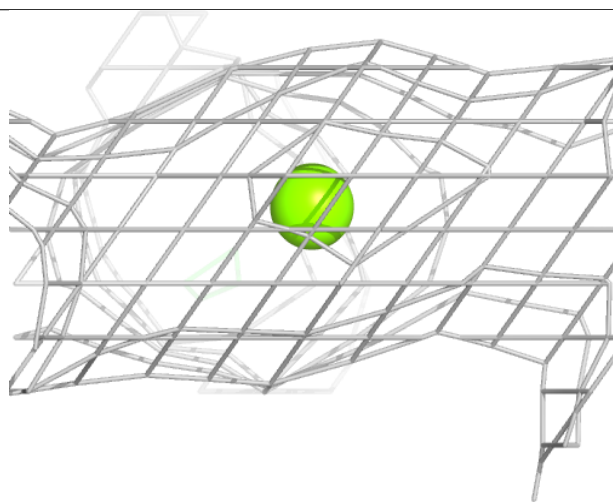
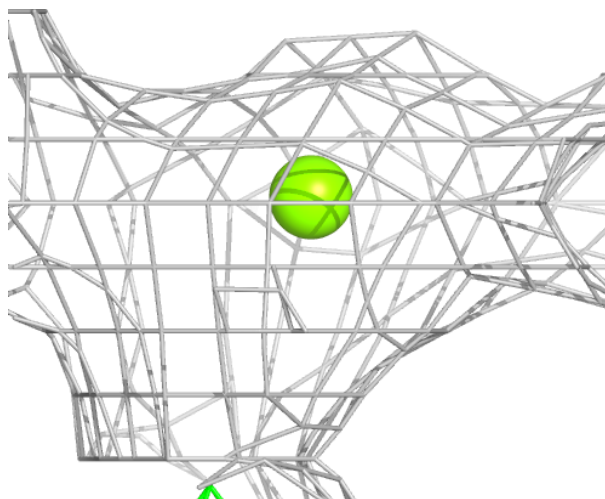
**Electron density around MG C 402:**

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



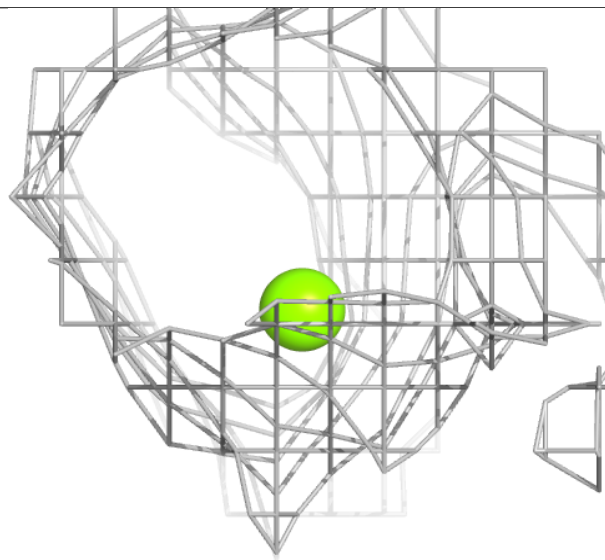
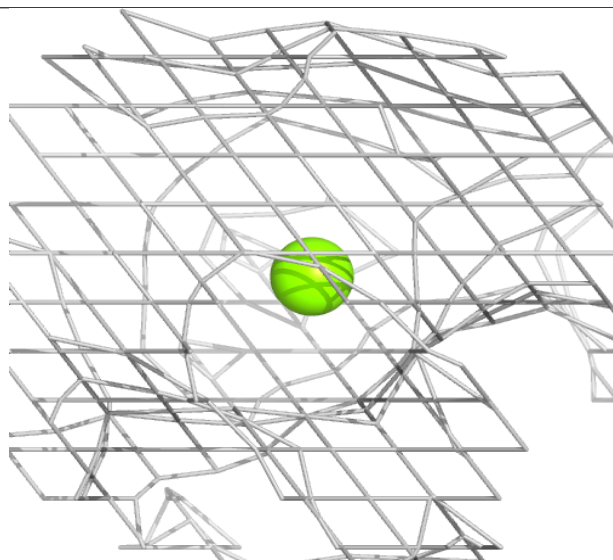
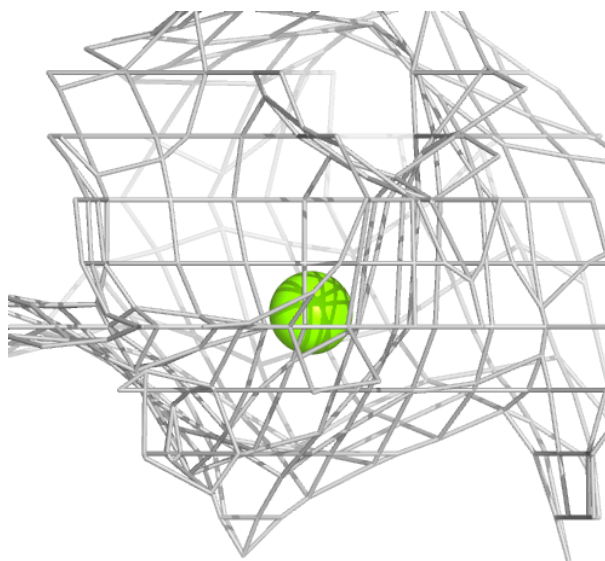
**Electron density around MG B 402:**

