



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 12, 2021 – 10:11 AM EDT

PDB ID : 7KMA  
Title : Crystal structure of eif2B $\alpha$  with a ligand.  
Authors : Nocek, B.; Hao, Q.; Remarcik, C.; Stoll, V.; Wong, Y.; Sidrauski, C.  
Deposited on : 2020-11-02  
Resolution : 2.70 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.22  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.22

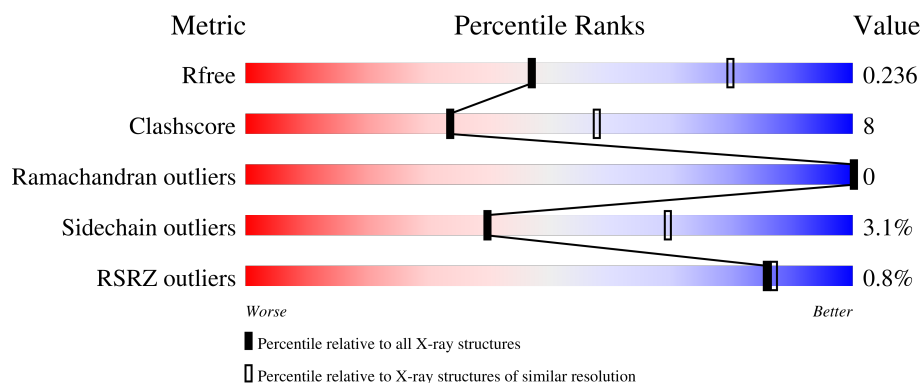
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	313	<div> <div></div> <div>79%13%8%</div> </div>
1	B	313	<div> <div></div> <div>71%14%14%</div> </div>
1	C	313	<div> <div></div> <div>77%15%6%</div> </div>
1	D	313	<div> <div></div> <div>71%19%9%</div> </div>
1	E	313	<div> <div></div> <div>70%19%11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	313	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>78%14%8%</div></div>
1	G	313	<div><div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div></div><div>81%11%7%</div></div>
1	H	313	<div><div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div></div><div>75%17%8%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17263 atoms, of which 91 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	2	0
			2145	1376	354	404	11			
1	B	268	Total	C	N	O	S	5	0	0
			1971	1269	325	368	9			
1	C	294	Total	C	N	O	S	0	1	0
			2172	1391	362	408	11			
1	D	284	Total	C	N	O	S	2	1	0
			2125	1367	357	390	11			
1	E	278	Total	C	N	O	S	0	0	0
			2029	1306	338	375	10			
1	F	287	Total	C	N	O	S	2	1	0
			2125	1371	352	391	11			
1	G	290	Total	C	N	O	S	0	1	0
			2164	1393	359	400	12			
1	H	289	Total	C	N	O	S	0	0	0
			2156	1391	351	402	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLY	-	expression tag	UNP Q14232
A	307	GLY	-	expression tag	UNP Q14232
A	308	GLU	-	expression tag	UNP Q14232
A	309	ASN	-	expression tag	UNP Q14232
A	310	LEU	-	expression tag	UNP Q14232
A	311	TYR	-	expression tag	UNP Q14232
A	312	PHE	-	expression tag	UNP Q14232
A	313	GLN	-	expression tag	UNP Q14232
B	306	GLY	-	expression tag	UNP Q14232
B	307	GLY	-	expression tag	UNP Q14232
B	308	GLU	-	expression tag	UNP Q14232
B	309	ASN	-	expression tag	UNP Q14232
B	310	LEU	-	expression tag	UNP Q14232

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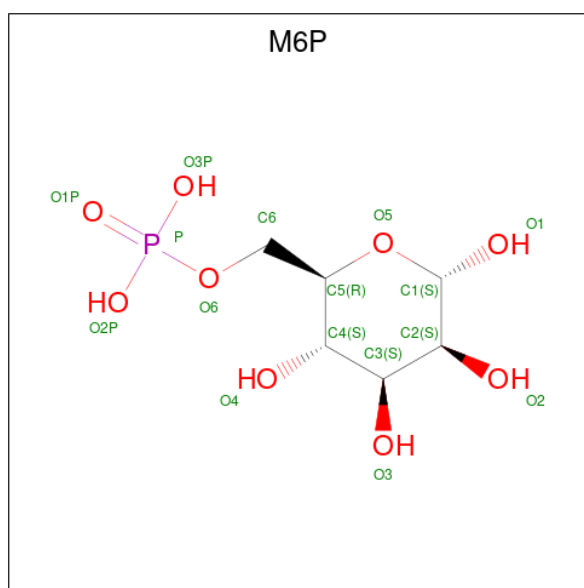
Chain	Residue	Modelled	Actual	Comment	Reference
B	311	TYR	-	expression tag	UNP Q14232
B	312	PHE	-	expression tag	UNP Q14232
B	313	GLN	-	expression tag	UNP Q14232
C	306	GLY	-	expression tag	UNP Q14232
C	307	GLY	-	expression tag	UNP Q14232
C	308	GLU	-	expression tag	UNP Q14232
C	309	ASN	-	expression tag	UNP Q14232
C	310	LEU	-	expression tag	UNP Q14232
C	311	TYR	-	expression tag	UNP Q14232
C	312	PHE	-	expression tag	UNP Q14232
C	313	GLN	-	expression tag	UNP Q14232
D	306	GLY	-	expression tag	UNP Q14232
D	307	GLY	-	expression tag	UNP Q14232
D	308	GLU	-	expression tag	UNP Q14232
D	309	ASN	-	expression tag	UNP Q14232
D	310	LEU	-	expression tag	UNP Q14232
D	311	TYR	-	expression tag	UNP Q14232
D	312	PHE	-	expression tag	UNP Q14232
D	313	GLN	-	expression tag	UNP Q14232
E	306	GLY	-	expression tag	UNP Q14232
E	307	GLY	-	expression tag	UNP Q14232
E	308	GLU	-	expression tag	UNP Q14232
E	309	ASN	-	expression tag	UNP Q14232
E	310	LEU	-	expression tag	UNP Q14232
E	311	TYR	-	expression tag	UNP Q14232
E	312	PHE	-	expression tag	UNP Q14232
E	313	GLN	-	expression tag	UNP Q14232
F	306	GLY	-	expression tag	UNP Q14232
F	307	GLY	-	expression tag	UNP Q14232
F	308	GLU	-	expression tag	UNP Q14232
F	309	ASN	-	expression tag	UNP Q14232
F	310	LEU	-	expression tag	UNP Q14232
F	311	TYR	-	expression tag	UNP Q14232
F	312	PHE	-	expression tag	UNP Q14232
F	313	GLN	-	expression tag	UNP Q14232
G	306	GLY	-	expression tag	UNP Q14232
G	307	GLY	-	expression tag	UNP Q14232
G	308	GLU	-	expression tag	UNP Q14232
G	309	ASN	-	expression tag	UNP Q14232
G	310	LEU	-	expression tag	UNP Q14232
G	311	TYR	-	expression tag	UNP Q14232
G	312	PHE	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
G	313	GLN	-	expression tag	UNP Q14232
H	306	GLY	-	expression tag	UNP Q14232
H	307	GLY	-	expression tag	UNP Q14232
H	308	GLU	-	expression tag	UNP Q14232
H	309	ASN	-	expression tag	UNP Q14232
H	310	LEU	-	expression tag	UNP Q14232
H	311	TYR	-	expression tag	UNP Q14232
H	312	PHE	-	expression tag	UNP Q14232
H	313	GLN	-	expression tag	UNP Q14232

- Molecule 2 is 6-O-phosphono-alpha-D-mannopyranose (three-letter code: M6P) (formula:  $C_6H_{13}O_9P$ ) (labeled as "Ligand of Interest" by depositor).



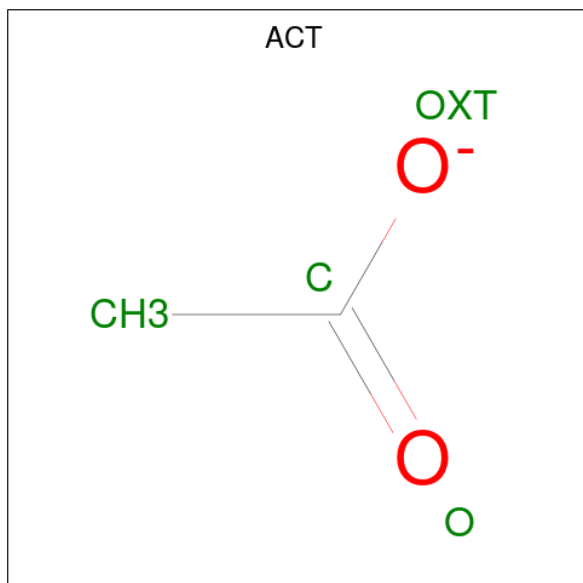
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	B	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	C	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	D	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	E	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	F	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
2	H	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	28	Total	O	0	0
			28	28		
4	C	19	Total	O	0	0
			19	19		
4	D	14	Total	O	0	0
			14	14		
4	E	10	Total	O	0	0
			10	10		
4	F	17	Total	O	0	0
			17	17		

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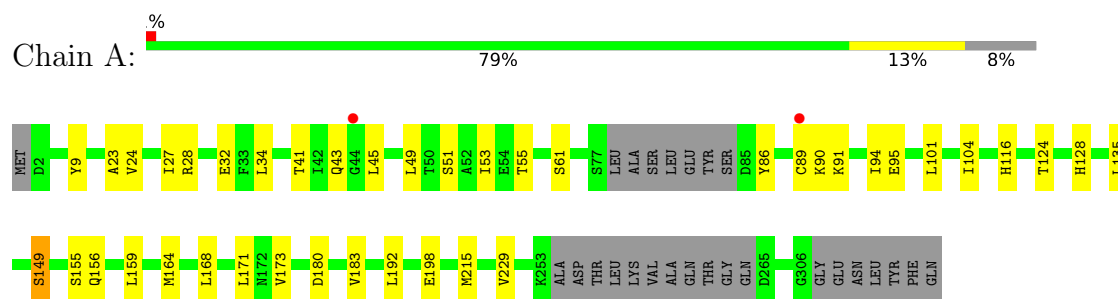
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	18	Total	O	0	0
			18	18		
4	H	25	Total	O	0	0
			25	25		



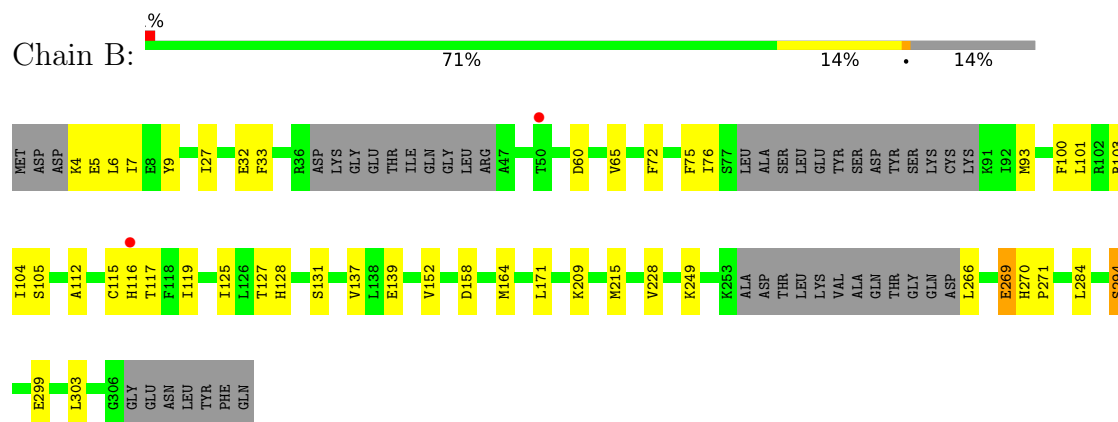
### 3 Residue-property plots [i](#)

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.

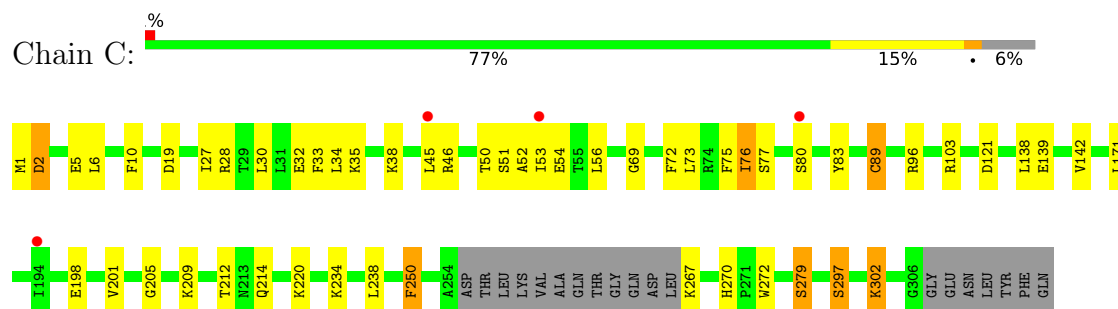
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 1: Translation initiation factor eIF-2B subunit alpha

