



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 11:34 PM UTC

PDB ID : 6K8P / pdb_00006k8p
Title : Structural and catalytic analysis of two diverse uridine phosphorylases in the oomycete *Phytophthora capsici*.
Authors : Yang, C.C.; Zhang, X.G.
Deposited on : 2019-06-13
Resolution : 1.97 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

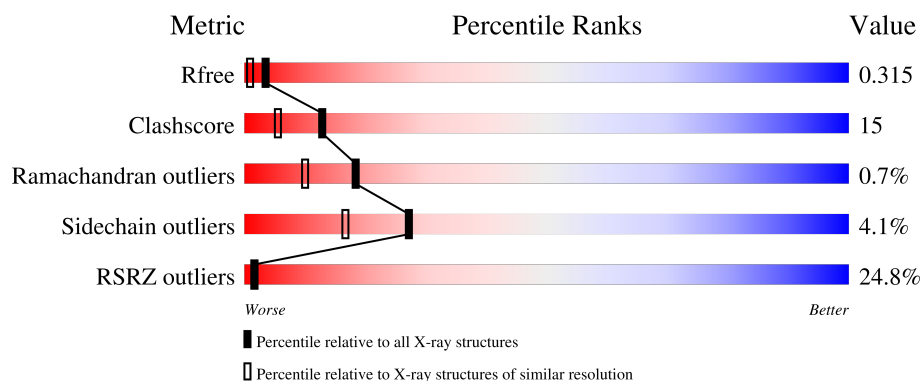
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
1	C	309	
1	D	309	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TDR	B	402	-	X	-	-
5	TDR	D	402	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17908 atoms, of which 8638 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	0	0	0
			4391	1372	2190	385	432	12			
1	B	280	Total	C	H	N	O	S	0	0	0
			4200	1311	2103	366	409	11			
1	C	294	Total	C	H	N	O	S	0	0	0
			4392	1372	2191	385	432	12			
1	D	280	Total	C	H	N	O	S	0	0	0
			4195	1311	2098	366	409	11			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A0A410UCT3
A	0	GLY	-	expression tag	UNP A0A410UCT3
A	297	ALA	-	expression tag	UNP A0A410UCT3
A	298	ALA	-	expression tag	UNP A0A410UCT3
A	299	ALA	-	expression tag	UNP A0A410UCT3
A	300	LEU	-	expression tag	UNP A0A410UCT3
A	301	GLU	-	expression tag	UNP A0A410UCT3
A	302	HIS	-	expression tag	UNP A0A410UCT3
A	303	HIS	-	expression tag	UNP A0A410UCT3
A	304	HIS	-	expression tag	UNP A0A410UCT3
A	305	HIS	-	expression tag	UNP A0A410UCT3
A	306	HIS	-	expression tag	UNP A0A410UCT3
A	307	HIS	-	expression tag	UNP A0A410UCT3
B	-1	MET	-	expression tag	UNP A0A410UCT3
B	0	GLY	-	expression tag	UNP A0A410UCT3
B	297	ALA	-	expression tag	UNP A0A410UCT3
B	298	ALA	-	expression tag	UNP A0A410UCT3
B	299	ALA	-	expression tag	UNP A0A410UCT3
B	300	LEU	-	expression tag	UNP A0A410UCT3
B	301	GLU	-	expression tag	UNP A0A410UCT3
B	302	HIS	-	expression tag	UNP A0A410UCT3