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



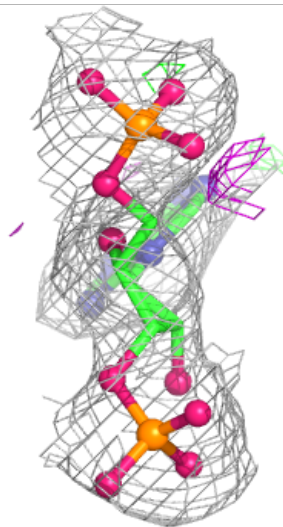
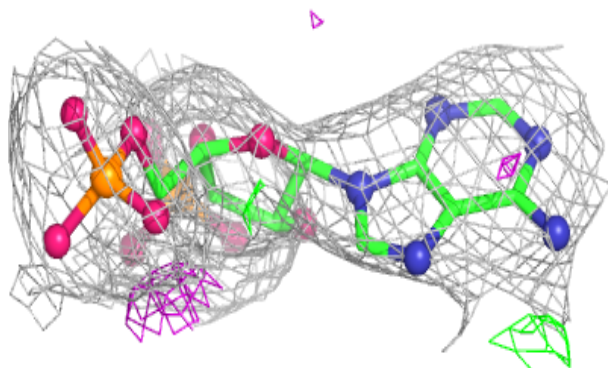
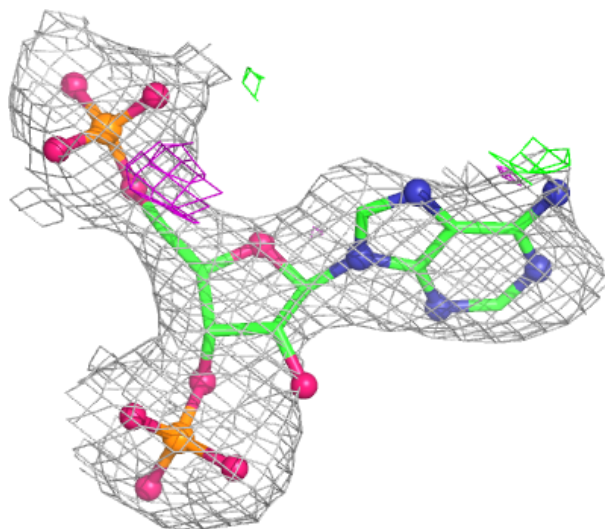
**Electron density around MG G 402:**

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



**Electron density around A3P B 401:**

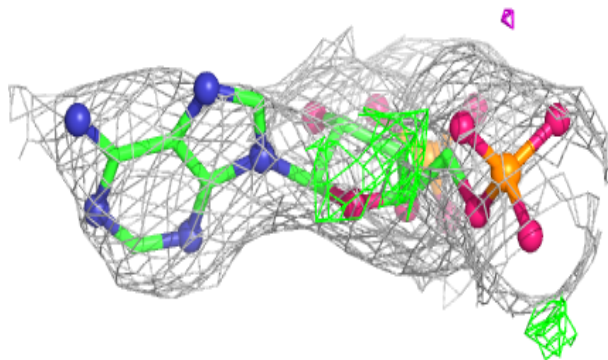
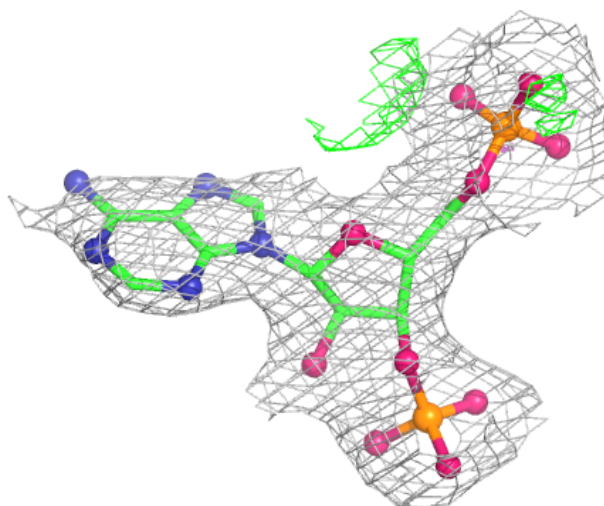
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





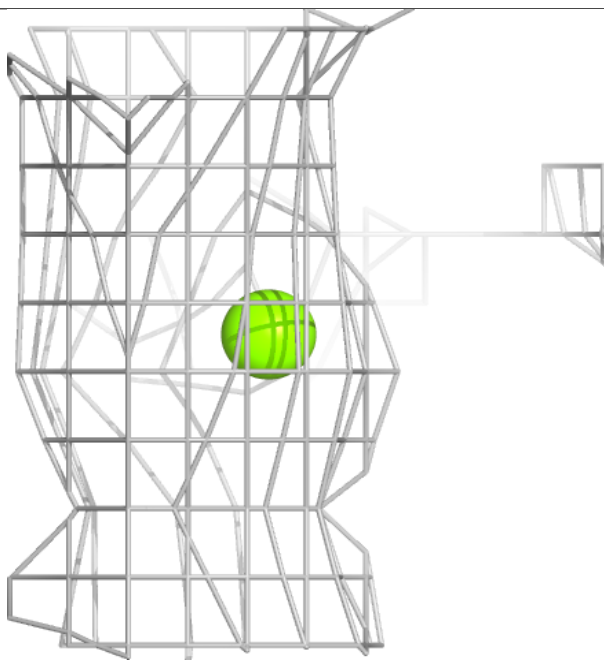
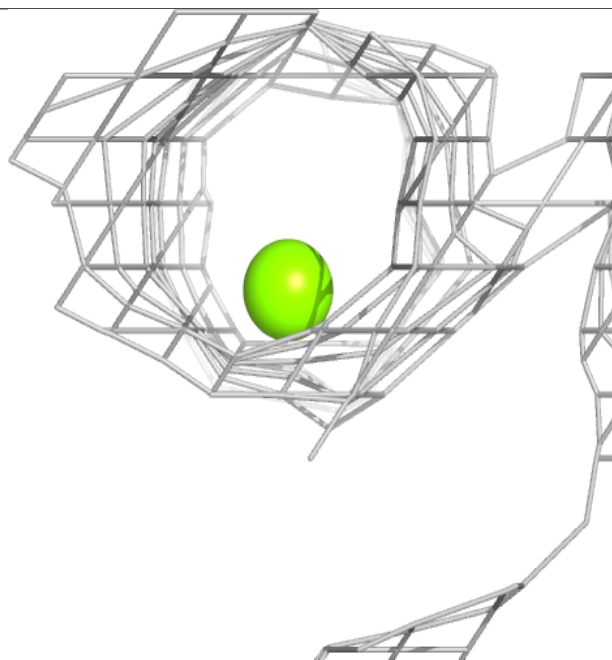
**Electron density around A3P F 401:**