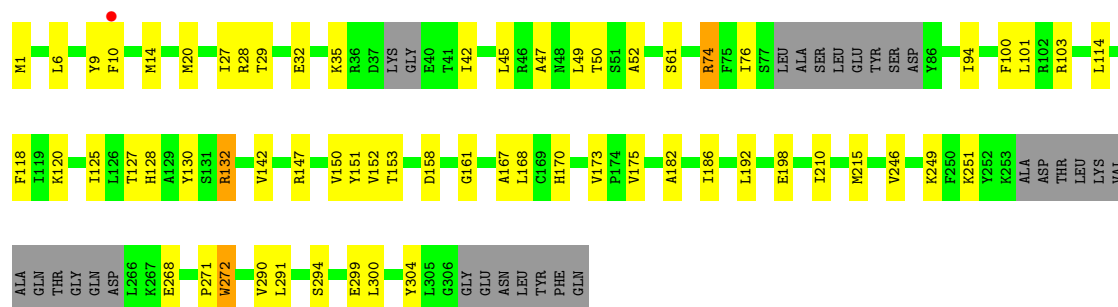


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

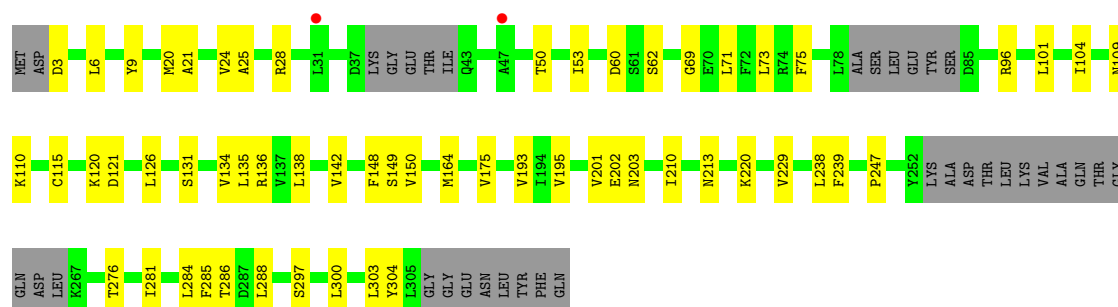


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

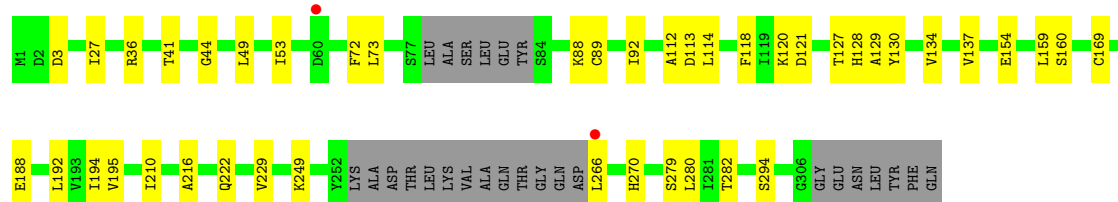
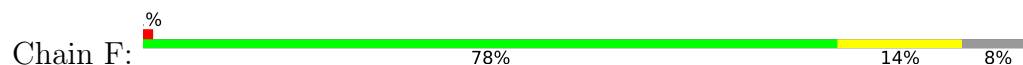




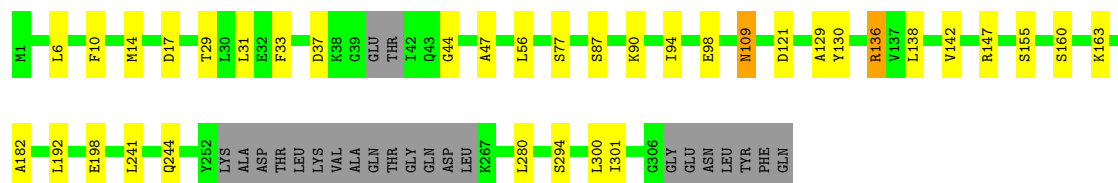
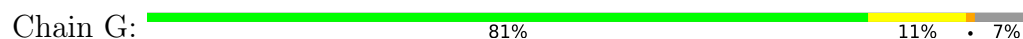
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



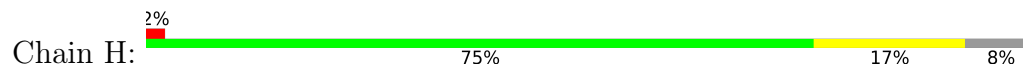
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

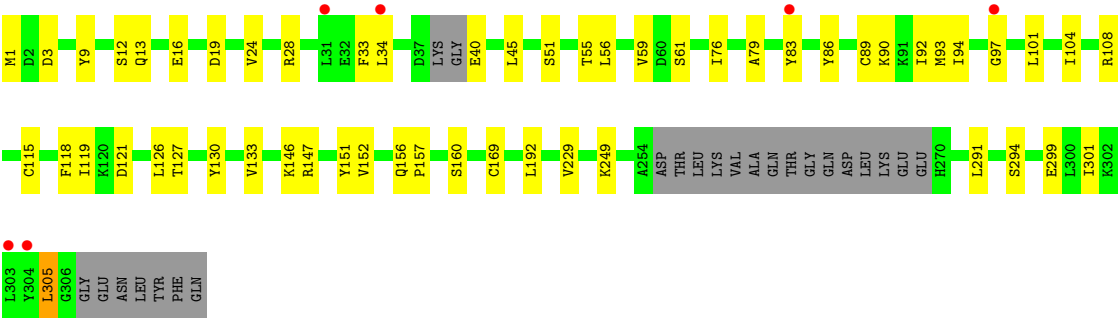


- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 1: Translation initiation factor eIF-2B subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.20Å 155.54Å 140.11Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	55.61 – 2.70 136.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (55.61-2.70) 93.7 (136.01-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.69Å)	Xtriage
Refinement program	PHENIX dev_3916	Depositor
R, $R_{free}$	0.191 , 0.238 0.189 , 0.236	Depositor DCC
$R_{free}$ test set	3882 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: M6P, ACT

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	0.32	0/2178	0.48	0/2959
1	B	0.43	0/2003	0.55	0/2722
1	C	0.41	1/2207 (0.0%)	0.52	0/2999
1	D	0.36	0/2158	0.49	0/2929
1	E	0.39	0/2059	0.54	0/2798
1	F	0.34	0/2159	0.47	0/2933
1	G	0.44	1/2201 (0.0%)	0.53	0/2985
1	H	0.40	0/2191	0.52	0/2972
All	All	0.39	2/17156 (0.0%)	0.51	0/23297

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	17	ASP	C-N	8.29	1.50	1.34
1	C	89	CYS	CB-SG	-7.28	1.69	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	109	ASN	Sidechain