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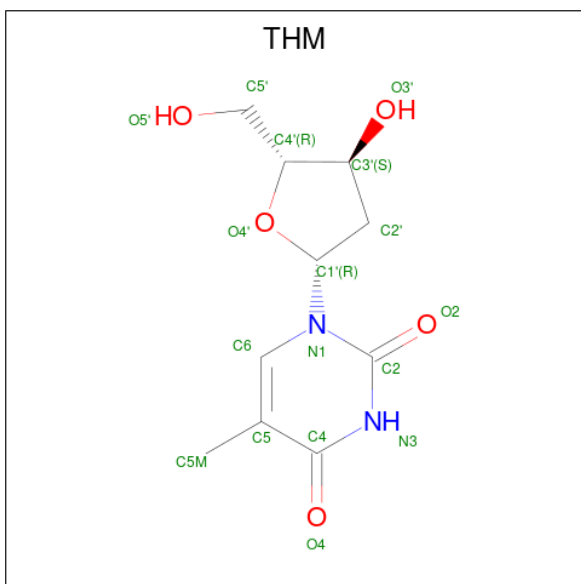
Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP A0A410UCT3
B	304	HIS	-	expression tag	UNP A0A410UCT3
B	305	HIS	-	expression tag	UNP A0A410UCT3
B	306	HIS	-	expression tag	UNP A0A410UCT3
B	307	HIS	-	expression tag	UNP A0A410UCT3
C	-1	MET	-	expression tag	UNP A0A410UCT3
C	0	GLY	-	expression tag	UNP A0A410UCT3
C	297	ALA	-	expression tag	UNP A0A410UCT3
C	298	ALA	-	expression tag	UNP A0A410UCT3
C	299	ALA	-	expression tag	UNP A0A410UCT3
C	300	LEU	-	expression tag	UNP A0A410UCT3
C	301	GLU	-	expression tag	UNP A0A410UCT3
C	302	HIS	-	expression tag	UNP A0A410UCT3
C	303	HIS	-	expression tag	UNP A0A410UCT3
C	304	HIS	-	expression tag	UNP A0A410UCT3
C	305	HIS	-	expression tag	UNP A0A410UCT3
C	306	HIS	-	expression tag	UNP A0A410UCT3
C	307	HIS	-	expression tag	UNP A0A410UCT3
D	-1	MET	-	expression tag	UNP A0A410UCT3
D	0	GLY	-	expression tag	UNP A0A410UCT3
D	297	ALA	-	expression tag	UNP A0A410UCT3
D	298	ALA	-	expression tag	UNP A0A410UCT3
D	299	ALA	-	expression tag	UNP A0A410UCT3
D	300	LEU	-	expression tag	UNP A0A410UCT3
D	301	GLU	-	expression tag	UNP A0A410UCT3
D	302	HIS	-	expression tag	UNP A0A410UCT3
D	303	HIS	-	expression tag	UNP A0A410UCT3
D	304	HIS	-	expression tag	UNP A0A410UCT3
D	305	HIS	-	expression tag	UNP A0A410UCT3
D	306	HIS	-	expression tag	UNP A0A410UCT3
D	307	HIS	-	expression tag	UNP A0A410UCT3

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is THYMIDINE (CCD ID: THM) (formula: $C_{10}H_{14}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



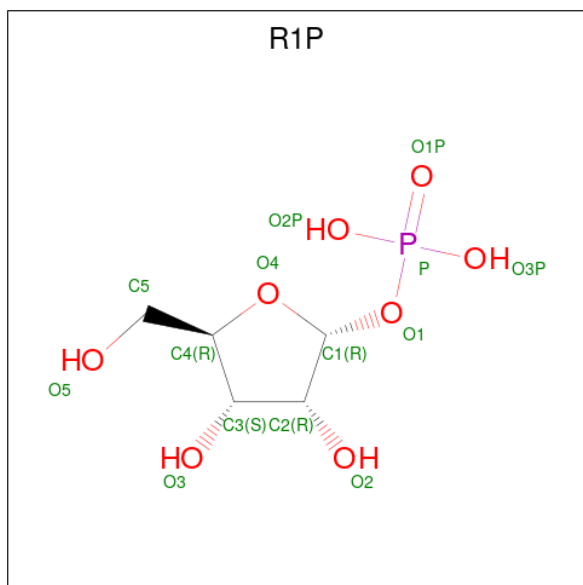
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			31	10	14	2	5		