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



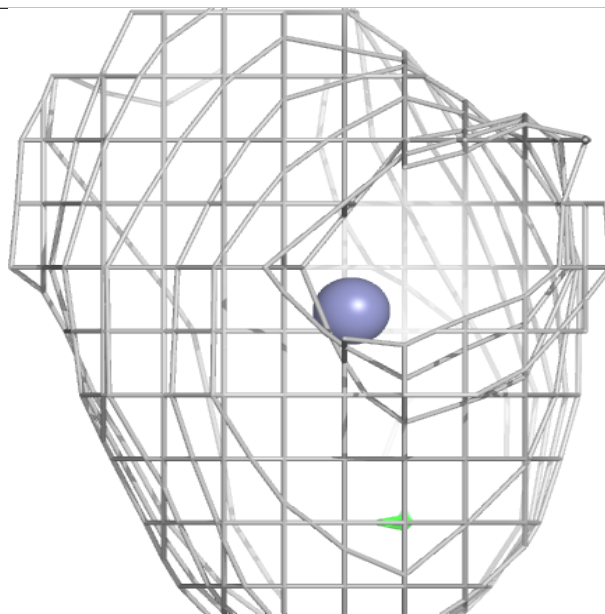
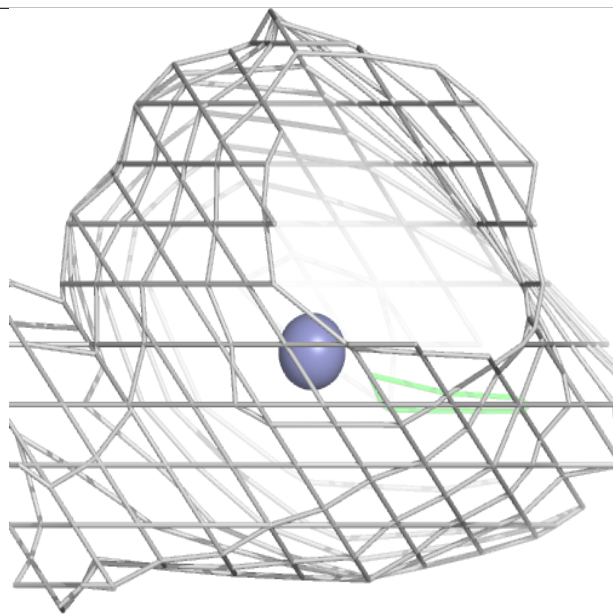
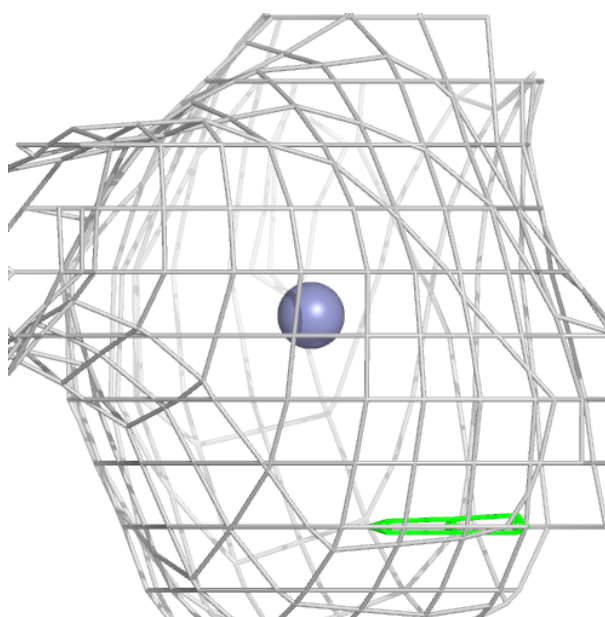
**Electron density around MG D 402:**