## 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	2145	0	2113	29	0
1	B	1971	0	1920	30	0
1	C	2172	0	2129	38	0
1	D	2125	0	2109	50	0
1	E	2029	0	1989	37	0
1	F	2125	0	2108	32	0
1	G	2164	0	2157	30	0
1	H	2156	0	2155	53	0
2	A	16	11	11	1	0
2	B	16	11	11	1	0
2	C	16	11	11	3	0
2	D	16	11	11	3	0
2	E	16	11	11	0	0
2	F	16	11	11	0	0
2	G	16	11	11	1	0
2	H	16	11	11	0	0
3	A	4	3	3	0	0
4	A	22	0	0	1	0
4	B	28	0	0	3	0
4	C	19	0	0	5	0
4	D	14	0	0	1	0
4	E	10	0	0	1	0
4	F	17	0	0	2	0
4	G	18	0	0	1	0
4	H	25	0	0	2	0
All	All	17172	91	16771	286	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 8.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124[B]:THR:HG22	1:A:149:SER:OG	1.72	0.89
1:H:45:LEU:HD21	1:H:93:MET:HE1	1.58	0.86
1:E:71:LEU:HD11	1:E:303:LEU:HD21	1.61	0.82
1:G:300:LEU:HD23	1:G:300:LEU:O	1.79	0.82
1:B:270:HIS:HB2	4:B:513:HOH:O	1.79	0.81
1:G:6:LEU:HD11	1:G:29:THR:HG22	1.63	0.80
1:D:127:THR:HG23	1:D:152:VAL:HG23	1.63	0.79
1:E:286:THR:HG23	1:E:288:LEU:H	1.50	0.77
1:D:151:TYR:CE1	1:D:186:ILE:HD11	2.21	0.76
1:D:132:ARG:N	2:D:401:M6P:O2P	2.19	0.73
1:H:156:GLN:HG3	1:H:157:PRO:HA	1.70	0.73
1:H:83:TYR:HE2	1:H:92:ILE:HG13	1.51	0.73
1:B:6:LEU:HG	1:B:33:PHE:HD1	1.54	0.73
1:G:6:LEU:CD1	1:G:29:THR:HG22	2.19	0.71
1:A:135:LEU:HD13	1:A:164:MET:HE3	1.73	0.71
1:H:156:GLN:CG	4:H:511:HOH:O	2.38	0.71
1:H:305:LEU:C	1:H:305:LEU:HD23	2.11	0.71
1:H:156:GLN:HG3	4:H:511:HOH:O	1.89	0.71
1:G:121:ASP:OD2	1:G:147:ARG:NE	2.24	0.70
1:D:167:ALA:HA	1:D:170:HIS:HD2	1.55	0.70
1:D:168:LEU:HD22	1:D:173:VAL:HG21	1.74	0.70
1:A:24:VAL:HG22	1:A:104:ILE:HD12	1.74	0.68
1:B:294:SER:O	4:B:501:HOH:O	2.12	0.68
1:D:35:LYS:HG2	1:D:94:ILE:HD13	1.76	0.67
1:F:127:THR:HG23	1:F:194:ILE:O	1.95	0.66
1:H:115:CYS:HA	1:H:118:PHE:CD2	2.30	0.66
1:F:249:LYS:HD3	1:F:249:LYS:N	2.11	0.66
1:A:49:LEU:O	1:A:53:ILE:HG22	1.96	0.66
1:B:209:LYS:HB2	2:B:401:M6P:H2	1.77	0.65
1:C:72:PHE:O	1:C:76:ILE:HG23	1.96	0.65
1:G:280:LEU:O	4:G:501:HOH:O	2.14	0.65
1:A:23:ALA:O	1:A:27:ILE:HD12	1.96	0.65
1:C:1:MET:HE2	1:C:6:LEU:HD23	1.78	0.64
1:F:88:LYS:O	1:F:92:ILE:HD12	1.98	0.64
1:B:119:ILE:HG23	1:B:125:ILE:HD11	1.80	0.64
1:E:71:LEU:HD11	1:E:303:LEU:CD2	2.29	0.62
1:C:209:LYS:HB2	2:C:401:M6P:H2	1.82	0.62
1:G:109:ASN:OD1	1:G:136:ARG:NH1	2.31	0.61
1:D:151:TYR:CZ	1:D:186:ILE:HD11	2.35	0.61
1:G:300:LEU:HD23	1:G:300:LEU:C	2.20	0.61
1:H:1:MET:HE3	1:H:33:PHE:HA	1.83	0.61
1:E:53:ILE:HD11	1:E:69:GLY:HA3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:LEU:HD13	1:E:164:MET:CE	2.30	0.60
1:B:266:LEU:HD13	1:H:169:CYS:SG	2.42	0.60
1:D:35:LYS:HG2	1:D:94:ILE:CD1	2.32	0.60
1:B:75:PHE:HD2	1:B:100:PHE:HB2	1.65	0.60
1:E:138:LEU:HD22	1:E:148:PHE:CE2	2.36	0.60
1:C:272:TRP:HB3	4:C:514:HOH:O	2.02	0.60
1:F:282[A]:THR:HG22	4:F:509:HOH:O	2.01	0.60
1:D:9:TYR:CE2	1:D:32:GLU:HG3	2.38	0.59
1:E:238:LEU:HD21	1:E:247:PRO:HD3	1.84	0.59
1:C:80:SER:HA	1:C:89:CYS:SG	2.42	0.59
1:B:299:GLU:HA	1:B:299:GLU:OE1	2.00	0.59
1:C:139:GLU:HG3	1:C:171:LEU:HD21	1.85	0.59
1:B:139:GLU:HG2	1:B:171:LEU:HD11	1.85	0.59
1:F:188:GLU:HA	1:F:222:GLN:HE22	1.67	0.59
1:D:128:HIS:HB2	1:D:215:MET:CE	2.33	0.59
1:E:75:PHE:O	1:E:96:ARG:NH1	2.35	0.59
1:E:138:LEU:O	1:E:142:VAL:HG23	2.03	0.58
1:H:115:CYS:HA	1:H:118:PHE:CE2	2.38	0.58
1:G:6:LEU:CD1	1:G:29:THR:CG2	2.82	0.58
1:H:305:LEU:HD23	1:H:305:LEU:O	2.03	0.58
1:B:4:LYS:HA	1:B:7:ILE:HB	1.84	0.58
1:F:279:SER:OG	4:F:501:HOH:O	2.17	0.58
1:G:6:LEU:HD12	1:G:29:THR:CG2	2.33	0.57
1:E:50:THR:O	1:E:53:ILE:HG22	2.05	0.57
1:H:108:ARG:HD3	1:H:133:VAL:HG22	1.87	0.57
1:F:266:LEU:HD23	1:F:266:LEU:O	2.04	0.57
1:C:1:MET:CE	1:C:6:LEU:HD23	2.35	0.56
1:E:24:VAL:HG12	1:E:104:ILE:HD12	1.86	0.56
1:D:28:ARG:HG3	1:D:101:LEU:HD11	1.87	0.56
1:D:158:ASP:OD2	1:D:272:TRP:HH2	1.88	0.56
1:D:130:TYR:O	2:D:401:M6P:O2	2.23	0.56
1:C:6:LEU:HD21	1:C:33:PHE:HD2	1.71	0.56
1:C:32:GLU:HA	1:C:35:LYS:HE2	1.87	0.56
1:G:198:GLU:HG3	2:G:401:M6P:O1	2.06	0.56
1:G:31:LEU:HD21	1:G:98:GLU:HG3	1.88	0.56
1:E:135:LEU:HD13	1:E:164:MET:HE3	1.88	0.55
1:B:269:GLU:HG3	1:B:271:PRO:HD3	1.88	0.55
1:H:83:TYR:CE2	1:H:92:ILE:HG13	2.35	0.55
1:H:51:SER:O	1:H:55:THR:HG22	2.06	0.55
1:D:128:HIS:HB2	1:D:215:MET:HE3	1.89	0.55
1:D:147:ARG:HA	4:D:509:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD12	1:B:72:PHE:HB2	1.89	0.54
1:C:46:ARG:O	1:C:50:THR:HG23	2.08	0.54
1:H:192:LEU:N	1:H:192:LEU:HD23	2.21	0.54
1:A:124[B]:THR:HG21	4:A:512:HOH:O	2.07	0.54
1:C:297:SER:OG	1:E:202:GLU:OE1	2.25	0.54
1:E:20:MET:CE	1:E:25:ALA:HB2	2.37	0.54
1:A:183:VAL:HB	1:C:214:GLN:HE21	1.73	0.53
1:D:10:PHE:CZ	1:D:14:MET:HE1	2.43	0.53
1:D:47:ALA:O	1:D:50:THR:OG1	2.25	0.53
1:D:210:ILE:HD13	1:D:271:PRO:HG2	1.90	0.53
1:C:220:LYS:HE2	4:C:516:HOH:O	2.09	0.52
1:B:128:HIS:O	4:B:502:HOH:O	2.19	0.52
1:D:125:ILE:HG12	1:D:192:LEU:HD21	1.92	0.52
1:H:34:LEU:HD11	1:H:93:MET:CE	2.39	0.52
1:E:300:LEU:HD11	1:E:304:TYR:CE1	2.45	0.52
1:A:156:GLN:NE2	1:A:159:LEU:HD21	2.25	0.52
1:E:20:MET:HE3	1:E:25:ALA:HB2	1.92	0.51
1:C:302:LYS:HD2	1:C:302:LYS:O	2.10	0.51
1:B:158:ASP:OD1	1:B:209:LYS:NZ	2.43	0.51
1:D:158:ASP:OD2	1:D:272:TRP:CH2	2.64	0.51
1:H:79:ALA:HB3	1:H:93:MET:HG3	1.93	0.51
1:D:42:ILE:HD12	1:D:42:ILE:H	1.75	0.51
1:B:60:ASP:HB3	1:B:65:VAL:HG11	1.92	0.51
1:E:28:ARG:HH12	1:E:101:LEU:HD11	1.76	0.51
1:A:168:LEU:HD22	1:A:173:VAL:HG21	1.93	0.50
1:E:60:ASP:OD1	1:E:62:SER:N	2.39	0.50
1:F:266:LEU:HD23	1:F:266:LEU:C	2.32	0.50
1:H:40:GLU:N	1:H:86:TYR:CE2	2.79	0.50
1:H:19:ASP:O	1:H:108:ARG:NH2	2.45	0.50
1:G:10:PHE:CB	1:G:56:LEU:HD21	2.42	0.50
1:G:10:PHE:HB2	1:G:56:LEU:HD21	1.94	0.50
1:C:30:LEU:HD21	1:C:56:LEU:HD12	1.94	0.49
1:D:6:LEU:HD23	1:D:29:THR:HG22	1.94	0.49
1:E:238:LEU:HD12	1:E:239:PHE:H	1.78	0.49
1:F:188:GLU:OE2	1:G:244:GLN:HG3	2.12	0.49
1:H:115:CYS:HB3	1:H:118:PHE:CD2	2.47	0.49
1:H:86:TYR:CE1	1:H:90:LYS:HB2	2.48	0.49
1:F:114:LEU:O	1:F:118:PHE:CE1	2.66	0.49
1:F:127:THR:HG22	1:F:128:HIS:H	1.77	0.49
1:F:154:GLU:O	1:F:159:LEU:HA	2.14	0.48
1:H:119:ILE:O	1:H:146:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLU:HG3	2:C:401:M6P:O1	2.13	0.48
1:E:131:SER:HB3	1:E:134:VAL:HB	1.95	0.48
1:B:75:PHE:CD2	1:B:100:PHE:HB2	2.47	0.48
1:D:20:MET:CE	1:D:28:ARG:HD3	2.43	0.48
1:D:114:LEU:HD21	1:D:290:VAL:CG2	2.43	0.48
1:F:114:LEU:O	1:F:114:LEU:HD23	2.14	0.48
1:D:27:ILE:HG22	1:D:101:LEU:HD13	1.95	0.48
1:B:103:ARG:HH21	1:B:104:ILE:HG22	1.80	0.47
1:D:74:ARG:NH2	1:D:304:TYR:O	2.46	0.47
1:A:45:LEU:C	1:A:45:LEU:HD23	2.35	0.47
1:H:127:THR:HG23	1:H:152:VAL:HG23	1.95	0.47
1:C:1:MET:HB3	1:C:5:GLU:CB	2.43	0.47
1:C:234:LYS:NZ	2:C:401:M6P:O3P	2.30	0.47
1:A:116:HIS:NE2	1:F:113:ASP:OD2	2.48	0.47
1:A:171:LEU:HD12	1:A:171:LEU:N	2.30	0.47
1:B:101:LEU:O	1:B:105:SER:OG	2.25	0.47
1:H:291:LEU:HD21	1:H:299:GLU:HG3	1.97	0.47
1:E:71:LEU:CD1	1:E:304:TYR:CE1	2.98	0.47
1:A:34:LEU:HD13	1:A:49:LEU:HD11	1.96	0.47
1:F:89:CYS:HA	1:F:92:ILE:CD1	2.45	0.46
1:H:93:MET:O	1:H:97:GLY:N	2.47	0.46
1:A:9:TYR:CE2	1:A:32:GLU:HG2	2.50	0.46
1:A:41:THR:HG22	1:A:43:GLN:H	1.81	0.46
1:E:201:VAL:HG23	1:E:203:ASN:OD1	2.15	0.46
1:B:127:THR:HG23	1:B:152:VAL:HG23	1.97	0.46
1:C:69:GLY:O	1:C:73:LEU:HD12	2.14	0.46
1:G:37:ASP:O	1:G:90:LYS:NZ	2.41	0.46
1:G:129:ALA:HB2	1:G:155:SER:OG	2.15	0.46
1:H:61:SER:HB2	1:H:249:LYS:O	2.16	0.46
1:D:27:ILE:HD13	1:D:100:PHE:HE2	1.80	0.46
1:G:301:ILE:HG12	1:H:301:ILE:HG13	1.97	0.46
1:B:6:LEU:HG	1:B:33:PHE:CD1	2.43	0.46
1:C:30:LEU:CD2	1:C:56:LEU:HD12	2.44	0.46
1:D:76:ILE:HG13	1:D:76:ILE:O	2.16	0.46
1:G:138:LEU:O	1:G:142:VAL:HG12	2.16	0.46
1:B:128:HIS:HB2	1:B:215:MET:CE	2.46	0.46
1:A:229:VAL:O	1:A:229:VAL:HG23	2.15	0.46
1:B:131:SER:H	1:B:164:MET:CE	2.28	0.46
1:H:40:GLU:N	1:H:86:TYR:HH	2.13	0.46
1:F:127:THR:HG21	1:F:134:VAL:HG11	1.98	0.46
1:H:130:TYR:HB2	1:H:160:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:O	1:A:94:ILE:HG13	2.17	0.46
1:A:180:ASP:O	1:C:214:GLN:NE2	2.36	0.46
1:B:9:TYR:OH	1:B:32:GLU:HG3	2.16	0.46
1:D:114:LEU:HD21	1:D:290:VAL:HG22	1.97	0.46
1:E:229:VAL:HG12	1:E:285:PHE:HB2	1.98	0.46
1:E:300:LEU:CD1	1:E:304:TYR:CE1	2.99	0.46
1:F:222:GLN:HE21	1:F:222:GLN:HB3	1.55	0.45
1:B:5:GLU:HG2	1:B:6:LEU:HD23	1.98	0.45
1:G:130:TYR:HB3	1:G:160:SER:OG	2.17	0.45
1:H:115:CYS:HB3	1:H:118:PHE:HD2	1.82	0.45
1:A:171:LEU:HD12	1:A:171:LEU:H	1.81	0.45
1:B:228:VAL:HB	1:B:284:LEU:HG	1.98	0.45
1:B:266:LEU:HB2	1:H:169:CYS:SG	2.57	0.45
1:H:9:TYR:O	1:H:13:GLN:HG2	2.17	0.45
1:A:155:SER:HA	1:A:180:ASP:OD1	2.16	0.45
1:D:198:GLU:OE1	2:D:401:M6P:O1	2.24	0.45
1:G:121:ASP:OD1	1:G:147:ARG:HG2	2.16	0.45
1:B:27:ILE:HD12	1:B:72:PHE:CB	2.47	0.45
1:D:9:TYR:CZ	1:D:32:GLU:HG3	2.52	0.45
1:D:130:TYR:HE2	1:D:132:ARG:HD3	1.82	0.45
1:E:126:LEU:HB3	1:E:193:VAL:HG22	1.98	0.45
1:A:51:SER:O	1:A:55:THR:OG1	2.32	0.45
1:D:1:MET:CE	1:D:6:LEU:HA	2.46	0.44
1:D:6:LEU:CD2	1:D:29:THR:HG22	2.47	0.44
1:B:76:ILE:HG21	1:B:93:MET:CB	2.47	0.44
1:C:220:LYS:CE	4:C:516:HOH:O	2.64	0.44
1:C:238:LEU:HD11	1:C:250:PHE:CE2	2.53	0.44
1:F:229:VAL:O	1:F:229:VAL:HG23	2.17	0.44
1:D:45:LEU:O	1:D:49:LEU:HB2	2.18	0.44
1:G:10:PHE:CZ	1:G:14:MET:SD	3.10	0.44
1:C:302:LYS:HD2	1:C:302:LYS:C	2.37	0.44
1:D:150:VAL:O	1:D:175:VAL:HA	2.17	0.44
1:D:132:ARG:HE	1:D:132:ARG:HB2	1.42	0.44
1:H:1:MET:CE	1:H:33:PHE:HA	2.47	0.44
1:E:60:ASP:OD1	1:E:62:SER:HB3	2.17	0.44
1:E:109:ASN:ND2	1:E:136:ARG:HE	2.16	0.44
1:E:238:LEU:HD12	1:E:239:PHE:N	2.32	0.44
1:F:130:TYR:O	1:F:130:TYR:CD2	2.71	0.44
1:H:83:TYR:HD2	1:H:89:CYS:HA	1.83	0.44
1:C:201:VAL:HG22	1:C:205:GLY:O	2.17	0.44
1:D:246:VAL:HB	1:D:251:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:H	1:C:5:GLU:CB	2.30	0.44
1:H:90:LYS:O	1:H:94:ILE:HG13	2.17	0.44
1:C:30:LEU:CD2	1:C:56:LEU:CD1	2.96	0.44
1:D:61:SER:HB2	1:D:249:LYS:O	2.18	0.44
1:G:130:TYR:CD1	1:G:163:LYS:HG2	2.53	0.44
1:E:73:LEU:C	1:E:73:LEU:HD23	2.38	0.43
1:F:129:ALA:HB1	1:F:160:SER:OG	2.17	0.43
1:E:3:ASP:HA	1:E:6:LEU:HD12	1.99	0.43
1:E:150:VAL:O	1:E:175:VAL:HA	2.17	0.43
1:H:12:SER:O	1:H:16:GLU:HG3	2.19	0.43
1:C:6:LEU:HD13	1:C:52:ALA:HB1	1.99	0.43
1:D:147:ARG:HG3	1:D:147:ARG:O	2.18	0.43
1:E:135:LEU:HD13	1:E:164:MET:HE1	2.00	0.43
1:G:300:LEU:C	1:G:300:LEU:CD2	2.85	0.43
1:H:79:ALA:CB	1:H:93:MET:HG3	2.48	0.43
1:A:28:ARG:CG	1:A:101:LEU:HD11	2.49	0.43
1:G:94:ILE:O	1:G:98:GLU:N	2.51	0.43
1:A:91:LYS:O	1:A:95:GLU:HG3	2.19	0.43
1:F:41:THR:HG23	1:F:44:GLY:H	1.84	0.43
1:H:3:ASP:N	1:H:3:ASP:OD1	2.51	0.43
1:C:10:PHE:CD2	1:C:10:PHE:C	2.92	0.43
1:G:33:PHE:O	1:G:37:ASP:HB2	2.19	0.43
1:B:117:THR:HG21	1:D:114:LEU:CD1	2.49	0.43
1:F:49:LEU:HD23	1:F:73:LEU:HD13	2.00	0.43
1:C:34:LEU:HD12	1:C:45:LEU:HD11	2.00	0.42
1:D:291:LEU:HD21	1:D:299:GLU:HG3	2.00	0.42
1:F:120:LYS:H	1:F:120:LYS:HD2	1.84	0.42
1:H:147:ARG:HB2	1:H:147:ARG:CZ	2.50	0.42
1:C:27:ILE:CD1	1:C:72:PHE:HB2	2.50	0.42
1:C:53:ILE:HG23	1:C:54:GLU:N	2.34	0.42
1:C:138:LEU:O	1:C:142:VAL:HG12	2.18	0.42
1:C:212:THR:HB	4:C:502:HOH:O	2.18	0.42
1:E:21:ALA:O	1:E:24:VAL:HG22	2.19	0.42
1:F:192:LEU:HD23	1:F:192:LEU:N	2.35	0.42
1:G:241:LEU:HD11	1:H:294:SER:HB3	2.00	0.42
1:H:13:GLN:OE1	1:H:28:ARG:CD	2.67	0.42
1:H:101:LEU:HD23	1:H:101:LEU:O	2.19	0.42
1:H:229:VAL:HG23	1:H:229:VAL:O	2.19	0.42
1:A:61:SER:O	1:A:61:SER:OG	2.36	0.42
1:A:192:LEU:HD23	1:A:192:LEU:N	2.35	0.42
1:D:186:ILE:HG13	1:D:186:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ASN:HA	1:E:276:THR:HG22	2.02	0.41
1:G:44:GLY:O	1:G:47:ALA:HB3	2.20	0.41
1:H:24:VAL:HG22	1:H:104:ILE:CD1	2.50	0.41
1:H:34:LEU:HD12	1:H:45:LEU:HD11	2.01	0.41
1:H:56:LEU:O	1:H:59:VAL:HG12	2.20	0.41
1:A:198:GLU:HG3	2:A:401:M6P:O1	2.20	0.41
1:F:27:ILE:HD12	1:F:72:PHE:HB2	2.01	0.41
1:H:45:LEU:CD2	1:H:93:MET:HE1	2.40	0.41
1:H:76:ILE:O	1:H:93:MET:HG2	2.20	0.41
1:B:112:ALA:HA	1:B:137:VAL:HG22	2.02	0.41
1:F:210:ILE:HD11	1:G:182:ALA:HA	2.02	0.41
1:D:6:LEU:HD23	1:D:29:THR:CG2	2.51	0.41
1:F:49:LEU:O	1:F:53:ILE:HG13	2.20	0.41
1:G:192:LEU:N	1:G:192:LEU:HD23	2.35	0.41
1:H:305:LEU:O	1:H:305:LEU:CG	2.69	0.41
1:D:6:LEU:HD11	1:D:52:ALA:HB1	2.03	0.41
1:D:45:LEU:O	1:D:49:LEU:N	2.42	0.41
1:H:119:ILE:O	1:H:146:LYS:HE2	2.21	0.41
1:A:128:HIS:HB2	1:A:215:MET:HE1	2.02	0.41
1:D:153:THR:O	1:D:161:GLY:HA3	2.20	0.41
1:F:114:LEU:O	1:F:118:PHE:HE1	2.02	0.41
1:C:1:MET:SD	1:C:6:LEU:HD23	2.61	0.41
1:D:20:MET:HE1	1:D:28:ARG:HD3	2.03	0.41
1:E:120:LYS:NZ	4:E:501:HOH:O	2.54	0.41
1:F:112:ALA:HA	1:F:137:VAL:HG22	2.03	0.41
1:F:216:ALA:HB1	1:F:280:LEU:HB3	2.03	0.41
1:H:126:LEU:HD12	1:H:151:TYR:O	2.21	0.41
1:C:75:PHE:O	1:C:96:ARG:NH2	2.54	0.41
1:G:129:ALA:HB2	1:G:155:SER:CB	2.51	0.41
1:H:147:ARG:HB2	1:H:147:ARG:NH1	2.36	0.40
1:C:279[A]:SER:OG	4:C:501:HOH:O	2.22	0.40
1:D:182:ALA:HA	1:E:210:ILE:HD11	2.02	0.40
1:F:89:CYS:HA	1:F:92:ILE:HD12	2.01	0.40
1:H:34:LEU:CD2	1:H:94:ILE:HG12	2.50	0.40
1:A:86:TYR:CD1	1:A:86:TYR:C	2.94	0.40
1:C:83:TYR:O	1:C:89:CYS:SG	2.75	0.40
1:A:116:HIS:CE1	1:F:113:ASP:OD2	2.74	0.40
1:D:300:LEU:HD23	1:D:300:LEU:C	2.41	0.40
1:E:281:ILE:HG21	1:E:284:LEU:CD1	2.51	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	283/313 (90%)	267 (94%)	16 (6%)	0	100	100
1	B	260/313 (83%)	256 (98%)	4 (2%)	0	100	100
1	C	291/313 (93%)	277 (95%)	14 (5%)	0	100	100
1	D	277/313 (88%)	272 (98%)	5 (2%)	0	100	100
1	E	270/313 (86%)	262 (97%)	8 (3%)	0	100	100
1	F	282/313 (90%)	274 (97%)	8 (3%)	0	100	100
1	G	285/313 (91%)	276 (97%)	9 (3%)	0	100	100
1	H	283/313 (90%)	276 (98%)	7 (2%)	0	100	100
All	All	2231/2504 (89%)	2160 (97%)	71 (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	222/266 (84%)	220 (99%)	2 (1%)	78	92
1	B	199/266 (75%)	193 (97%)	6 (3%)	41	70
1	C	221/266 (83%)	205 (93%)	16 (7%)	14	34
1	D	218/266 (82%)	208 (95%)	10 (5%)	27	54
1	E	203/266 (76%)	195 (96%)	8 (4%)	32	61
1	F	217/266 (82%)	210 (97%)	7 (3%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	223/266 (84%)	219 (98%)	4 (2%)	59	83
1	H	225/266 (85%)	223 (99%)	2 (1%)	78	92
All	All	1728/2128 (81%)	1673 (97%)	55 (3%)	40	68