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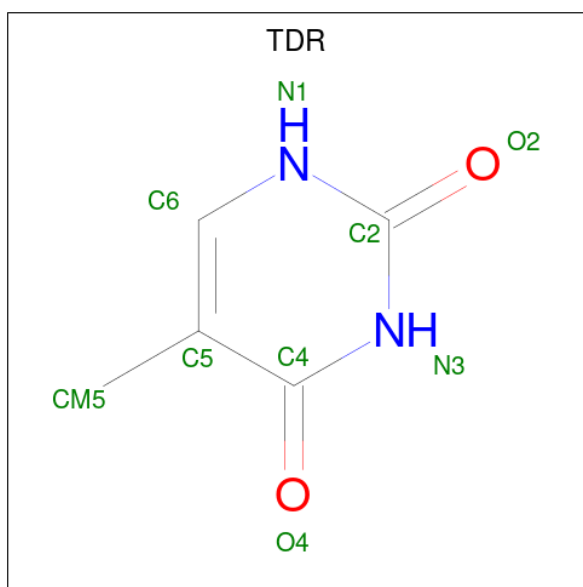
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			30	10	13	2	5		

- Molecule 4 is 1-O-phosphono-alpha-D-ribofuranose (CCD ID: R1P) (formula: $C_5H_{11}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	O	P	0	0
			23	5	9	8	1		
4	D	1	Total	C	H	O	P	0	0
			22	5	8	8	1		

- Molecule 5 is THYMINE (CCD ID: TDR) (formula: $C_5H_6N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	0	0
			15	5	6	2	2		
5	D	1	Total	C	H	N	O	0	0
			15	5	6	2	2		

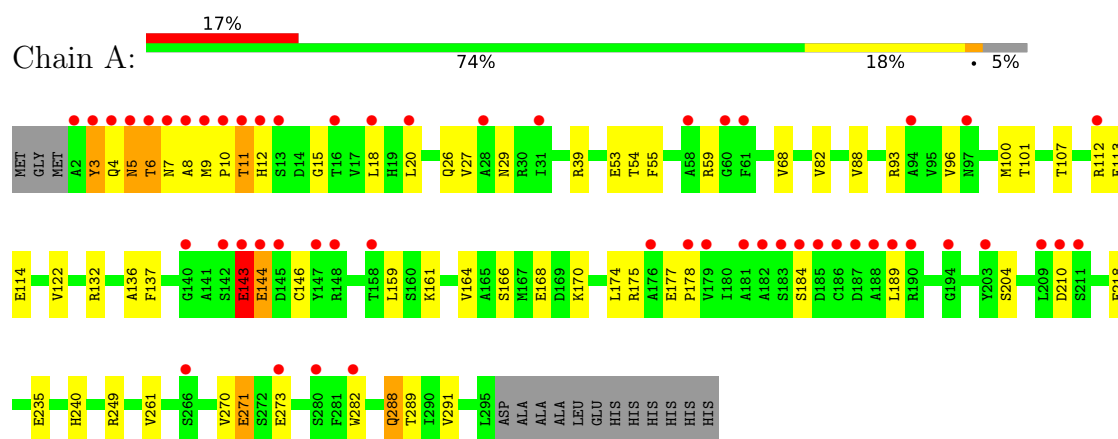
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		
6	B	136	Total	O	0	0
			136	136		
6	C	170	Total	O	0	0
			170	170		
6	D	122	Total	O	0	0
			122	122		