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



**Electron density around ZN H 403:**

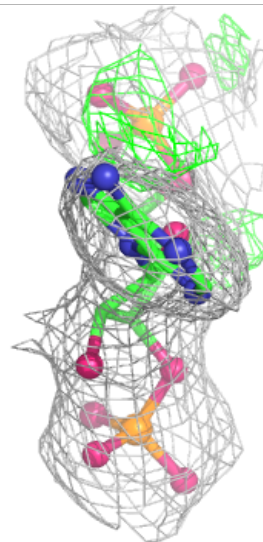
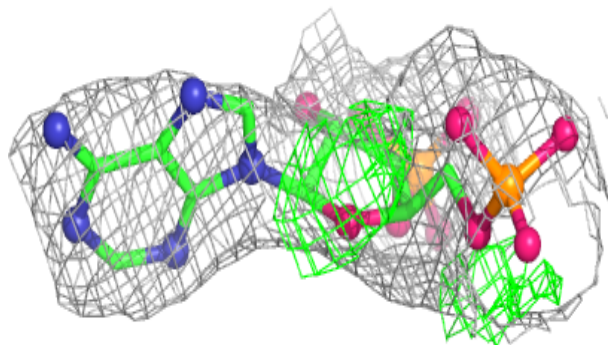
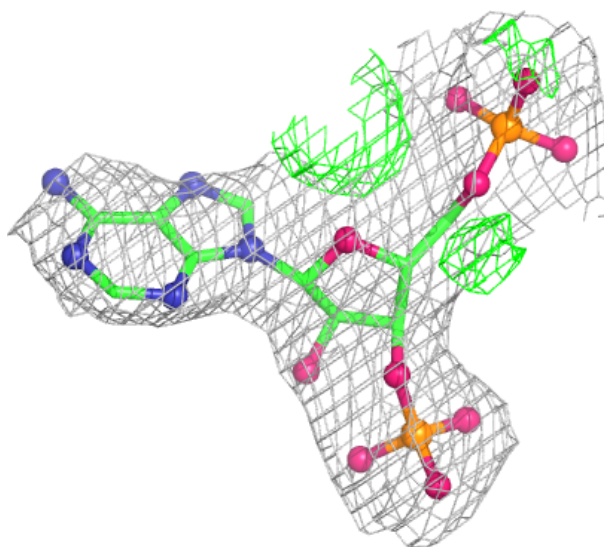
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





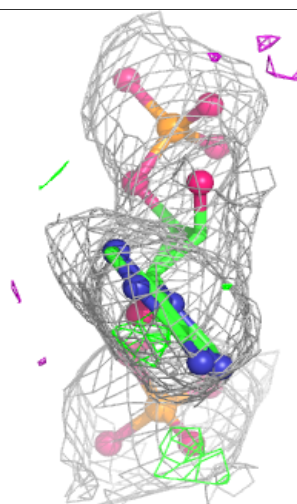
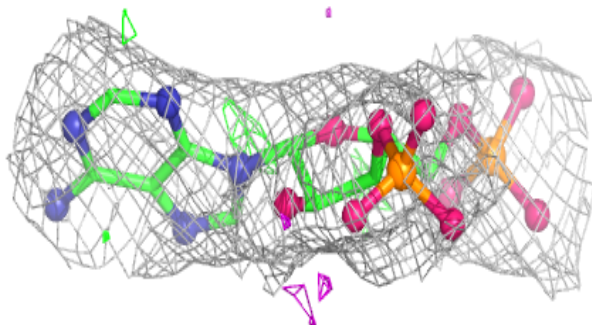
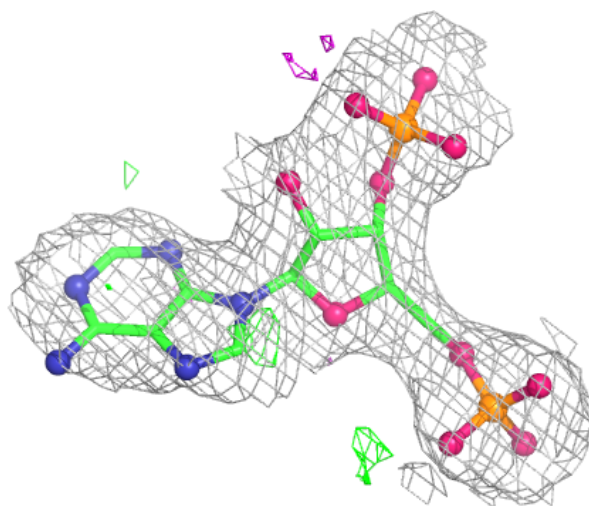
**Electron density around A3P D 401:**

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



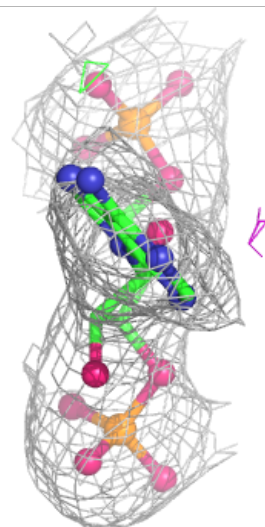
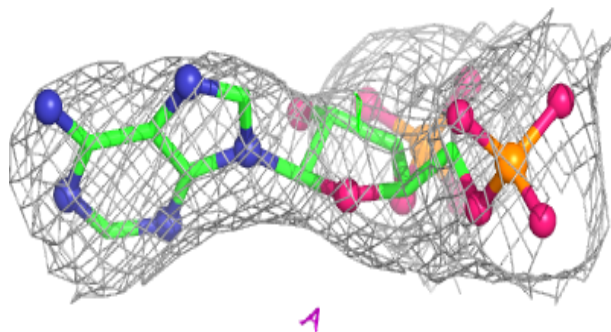
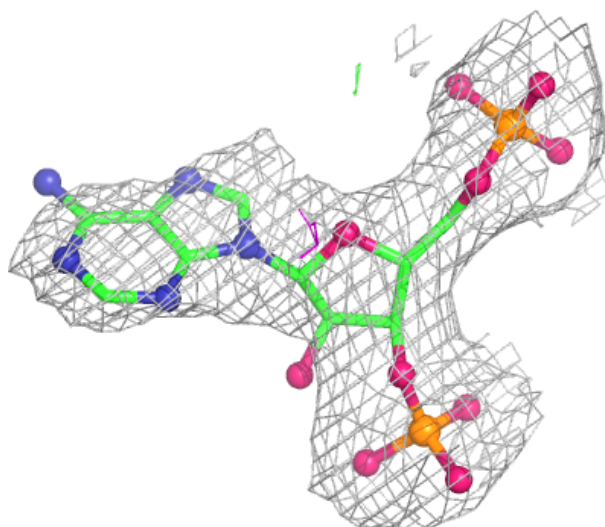
**Electron density around A3P A 401:**