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	CYS
1	A	149	SER
1	B	115	CYS
1	B	116	HIS
1	B	249	LYS
1	B	269	GLU
1	B	294	SER
1	B	303	LEU
1	C	2	ASP
1	C	19	ASP
1	C	28	ARG
1	C	38	LYS
1	C	51	SER
1	C	76	ILE
1	C	77	SER
1	C	103	ARG
1	C	121	ASP
1	C	250	PHE
1	C	267	LYS
1	C	270	HIS
1	C	279[A]	SER
1	C	279[B]	SER
1	C	297	SER
1	C	302	LYS
1	D	74	ARG
1	D	103[A]	ARG
1	D	103[B]	ARG
1	D	118	PHE
1	D	120	LYS
1	D	132	ARG
1	D	142	VAL
1	D	268	GLU
1	D	272	TRP
1	D	294	SER

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Mol	Chain	Res	Type
1	E	9	TYR
1	E	110	LYS
1	E	115	CYS
1	E	121	ASP
1	E	149	SER
1	E	195	VAL
1	E	220	LYS
1	E	297	SER
1	F	3	ASP
1	F	36	ARG
1	F	121	ASP
1	F	169	CYS
1	F	195	VAL
1	F	270	HIS
1	F	294	SER
1	G	77	SER
1	G	87	SER
1	G	136	ARG
1	G	294	SER
1	H	121	ASP
1	H	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	D	170	HIS
1	F	222	GLN

### 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 monosaccharides in this entry.



## 5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	M6P	H	401	-	16,16,16	1.34	2 (12%)	24,24,24	1.71	7 (29%)
2	M6P	A	401	-	16,16,16	1.56	4 (25%)	24,24,24	1.41	4 (16%)
2	M6P	B	401	-	16,16,16	1.52	3 (18%)	24,24,24	1.25	1 (4%)
2	M6P	D	401	-	16,16,16	1.21	2 (12%)	24,24,24	1.18	2 (8%)
3	ACT	A	402	-	1,3,3	2.87	1 (100%)	0,3,3	0.00	-
2	M6P	C	401	-	16,16,16	1.17	2 (12%)	24,24,24	1.34	4 (16%)
2	M6P	E	401	-	16,16,16	1.26	2 (12%)	24,24,24	1.72	7 (29%)
2	M6P	G	401	-	16,16,16	1.13	2 (12%)	24,24,24	1.35	4 (16%)
2	M6P	F	401	-	16,16,16	1.21	2 (12%)	24,24,24	1.64	5 (20%)

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	M6P	H	401	-	-	5/6/26/26	0/1/1/1
2	M6P	A	401	-	-	5/6/26/26	0/1/1/1
2	M6P	B	401	-	-	2/6/26/26	0/1/1/1
2	M6P	D	401	-	-	3/6/26/26	0/1/1/1
2	M6P	C	401	-	-	3/6/26/26	0/1/1/1
2	M6P	E	401	-	-	5/6/26/26	0/1/1/1
2	M6P	G	401	-	-	5/6/26/26	0/1/1/1
2	M6P	F	401	-	-	5/6/26/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	M6P	P-O2P	-3.03	1.43	1.54
3	A	402	ACT	CH3-C	2.87	1.52	1.48
2	A	401	M6P	P-O3P	-2.85	1.43	1.54
2	B	401	M6P	P-O2P	-2.77	1.44	1.54
2	B	401	M6P	P-O3P	-2.61	1.44	1.54
2	H	401	M6P	P-O2P	-2.60	1.44	1.54
2	C	401	M6P	P-O3P	-2.43	1.45	1.54
2	F	401	M6P	P-O3P	-2.41	1.45	1.54
2	E	401	M6P	P-O2P	-2.37	1.45	1.54
2	H	401	M6P	P-O3P	-2.34	1.45	1.54
2	D	401	M6P	P-O2P	-2.33	1.45	1.54
2	G	401	M6P	P-O2P	-2.32	1.45	1.54
2	G	401	M6P	P-O3P	-2.30	1.46	1.54
2	C	401	M6P	P-O2P	-2.29	1.46	1.54
2	F	401	M6P	P-O2P	-2.27	1.46	1.54
2	E	401	M6P	P-O3P	-2.26	1.46	1.54
2	A	401	M6P	P-O1P	-2.16	1.43	1.50
2	B	401	M6P	P-O1P	-2.15	1.43	1.50
2	D	401	M6P	P-O3P	-2.14	1.46	1.54
2	A	401	M6P	C4-C5	-2.07	1.48	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	M6P	O5-C5-C6	3.73	114.19	106.67
2	E	401	M6P	O2P-P-O6	-3.60	97.16	106.73
2	E	401	M6P	O4-C4-C3	-3.31	102.70	110.35
2	F	401	M6P	O5-C5-C6	3.30	113.33	106.67
2	H	401	M6P	C6-C5-C4	-3.25	105.30	112.09
2	F	401	M6P	O5-C1-C2	3.18	115.97	110.28
2	H	401	M6P	O2P-P-O6	-3.17	98.29	106.73
2	A	401	M6P	C6-C5-C4	-3.14	105.53	112.09
2	A	401	M6P	O5-C5-C6	2.97	112.66	106.67
2	E	401	M6P	O5-C1-C2	2.92	115.49	110.28
2	C	401	M6P	O4-C4-C3	-2.87	103.72	110.35
2	A	401	M6P	O6-P-O1P	-2.84	98.51	106.47
2	G	401	M6P	O5-C5-C6	2.74	112.20	106.67
2	G	401	M6P	C6-C5-C4	-2.70	106.45	112.09
2	E	401	M6P	O3P-P-O2P	2.65	117.78	107.64
2	H	401	M6P	O3-C3-C4	-2.62	104.29	110.35
2	E	401	M6P	C3-C4-C5	2.61	114.90	110.24
2	G	401	M6P	O2P-P-O6	-2.49	100.11	106.73
2	E	401	M6P	O3-C3-C4	-2.47	104.65	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	M6P	O1-C1-C2	-2.42	102.22	109.03
2	C	401	M6P	O3-C3-C4	-2.40	104.80	110.35
2	C	401	M6P	O2P-P-O6	-2.37	100.44	106.73
2	B	401	M6P	O3-C3-C4	-2.35	104.92	110.35
2	E	401	M6P	O1-C1-O5	-2.33	103.38	110.38
2	C	401	M6P	O3P-P-O2P	2.32	116.51	107.64
2	D	401	M6P	O5-C5-C6	2.27	111.25	106.67
2	A	401	M6P	O3-C3-C4	-2.27	105.11	110.35
2	H	401	M6P	O2-C2-C3	-2.24	105.17	110.35
2	F	401	M6P	C4-C3-C2	-2.22	106.96	110.82
2	H	401	M6P	O3P-P-O2P	2.20	116.06	107.64
2	G	401	M6P	C3-C4-C5	2.14	114.05	110.24
2	D	401	M6P	O3-C3-C4	-2.13	105.42	110.35
2	F	401	M6P	C6-C5-C4	-2.10	107.72	112.09
2	H	401	M6P	O6-P-O1P	-2.07	100.67	106.47

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	M6P	C4-C5-C6-O6
2	A	401	M6P	O5-C5-C6-O6
2	A	401	M6P	C6-O6-P-O2P
2	A	401	M6P	C6-O6-P-O3P
2	B	401	M6P	C4-C5-C6-O6
2	B	401	M6P	O5-C5-C6-O6
2	C	401	M6P	C6-O6-P-O2P
2	C	401	M6P	C6-O6-P-O3P
2	D	401	M6P	O5-C5-C6-O6
2	E	401	M6P	C4-C5-C6-O6
2	E	401	M6P	O5-C5-C6-O6
2	E	401	M6P	C6-O6-P-O2P
2	F	401	M6P	C4-C5-C6-O6
2	F	401	M6P	O5-C5-C6-O6
2	F	401	M6P	C6-O6-P-O1P
2	F	401	M6P	C6-O6-P-O2P
2	F	401	M6P	C6-O6-P-O3P
2	G	401	M6P	C4-C5-C6-O6
2	G	401	M6P	O5-C5-C6-O6
2	G	401	M6P	C6-O6-P-O1P
2	G	401	M6P	C6-O6-P-O2P
2	G	401	M6P	C6-O6-P-O3P

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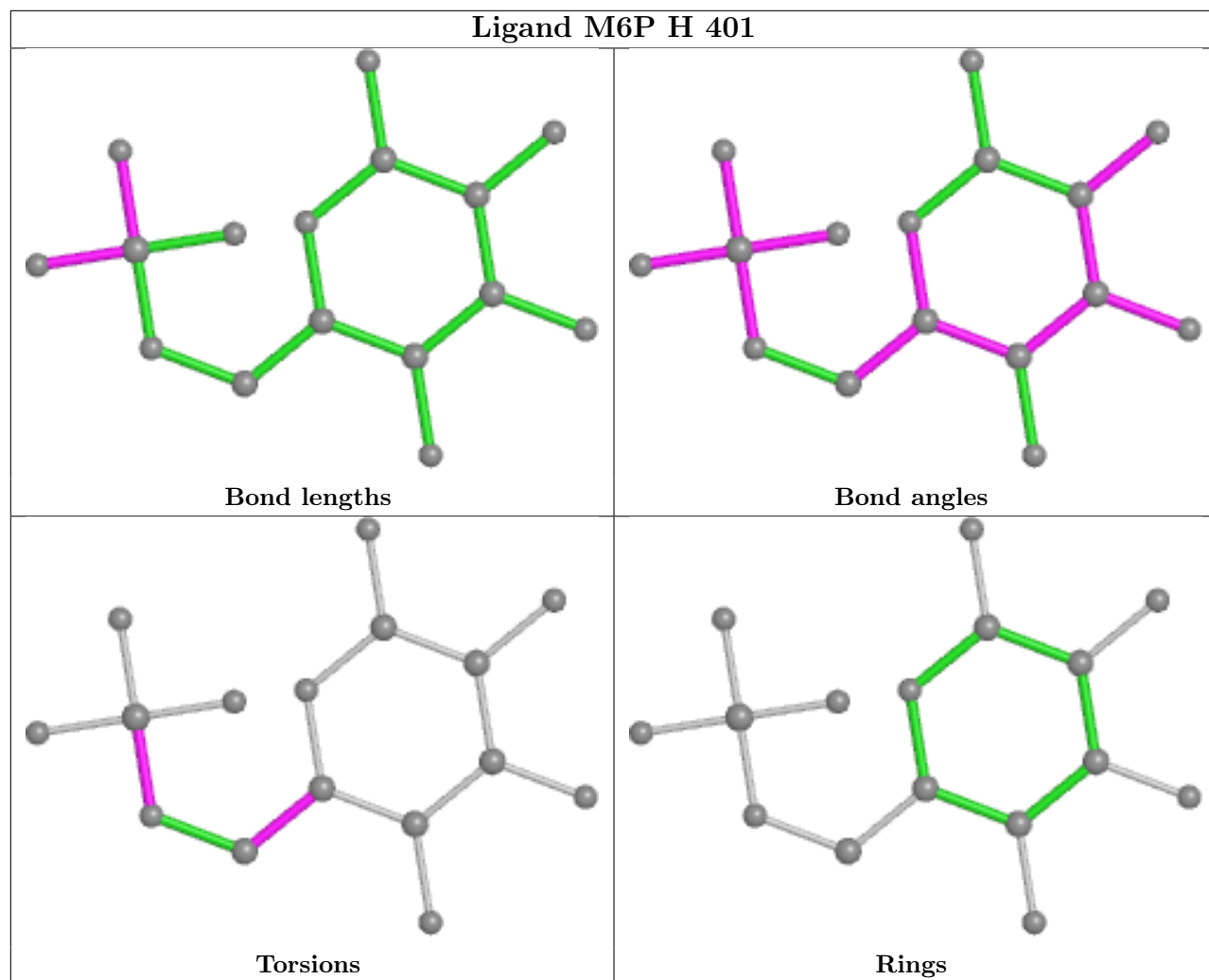
Mol	Chain	Res	Type	Atoms
2	H	401	M6P	C4-C5-C6-O6
2	H	401	M6P	O5-C5-C6-O6
2	H	401	M6P	C6-O6-P-O2P
2	H	401	M6P	C6-O6-P-O3P
2	A	401	M6P	C6-O6-P-O1P
2	C	401	M6P	C6-O6-P-O1P
2	D	401	M6P	C6-O6-P-O1P
2	E	401	M6P	C6-O6-P-O1P
2	H	401	M6P	C6-O6-P-O1P
2	D	401	M6P	C4-C5-C6-O6
2	E	401	M6P	C6-O6-P-O3P