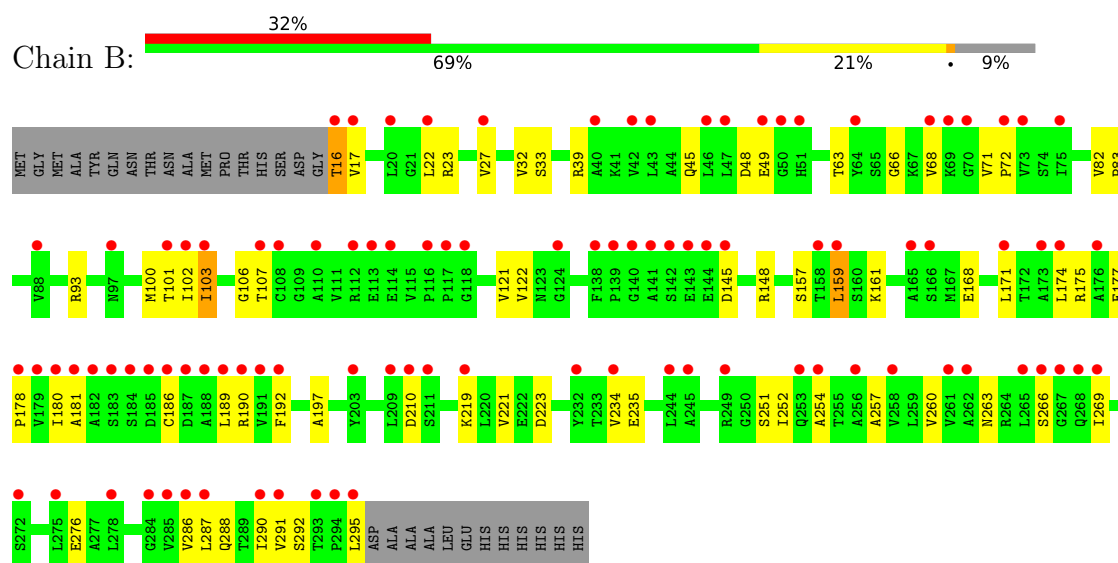
3 Residue-property plots [i](#)

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.