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



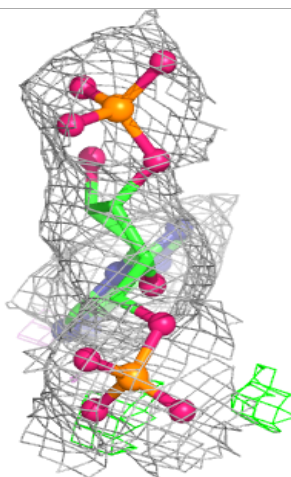
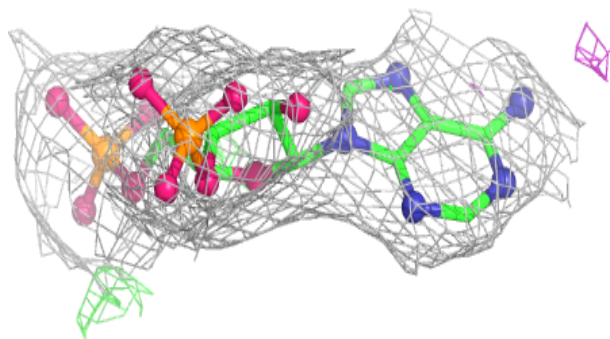
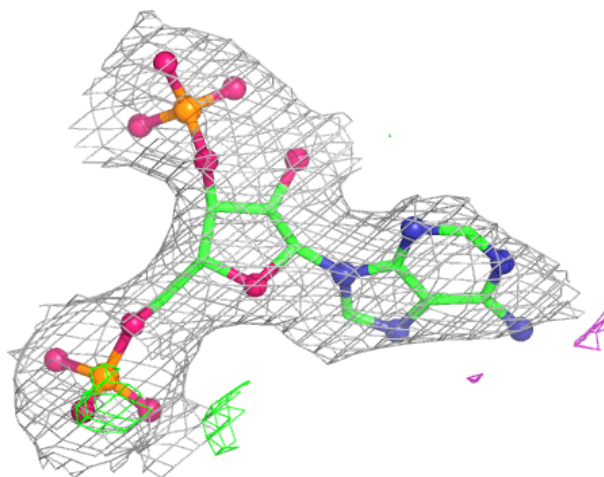
**Electron density around A3P H 401:**

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



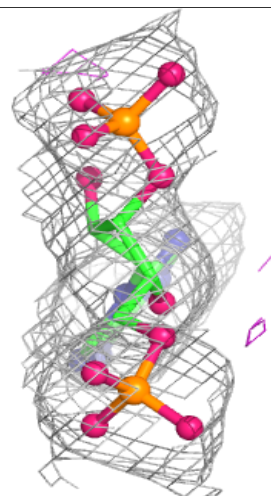
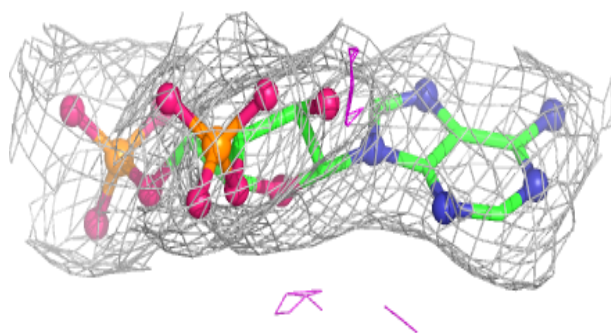
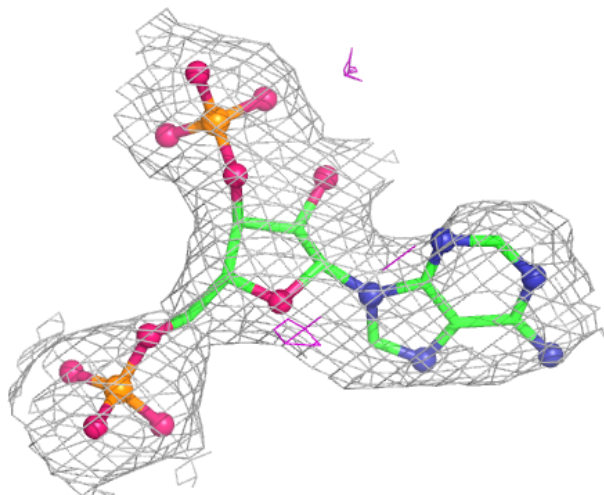
**Electron density around A3P C 401:**