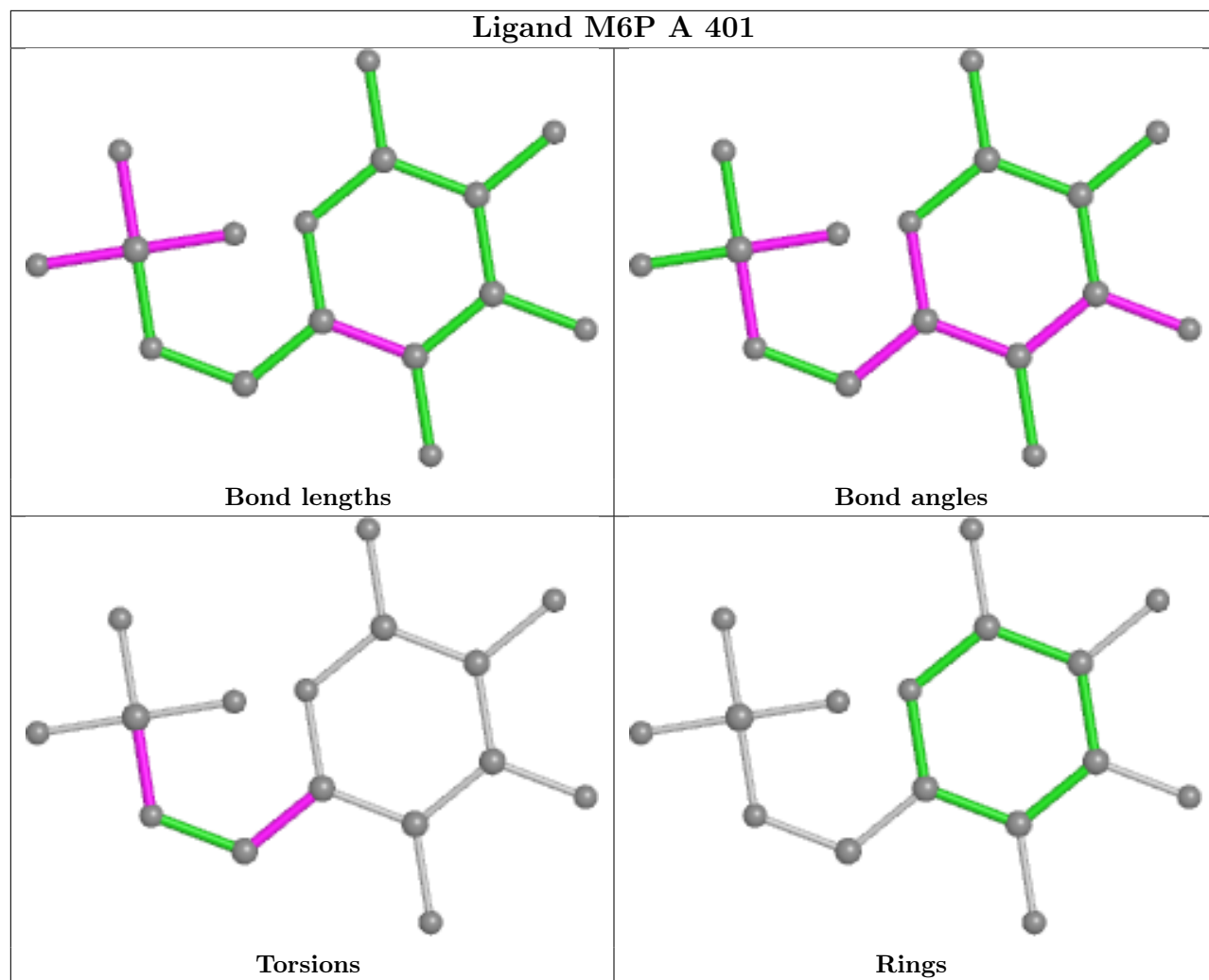
There are no ring outliers.

5 monomers are involved in 9 short contacts:

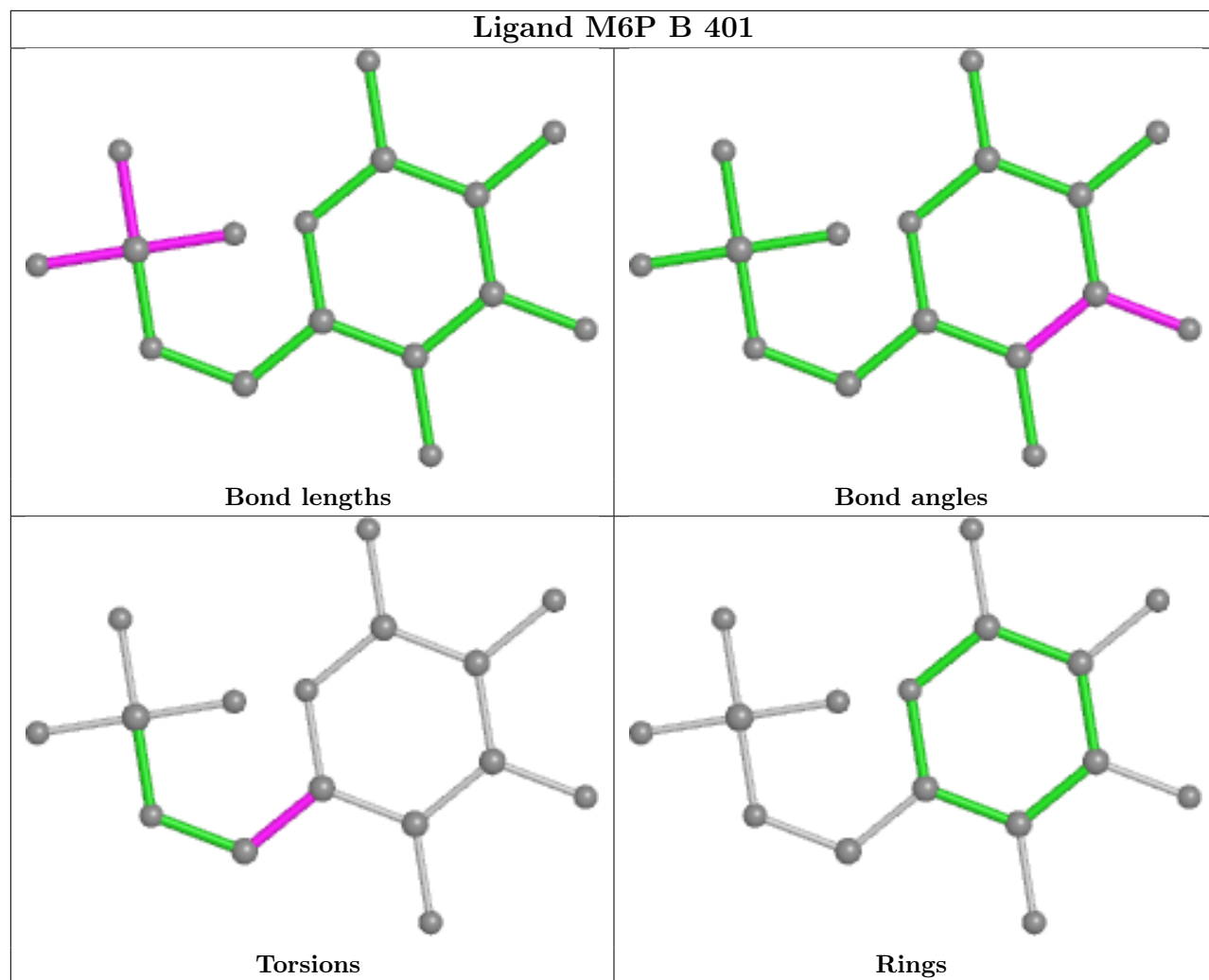
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	M6P	1	0
2	B	401	M6P	1	0
2	D	401	M6P	3	0
2	C	401	M6P	3	0
2	G	401	M6P	1	0

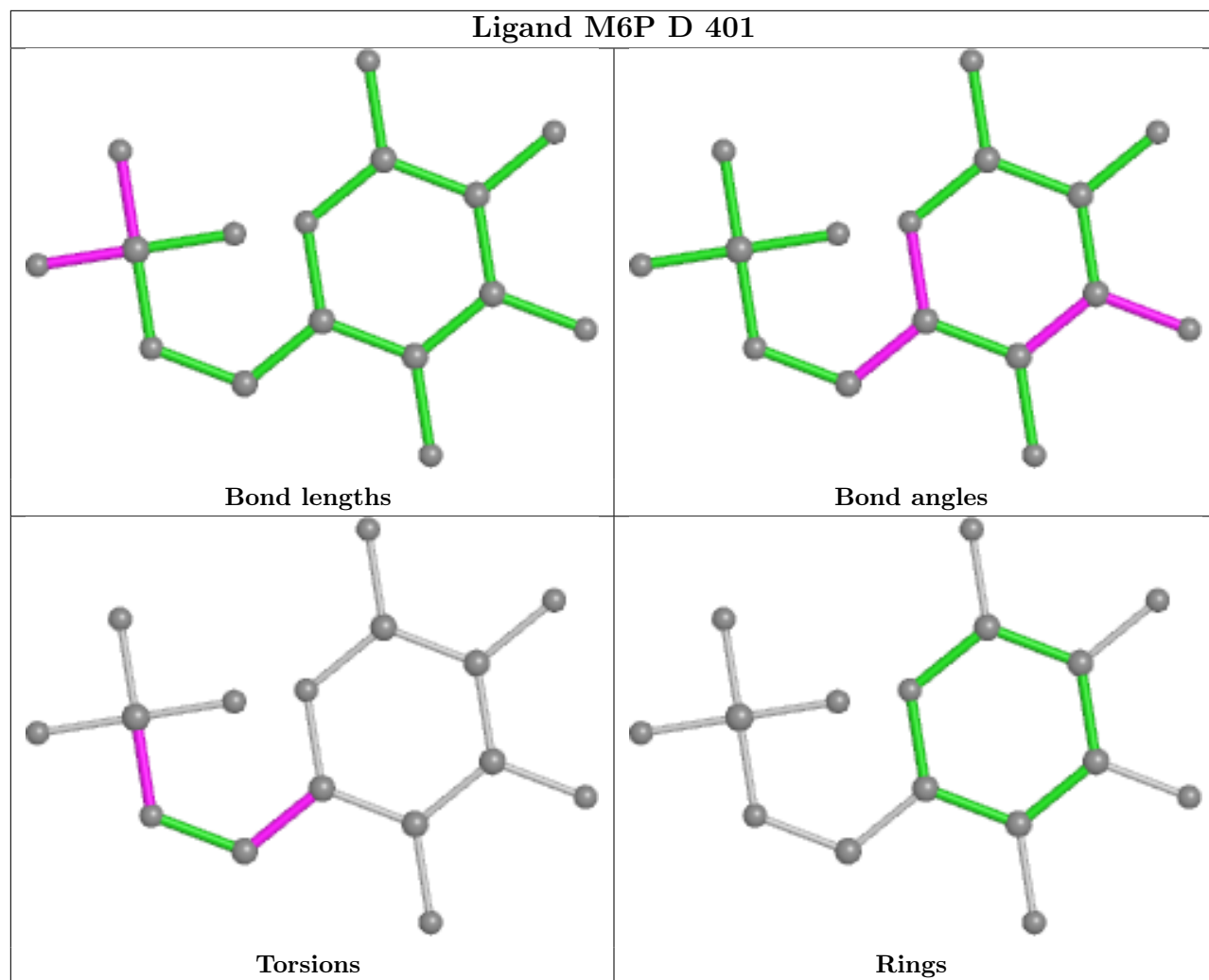
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