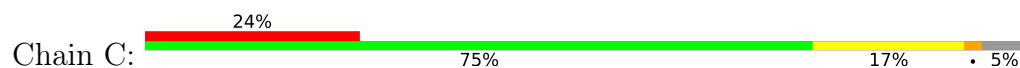
• Molecule 1: Uridine phosphorylase

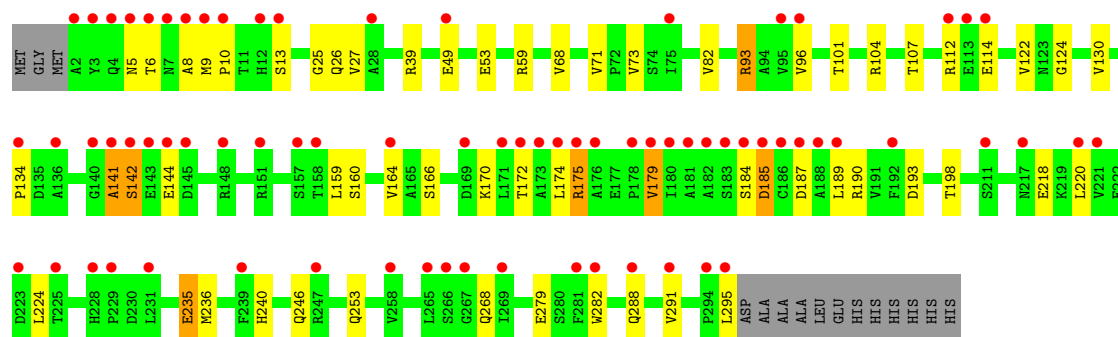


• Molecule 1: Uridine phosphorylase

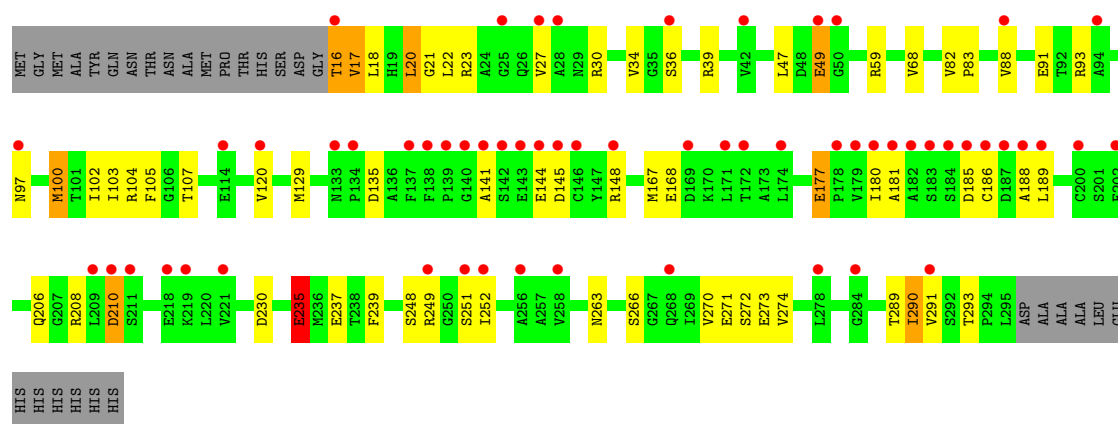


• Molecule 1: Uridine phosphorylase





● Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.96Å 97.33Å 188.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.46 – 1.97 38.46 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.46-1.97) 98.7 (38.46-1.97)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.265 , 0.316 0.265 , 0.315	Depositor DCC
R_{free} test set	4385 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17908	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4637e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, THM, R1P, TDR

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	0.64	1/2236 (0.0%)	0.79	0/3037
1	B	0.63	0/2129	0.79	0/2890
1	C	0.68	0/2236	0.83	0/3037
1	D	0.62	0/2129	0.83	3/2890 (0.1%)
All	All	0.64	1/8730 (0.0%)	0.81	3/11854 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	MET	CG-SD	-5.56	1.66	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	SER	N-CA-C	6.64	120.87	110.17
1	D	235	GLU	CG-CD-OE2	-5.30	106.20	118.40
1	D	235	GLU	N-CA-CB	-5.27	103.28	111.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Peptide
1	C	141	ALA	Peptide
1	D	181	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2201	2190	2190	72	1
1	B	2097	2103	2102	63	1
1	C	2201	2191	2190	60	0
1	D	2097	2098	2102	73	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
3	A	17	14	11	1	0
3	C	17	13	14	1	0
4	B	14	9	0	2	0
4	D	14	8	0	3	0
5	B	9	6	6	0	0
5	D	9	6	6	0	0
6	A	156	0	0	17	1
6	B	136	0	0	18	0
6	C	170	0	0	18	1
6	D	122	0	0	22	0
All	All	9270	8638	8621	262	2

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 15.