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



**Electron density around A3P G 401:**

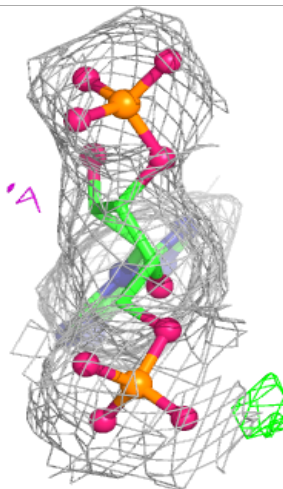
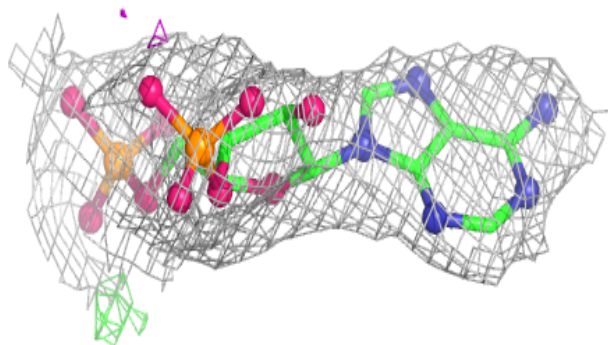
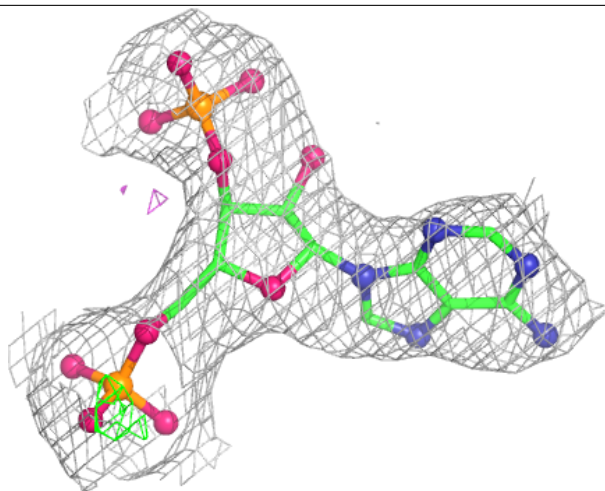
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





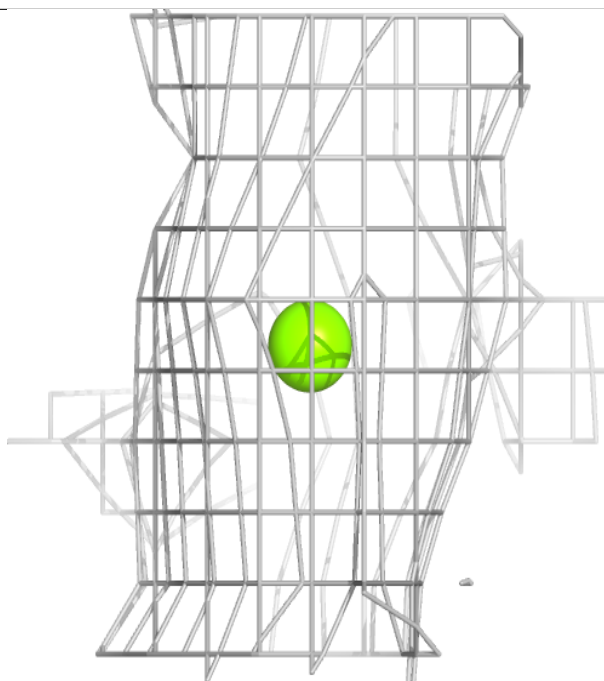
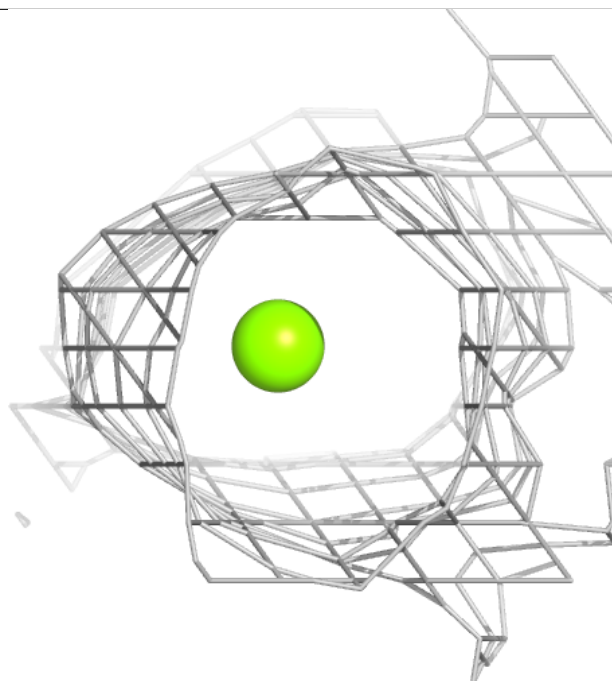
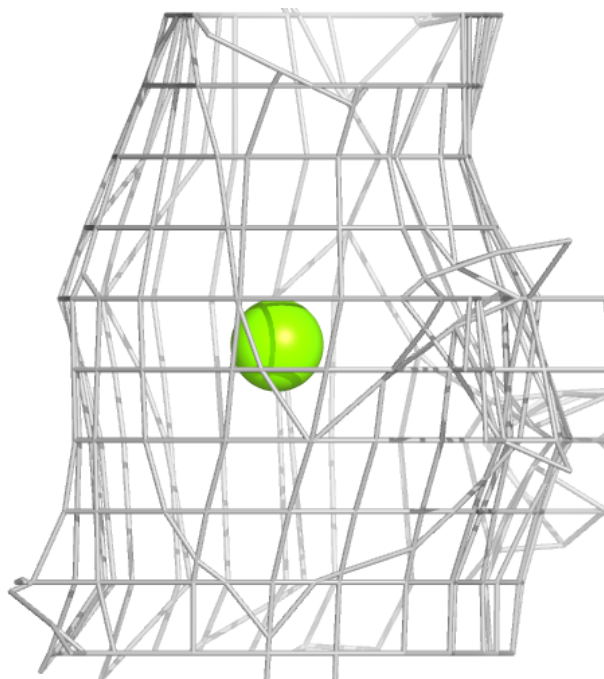
**Electron density around A3P E 401:**