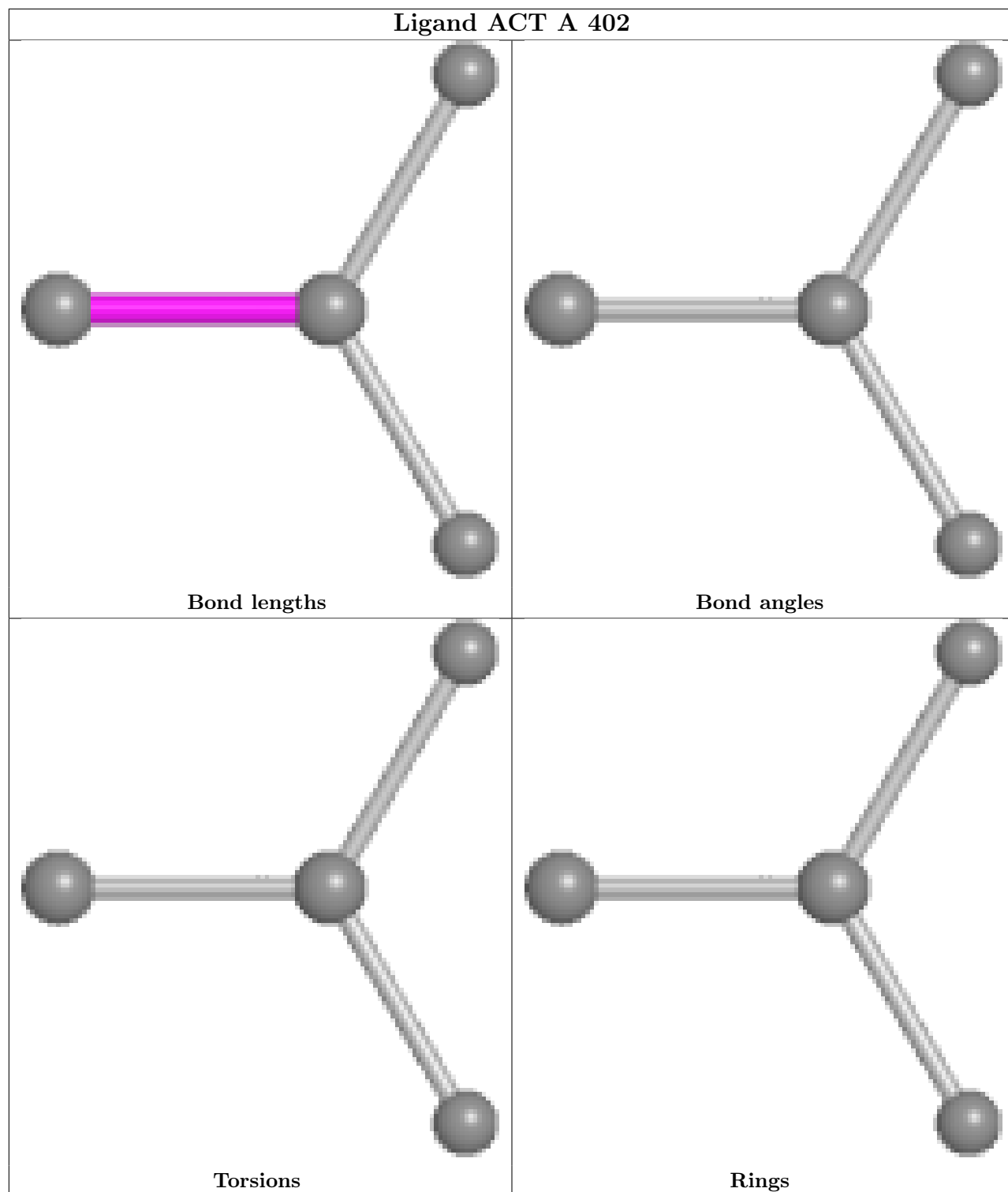


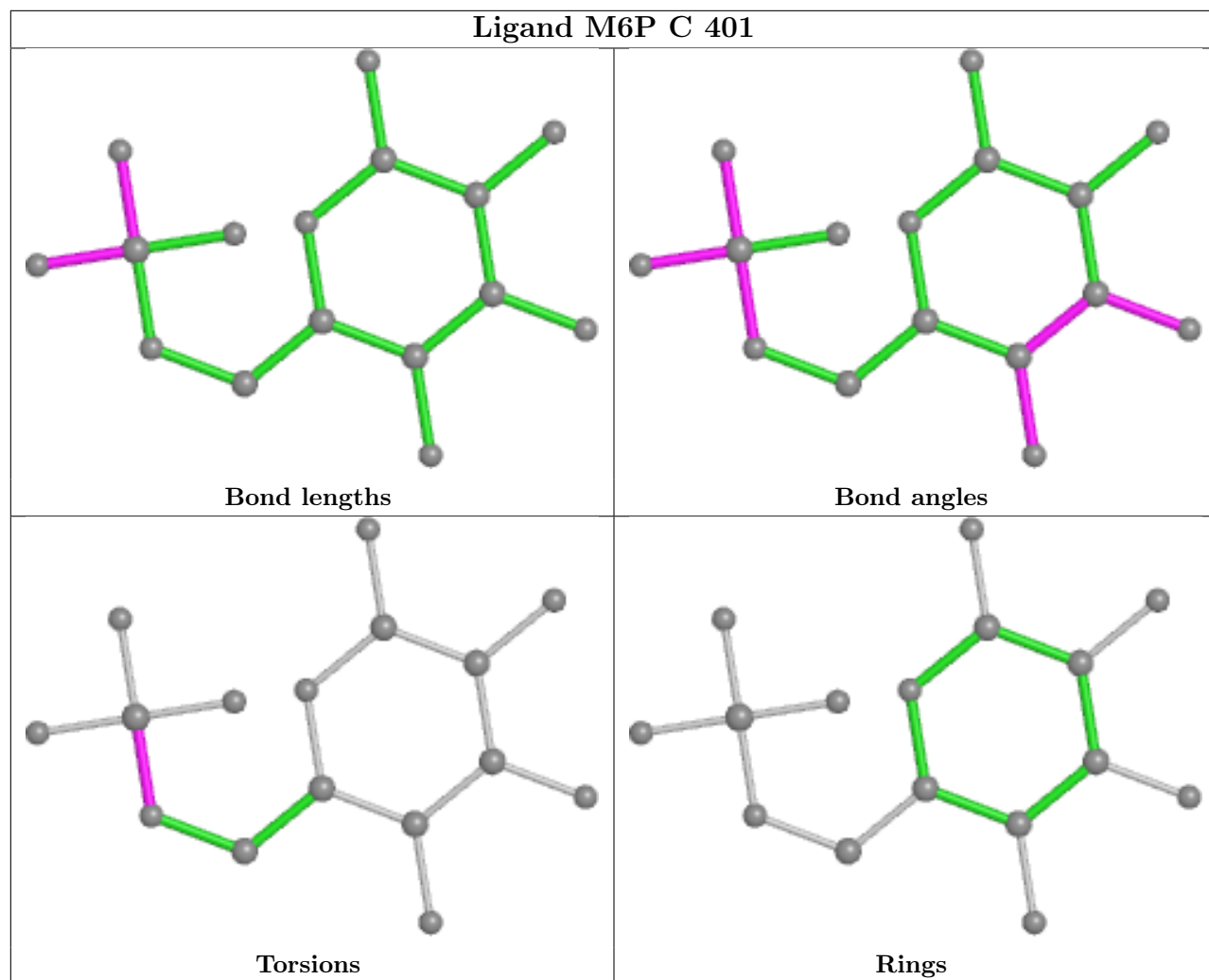
## Ligand M6P B 401



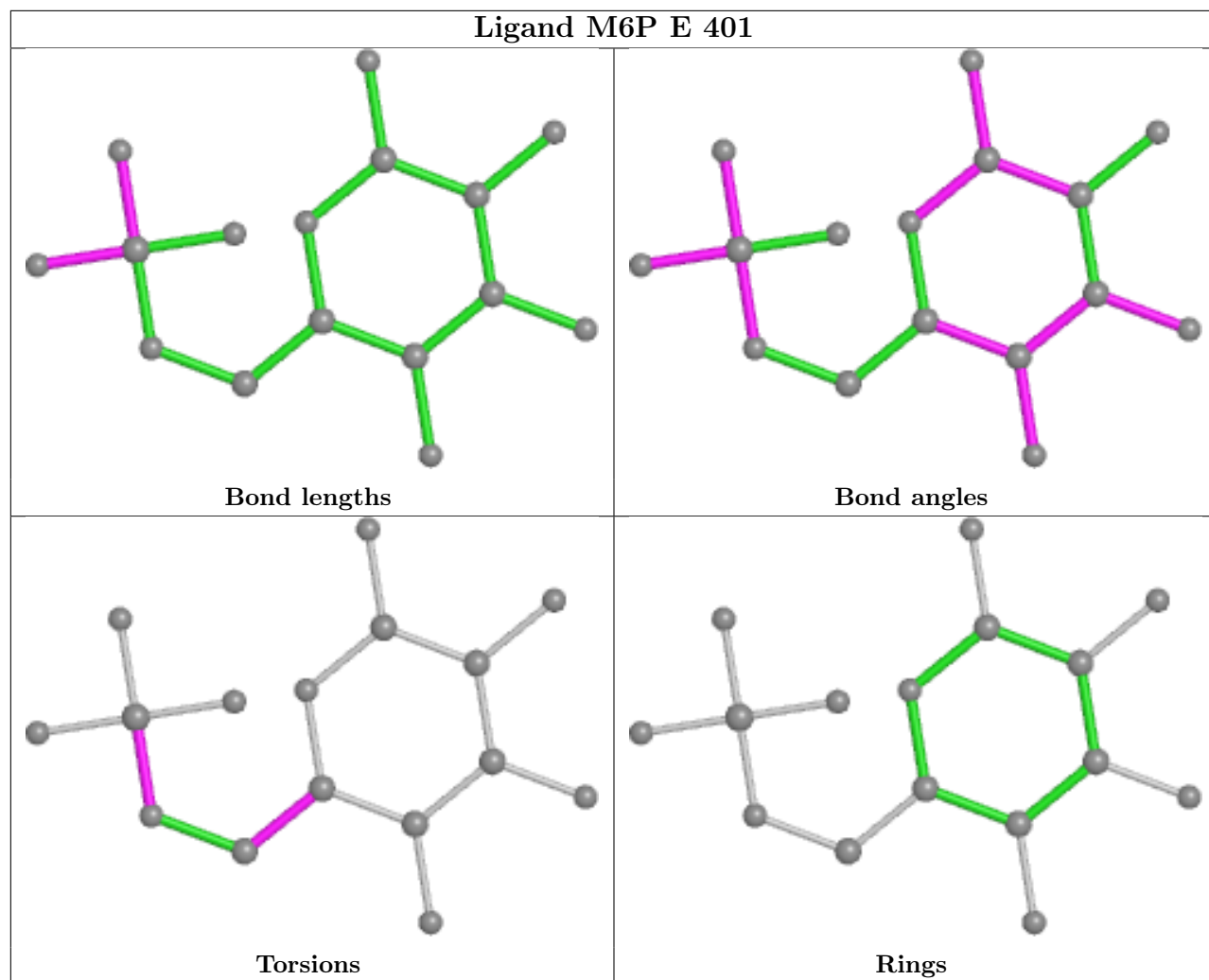


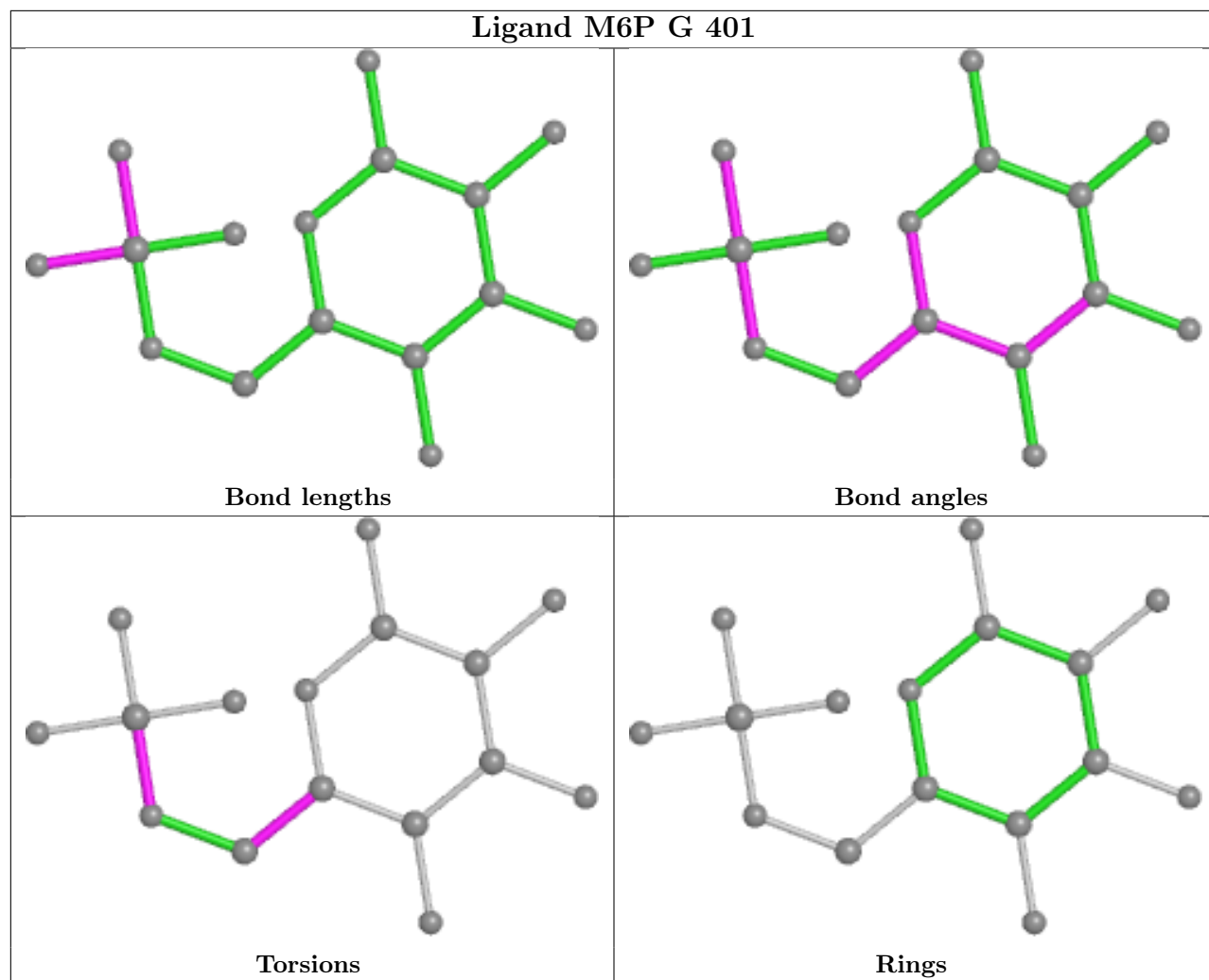


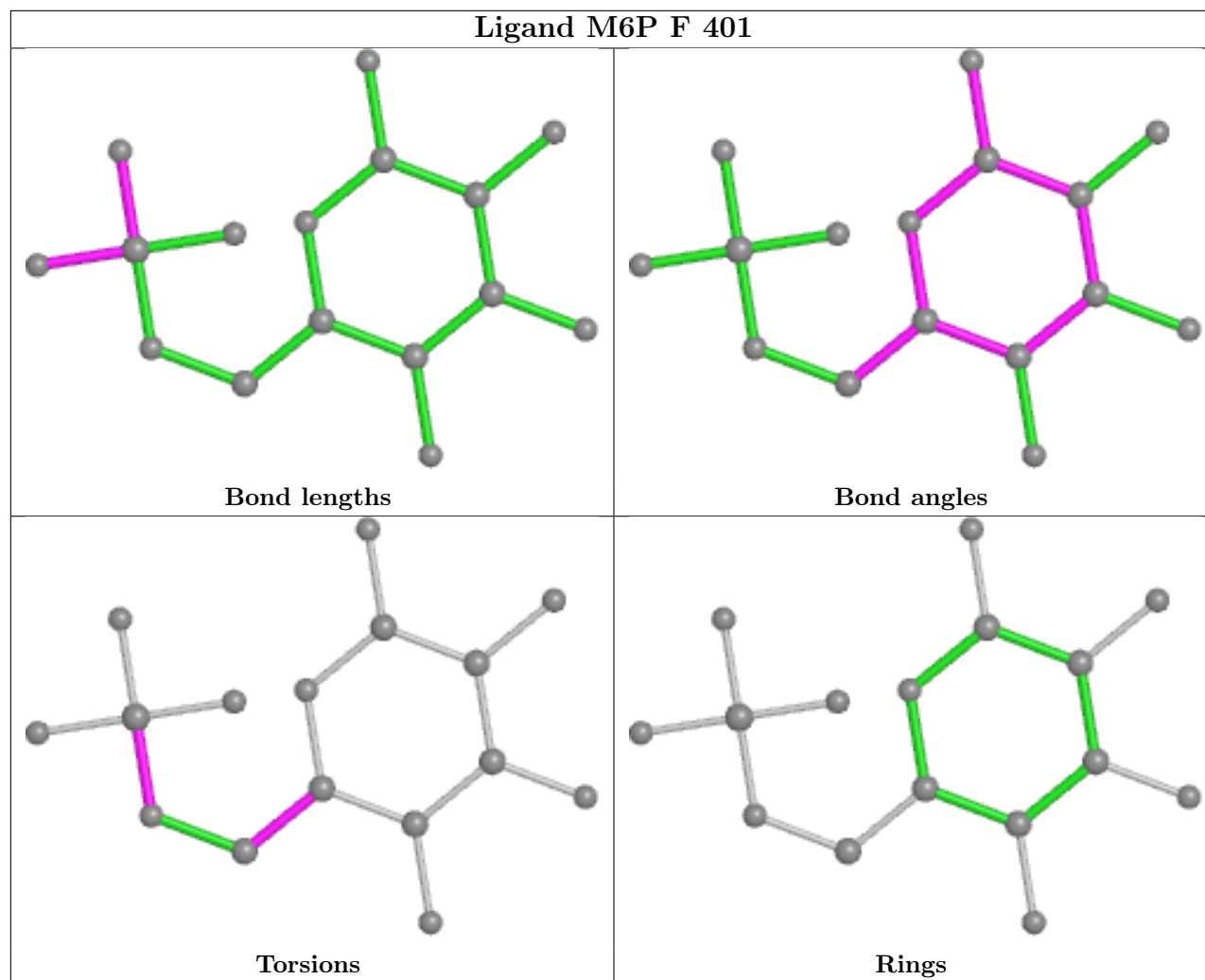




## Ligand M6P E 401







## 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	287/313 (91%)	-0.09	2 (0%) 87 89	32, 56, 117, 164	0
1	B	268/313 (85%)	-0.12	2 (0%) 87 89	31, 55, 132, 152	2 (0%)
1	C	294/313 (93%)	-0.00	4 (1%) 75 77	35, 67, 127, 149	0
1	D	284/313 (90%)	-0.06	1 (0%) 92 93	36, 64, 117, 153	3 (1%)
1	E	278/313 (88%)	-0.11	2 (0%) 87 89	39, 73, 126, 172	0
1	F	287/313 (91%)	-0.10	2 (0%) 87 89	37, 61, 114, 163	2 (0%)
1	G	290/313 (92%)	-0.13	0 100 100	37, 63, 109, 158	0
1	H	289/313 (92%)	-0.06	6 (2%) 63 65	31, 62, 119, 168	0
All	All	2277/2504 (90%)	-0.08	19 (0%) 86 87	31, 63, 121, 172	7 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	97	GLY	3.2
1	B	50	THR	3.1
1	E	47	ALA	2.8
1	H	304	TYR	2.8
1	E	31	LEU	2.5
1	H	34	LEU	2.4
1	A	89	CYS	2.3
1	F	266	LEU	2.3
1	H	303	LEU	2.3
1	C	80	SER	2.3
1	D	10	PHE	2.2
1	B	116	HIS	2.2
1	H	83	TYR	2.2
1	C	45	LEU	2.1
1	C	53	ILE	2.1