All (262) 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)
4:B:401:R1P:O4	4:B:401:R1P:C1	1.70	1.24
4:D:401:R1P:O4	4:D:401:R1P:C1	1.69	1.21
1:D:167:MET:SD	6:D:604:HOH:O	2.09	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:VAL:HG11	6:D:595:HOH:O	1.56	1.04
1:A:54:THR:HG21	6:A:510:HOH:O	1.60	1.01
1:D:22:LEU:N	6:D:501:HOH:O	1.93	0.99
1:B:16:THR:N	6:B:502:HOH:O	1.96	0.98
1:B:27:VAL:HG22	1:B:63:THR:HG21	1.49	0.95
1:D:22:LEU:HD13	1:D:27:VAL:HG21	1.46	0.94
1:B:22:LEU:HD13	1:B:27:VAL:HG21	1.51	0.93
1:B:45:GLN:OE1	6:B:501:HOH:O	1.86	0.90
1:A:101:THR:HG23	1:A:159:LEU:HD11	1.55	0.88
1:B:288:GLN:HG3	6:B:614:HOH:O	1.74	0.86
1:C:160:SER:O	1:C:164:VAL:HG23	1.73	0.86
1:B:260:VAL:HG23	6:B:510:HOH:O	1.74	0.85
1:A:5:ASN:OD1	1:A:8:ALA:HB3	1.80	0.81
1:B:189:LEU:HD12	1:B:189:LEU:O	1.81	0.81
1:C:179:VAL:O	6:C:503:HOH:O	1.98	0.81
1:D:82:VAL:HG11	6:D:617:HOH:O	1.82	0.80
1:A:39:ARG:HH22	1:A:107:THR:HG22	1.47	0.80
1:B:16:THR:HG21	6:B:596:HOH:O	1.82	0.79
1:B:295:LEU:O	6:B:503:HOH:O	1.99	0.79
1:A:8:ALA:HB2	1:D:249:ARG:NH2	1.97	0.79
1:A:5:ASN:HB2	1:D:97:ASN:OD1	1.83	0.78
1:A:3:TYR:HD2	1:A:18:LEU:HD13	1.48	0.78
1:A:39:ARG:NH2	1:A:107:THR:HG22	1.99	0.78
1:D:16:THR:N	6:D:506:HOH:O	2.17	0.76
1:D:22:LEU:HD13	1:D:27:VAL:CG2	2.16	0.75
1:C:82:VAL:N	6:C:501:HOH:O	1.94	0.75
1:B:22:LEU:HD13	1:B:27:VAL:CG2	2.18	0.74
1:D:20:LEU:HD11	1:D:88:VAL:HA	1.70	0.74
1:D:135:ASP:OD1	6:D:502:HOH:O	2.06	0.73
1:D:273:GLU:OE2	6:D:503:HOH:O	2.07	0.72
1:A:210:ASP:OD2	6:A:501:HOH:O	2.07	0.72
1:A:175:ARG:NH2	1:A:189:LEU:O	2.22	0.72
1:A:132:ARG:NE	6:A:507:HOH:O	2.23	0.71
1:D:185:ASP:O	1:D:188:ALA:N	2.24	0.71
1:C:39:ARG:HH22	1:C:107:THR:HG22	1.56	0.70
1:A:107:THR:HG23	2:A:401:PO4:O1	1.92	0.70
1:D:206:GLN:O	6:D:504:HOH:O	2.09	0.70
1:C:93:ARG:O	1:C:93:ARG:HD3	1.92	0.70
1:B:168:GLU:O	6:B:504:HOH:O	2.09	0.69
1:A:53:GLU:OE1	6:A:503:HOH:O	2.09	0.69
1:C:26:GLN:N	6:C:508:HOH:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLN:NE2	6:C:507:HOH:O	2.11	0.69
1:C:295:LEU:O	6:C:506:HOH:O	2.10	0.69
1:C:71:VAL:HB	1:C:291:VAL:HG13	1.74	0.69
1:A:107:THR:CB	6:A:505:HOH:O	2.41	0.68
1:B:22:LEU:CD1	1:B:27:VAL:HG21	2.23	0.68
1:B:68:VAL:HB	1:B:291:VAL:HG21	1.74	0.68
1:C:246:GLN:HB3	6:C:518:HOH:O	1.93	0.68
1:D:68:VAL:HB	1:D:291:VAL:HG21	1.75	0.68