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



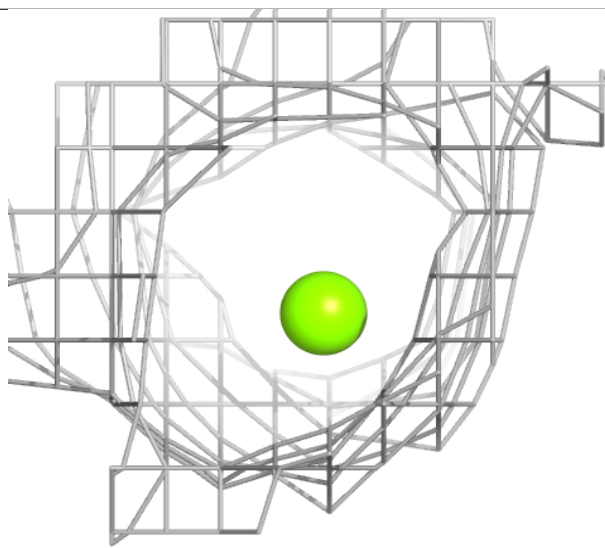
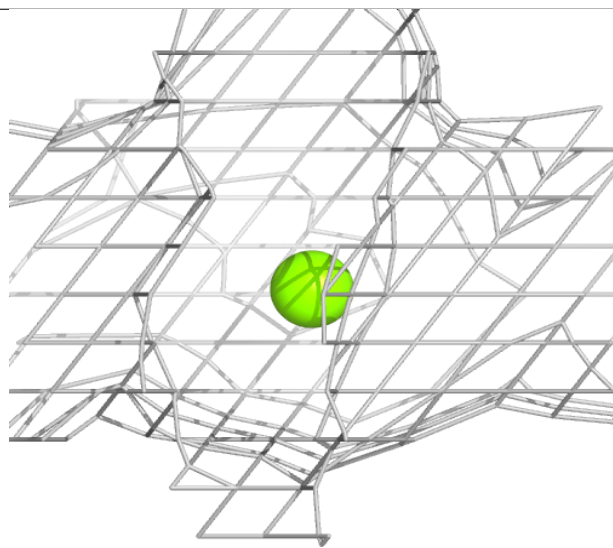
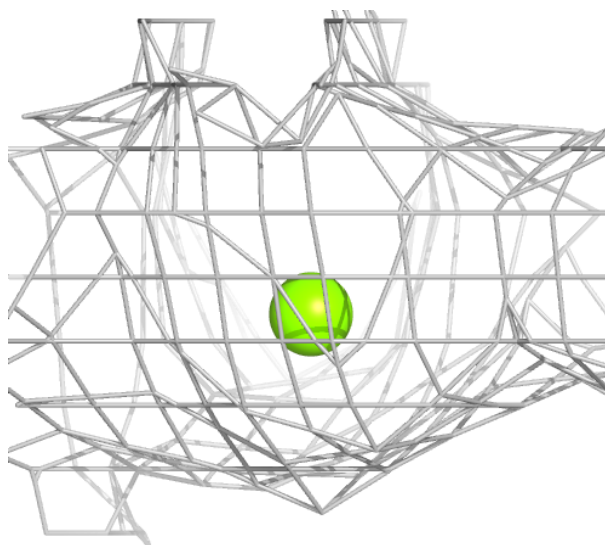
**Electron density around MG E 402:**

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



**Electron density around MG A 402:**

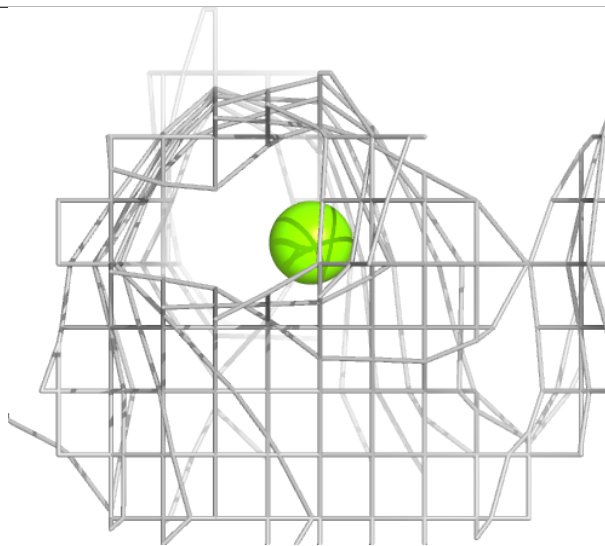
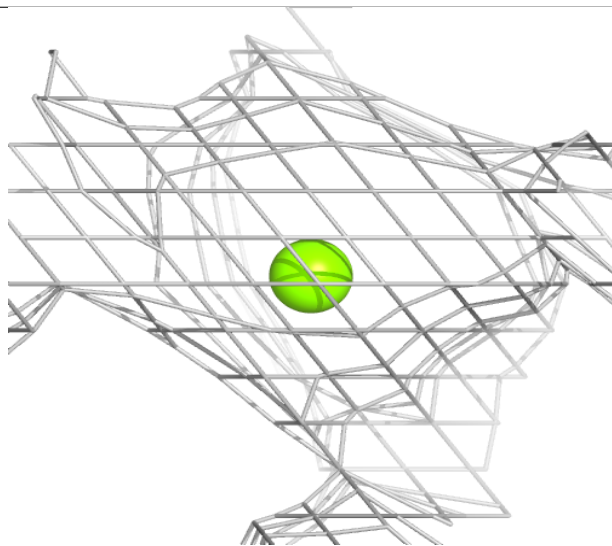
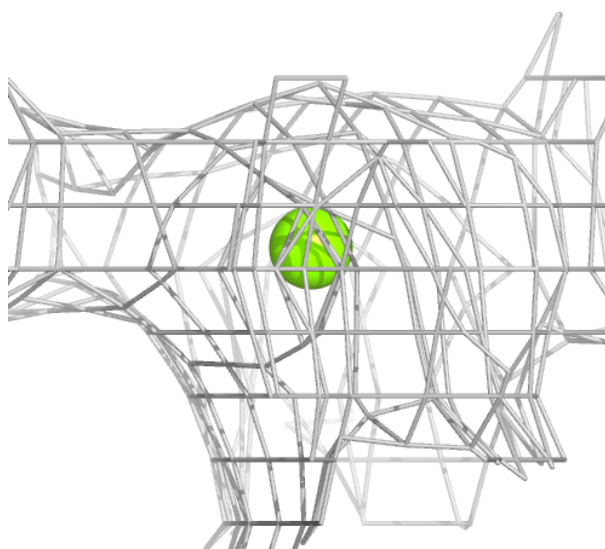
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