1	C	194	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	2.0
1	F	60	ASP	2.0
1	H	31	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

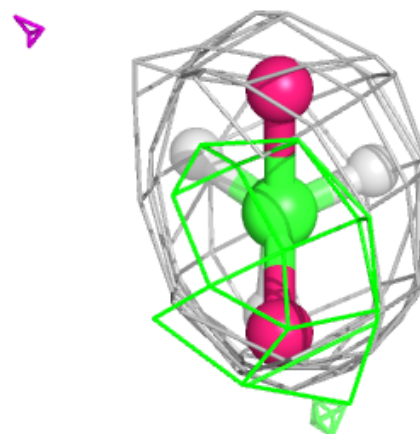
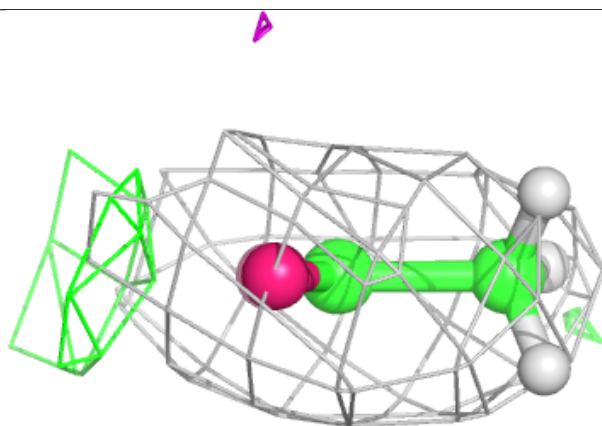
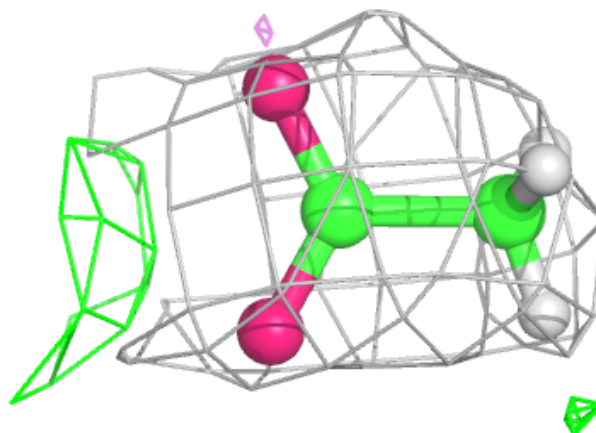
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	A	402	4/4	0.90	0.16	73,76,87,87	0
2	M6P	F	401	16/16	0.93	0.23	45,57,69,78	27
2	M6P	D	401	16/16	0.94	0.17	46,60,73,81	27
2	M6P	G	401	16/16	0.95	0.16	49,61,79,82	27
2	M6P	H	401	16/16	0.95	0.15	43,56,65,74	27
2	M6P	E	401	16/16	0.95	0.19	50,66,81,93	27
2	M6P	C	401	16/16	0.96	0.13	51,62,75,78	0
2	M6P	B	401	16/16	0.97	0.20	36,51,61,66	27
2	M6P	A	401	16/16	0.97	0.17	37,48,57,68	27

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 ACT A 402:**

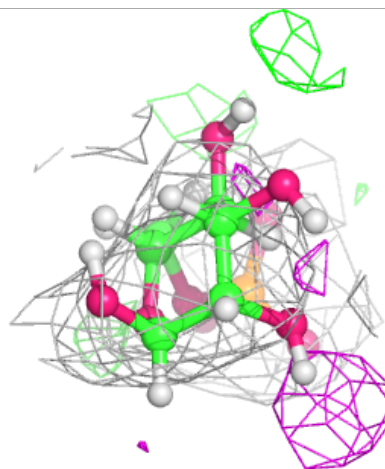
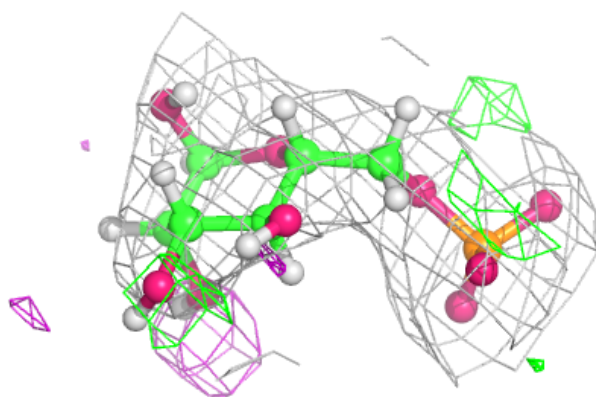
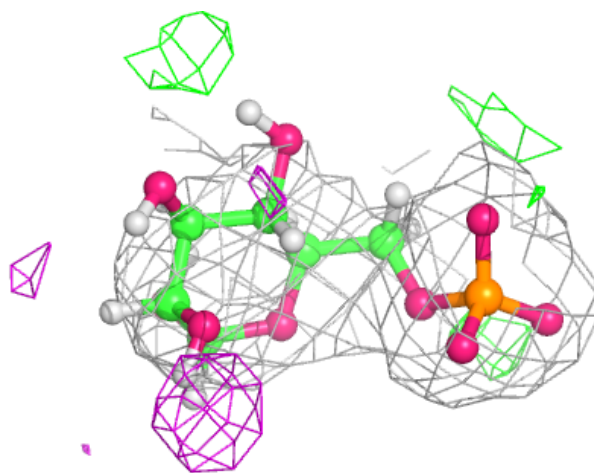
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





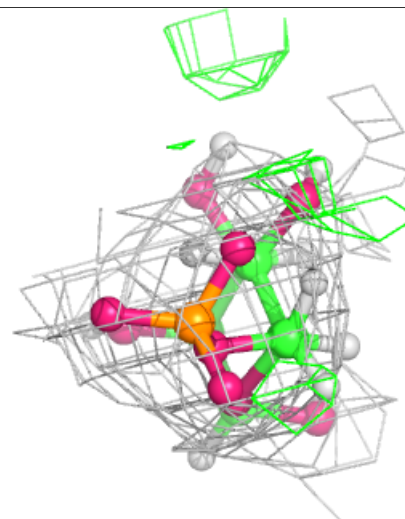
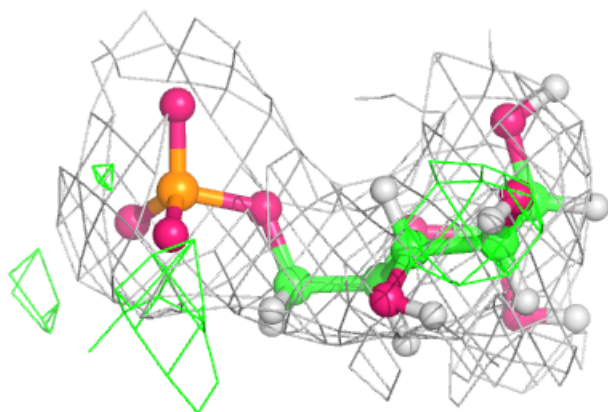
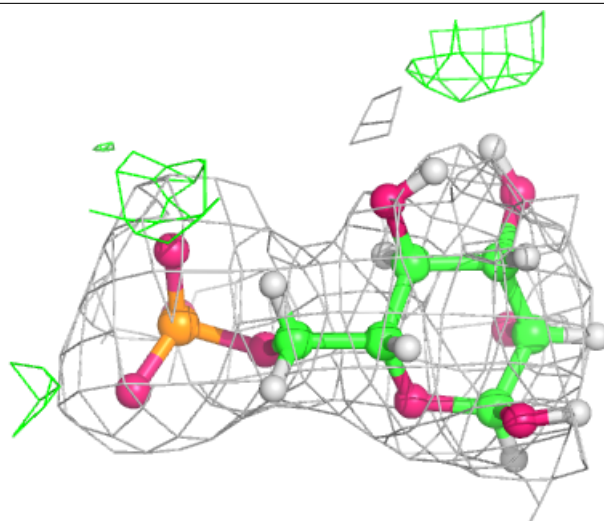
**Electron density around M6P F 401:**