1:C:174:LEU:HD22	1:C:282:TRP:CH2	2.29	0.67
1:C:39:ARG:NH2	1:C:107:THR:HG22	2.10	0.67
1:D:168:GLU:O	6:D:505:HOH:O	2.13	0.67
1:D:16:THR:HG22	1:D:23:ARG:CG	2.24	0.67
1:B:33:SER:O	6:B:505:HOH:O	2.12	0.66
1:D:120:VAL:HG11	1:D:167:MET:HE3	1.78	0.66
1:D:82:VAL:CG1	6:D:617:HOH:O	2.43	0.65
1:A:5:ASN:O	1:A:7:ASN:N	2.30	0.64
1:B:93:ARG:O	1:B:93:ARG:HD3	1.98	0.64
1:C:27:VAL:HG13	1:C:96:VAL:CG2	2.28	0.63
1:A:112:ARG:NH2	6:A:504:HOH:O	2.16	0.63
1:B:175:ARG:NH1	6:B:509:HOH:O	2.32	0.63
1:B:122:VAL:HG22	1:B:257:ALA:HB2	1.81	0.63
1:C:141:ALA:O	1:C:142:SER:HB2	2.00	0.61
1:D:93:ARG:O	1:D:93:ARG:HD3	2.00	0.61
1:B:39:ARG:HH22	1:B:106:GLY:HA2	1.65	0.61
1:C:82:VAL:HG13	1:C:240:HIS:CG	2.36	0.60
1:B:16:THR:HG22	1:B:23:ARG:CG	2.31	0.60
1:D:100:MET:HG3	1:D:252:ILE:CD1	2.31	0.60
1:C:220:LEU:N	6:C:505:HOH:O	2.34	0.60
1:C:253:GLN:NE2	6:C:509:HOH:O	2.16	0.60
1:C:9:MET:N	6:C:504:HOH:O	2.04	0.59
1:C:190:ARG:NE	6:C:512:HOH:O	2.23	0.59
1:A:122:VAL:HG11	1:A:164:VAL:HG23	1.84	0.59
1:D:100:MET:HG3	1:D:252:ILE:HD12	1.84	0.59
1:A:8:ALA:HB2	1:D:249:ARG:HH21	1.66	0.59
1:C:122:VAL:HG11	1:C:164:VAL:HG22	1.84	0.59
1:D:208:ARG:N	6:D:504:HOH:O	2.34	0.59
1:D:271:GLU:HB2	1:D:274:VAL:HG12	1.85	0.59
1:B:121:VAL:HG23	6:B:510:HOH:O	2.02	0.58
1:B:103:ILE:HG12	1:B:286:VAL:HG13	1.86	0.58
1:A:113:GLU:HG3	1:A:114:GLU:N	2.17	0.58
1:C:166:SER:O	1:C:170:LYS:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:THR:HA	1:C:175:ARG:HG3	1.86	0.58
1:B:16:THR:HG22	1:B:23:ARG:HG3	1.86	0.58
1:D:208:ARG:HG3	6:D:504:HOH:O	2.04	0.58
1:A:210:ASP:CB	6:A:501:HOH:O	2.52	0.57
1:C:49:GLU:HA	1:C:49:GLU:OE1	2.04	0.57
1:C:71:VAL:CB	1:C:291:VAL:HG13	2.35	0.57
1:A:3:TYR:CD2	1:A:18:LEU:HD13	2.35	0.57
1:C:53:GLU:OE1	6:C:510:HOH:O	2.18	0.57
1:A:107:THR:OG1	6:A:505:HOH:O	2.17	0.57
1:D:180:ILE:HG22	1:D:180:ILE:O	2.05	0.57
1:B:39:ARG:NH2	1:B:106:GLY:HA2	2.20	0.57
1:B:16:THR:CA	6:B:502:HOH:O	2.48	0.57
1:C:122:VAL:CB	1:C:164:VAL:HG22	2.33	0.57
1:A:3:TYR:HB2	1:A:18:LEU:HD22	1.85	0.57
1:A:174:LEU:HD22	1:A:282:TRP:CH2	2.40	0.57
1:B:171:LEU:HD21	1:B:175:ARG:NH2	2.19	0.57
1:C:93:ARG:HD3	1:C:93:ARG:C	2.29	0.57
1:C:246:GLN:NE2	6:C:518:HOH:O	2.37	0.56
1:A:5:ASN:N	1:D:97:ASN:OD1	2.39	0.56
1:A:132:ARG:HD2	6:A:507:HOH:O	2.06	0.56
1:C:134:PRO:HA	6:D:511:HOH:O	2.04	0.56