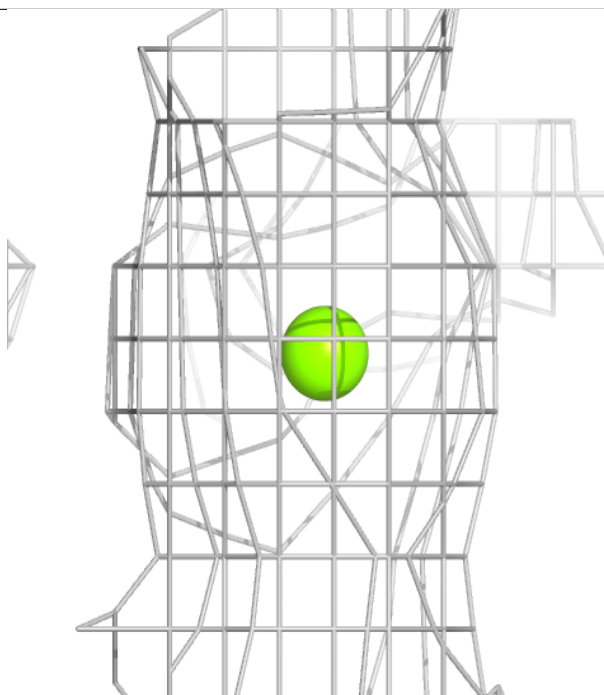
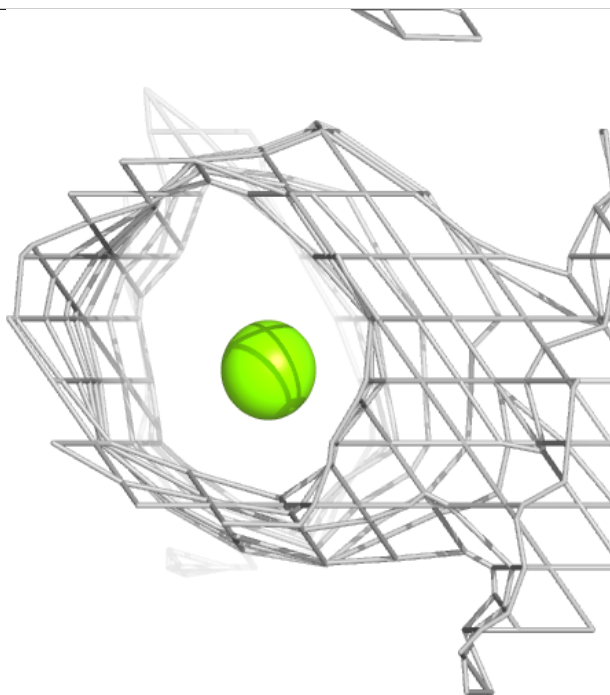
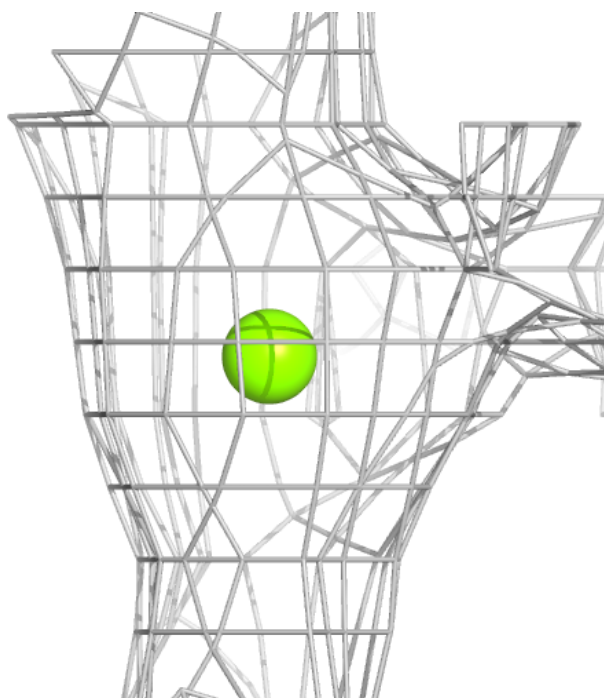
**Electron density around MG H 402:**

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



**Electron density around MG F 402:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.