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



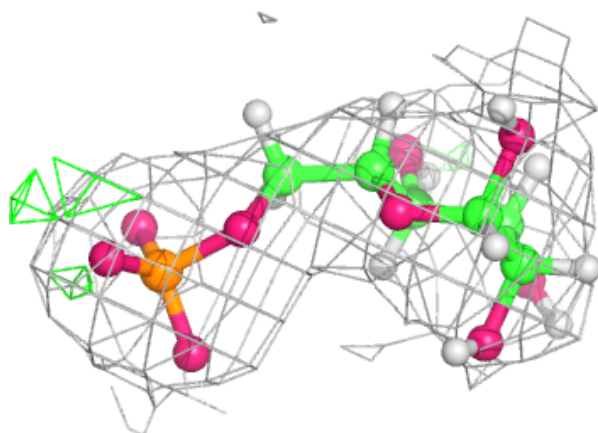
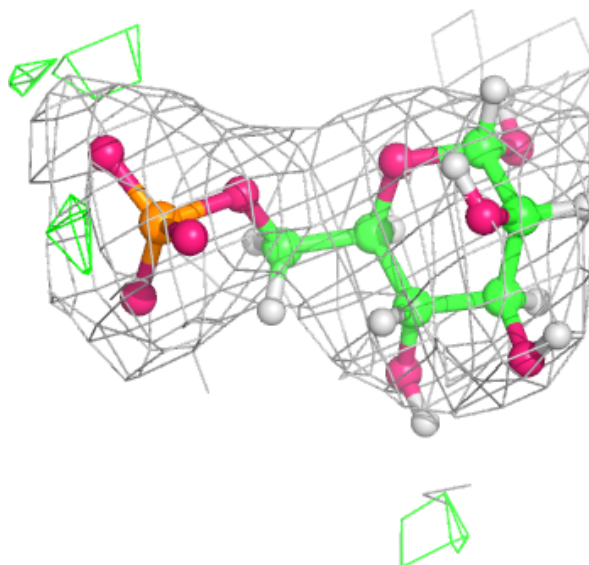
**Electron density around M6P D 401:**

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



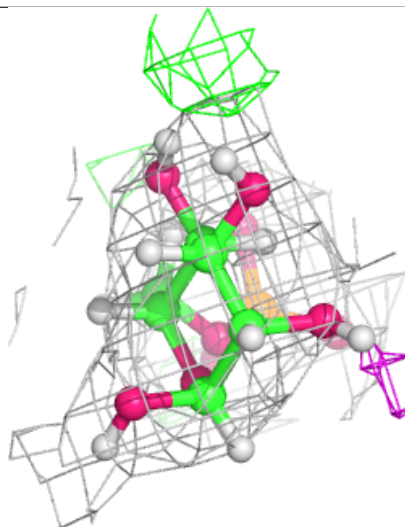
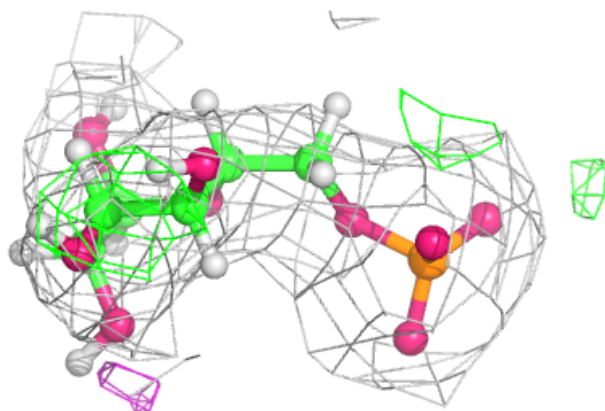
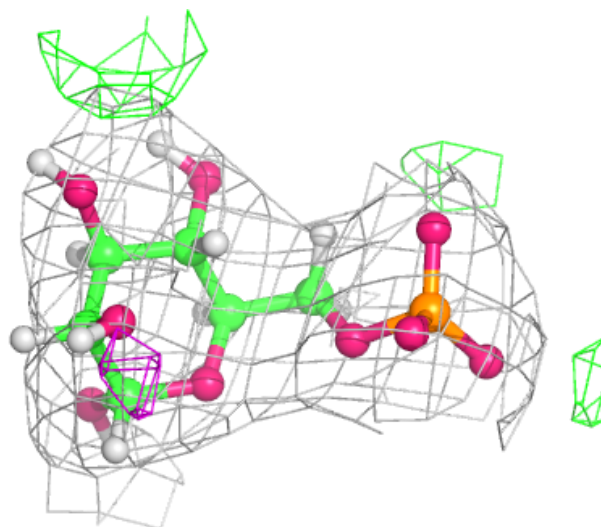
**Electron density around M6P G 401:**

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



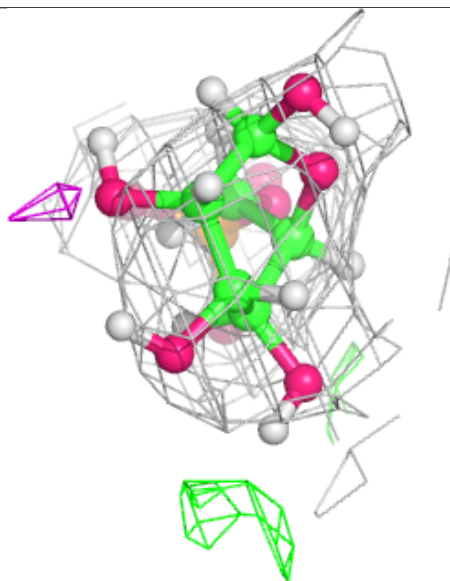
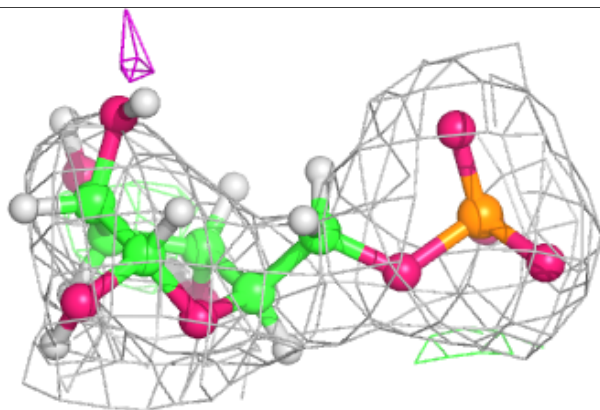
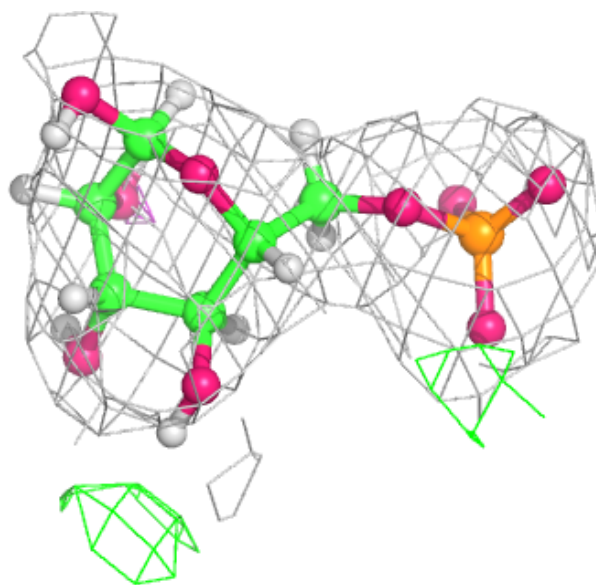
**Electron density around M6P H 401:**

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



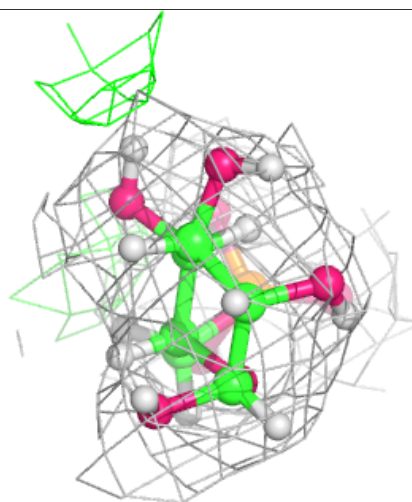
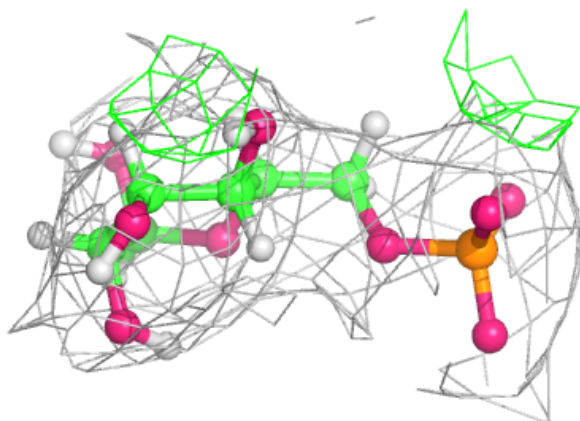
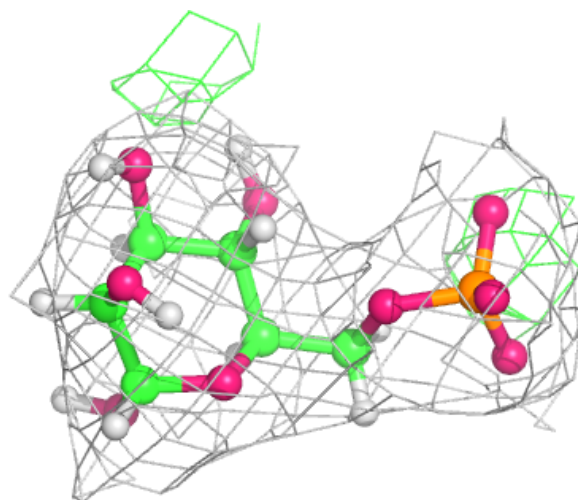
**Electron density around M6P E 401:**

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



**Electron density around M6P C 401:**

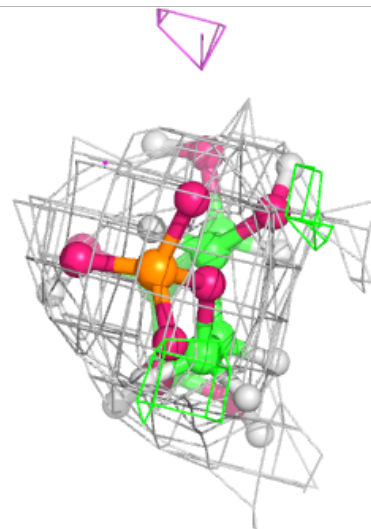
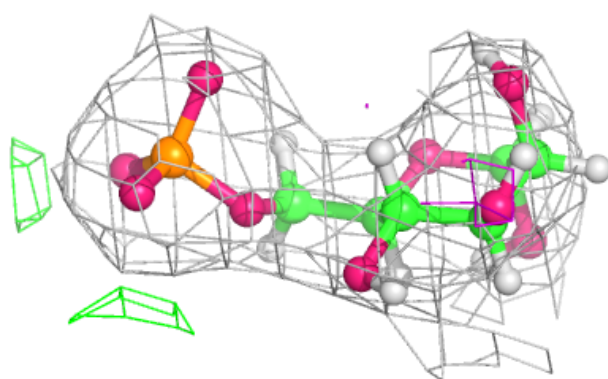
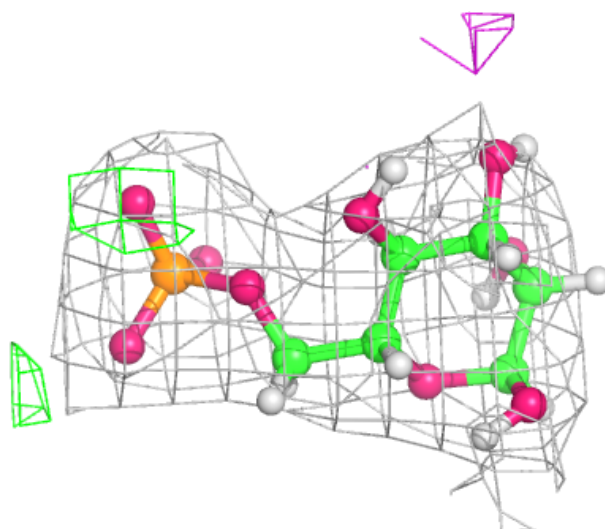
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





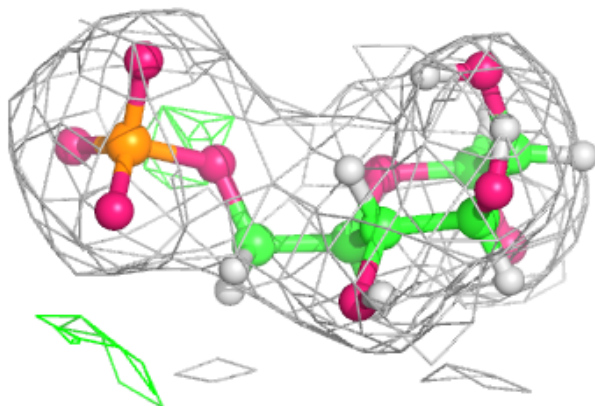
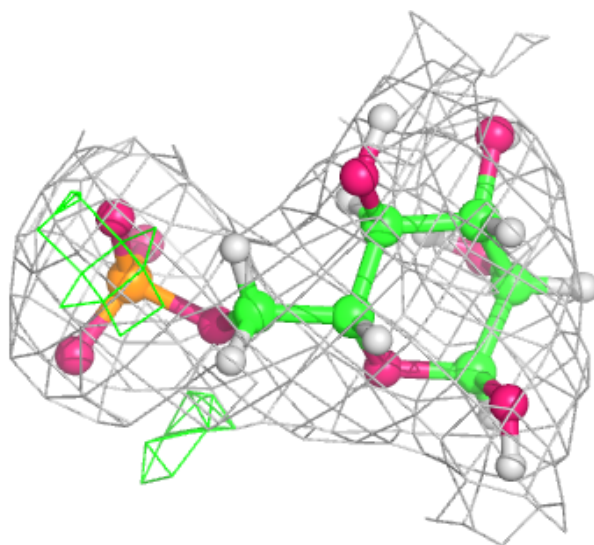
**Electron density around M6P B 401:**

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



**Electron density around M6P A 401:**

$2mF_o-DF_c$  (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.