1:D:16:THR:HG22	1:D:23:ARG:HG3	1.87	0.56
1:D:93:ARG:NH2	1:D:251:SER:HB2	2.20	0.56
1:A:136:ALA:HB2	1:A:144:GLU:HG2	1.88	0.56
1:D:206:GLN:C	6:D:504:HOH:O	2.47	0.56
1:D:39:ARG:NH1	1:D:105:PHE:O	2.40	0.55
1:A:9:MET:HG2	6:B:592:HOH:O	2.07	0.55
1:B:103:ILE:O	1:B:103:ILE:HG13	2.06	0.55
1:D:47:LEU:O	1:D:49:GLU:O	2.25	0.54
1:D:249:ARG:O	1:D:249:ARG:CD	2.55	0.54
1:D:177:GLU:HB3	6:D:536:HOH:O	2.06	0.54
1:D:248:SER:O	1:D:249:ARG:HG3	2.08	0.54
1:C:112:ARG:NH2	1:C:114:GLU:OE2	2.39	0.54
1:D:21:GLY:C	6:D:501:HOH:O	2.39	0.53
1:A:20:LEU:HD21	1:A:88:VAL:HA	1.89	0.53
1:B:292:SER:OG	6:B:506:HOH:O	2.18	0.53
1:A:26:GLN:HB3	1:A:55:PHE:CZ	2.44	0.53
1:A:184:SER:O	6:A:506:HOH:O	2.18	0.53
3:C:402:THM:H5'1	6:C:526:HOH:O	2.09	0.53
1:A:132:ARG:CD	6:A:507:HOH:O	2.56	0.53
1:B:107:THR:OG1	4:B:401:R1P:C1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:NH2	1:C:107:THR:CG2	2.73	0.52
1:A:5:ASN:HB3	1:A:10:PRO:HA	1.90	0.52
1:C:112:ARG:HH11	1:C:112:ARG:HG2	1.75	0.52
1:B:93:ARG:HH21	1:B:252:ILE:HD13	1.75	0.52
1:D:100:MET:HE2	1:D:102:ILE:HD11	1.91	0.51
1:B:82:VAL:HB	1:B:83:PRO:HD3	1.91	0.51
1:B:221:VAL:HG23	6:B:576:HOH:O	2.10	0.51
1:D:237:GLU:OE1	4:D:401:R1P:O2	2.26	0.51
1:B:157:SER:O	1:B:161:LYS:HG2	2.11	0.50
1:C:122:VAL:CG1	1:C:164:VAL:HG22	2.41	0.50
1:D:17:VAL:HG13	1:D:91:GLU:OE1	2.12	0.50
1:D:104:ARG:HH21	1:D:235:GLU:CG	2.24	0.50
1:A:4:GLN:O	1:A:6:THR:N	2.44	0.50
1:B:177:GLU:HB2	1:B:180:ILE:HD12	1.93	0.50
1:D:210:ASP:OD1	1:D:210:ASP:N	2.42	0.50
1:B:22:LEU:HD22	1:B:27:VAL:HG23	1.93	0.49
1:C:68:VAL:HB	1:C:291:VAL:HG21	1.93	0.49
1:A:3:TYR:HD2	1:A:18:LEU:CD1	2.24	0.49
1:A:107:THR:HB	6:A:505:HOH:O	2.06	0.49
1:C:122:VAL:HG11	1:C:164:VAL:CG2	2.42	0.49
1:A:271:GLU:HG2	1:A:273:GLU:OE1	2.13	0.49
1:B:39:ARG:HH22	1:B:106:GLY:CA	2.25	0.49
6:C:501:HOH:O	1:D:83:PRO:HG2	2.13	0.49
1:D:230:ASP:OD2	6:D:507:HOH:O	2.20	0.49
1:A:93:ARG:NH2	1:A:96:VAL:O	2.43	0.48
1:D:289:THR:O	1:D:293:THR:HG23	2.12	0.48
1:B:174:LEU:CD1	1:B:180:ILE:HD13	2.43	0.48
1:C:8:ALA:O	1:C:10:PRO:HD3	2.14	0.48
1:C:170:LYS:HD3	1:C:170:LYS:N	2.29	0.48
1:C:218:GLU:CD	1:C:218:GLU:H	2.22	0.48
1:B:171:LEU:O	1:B:175:ARG:HG3	2.13	0.48
1:A:170:LYS:N	1:A:170:LYS:HD3	2.29	0.48
1:D:185:ASP:O	1:D:189:LEU:N	2.47	0.48
1:A:4:GLN:HB3	1:D:97:ASN:OD1	2.12	0.48
1:A:3:TYR:CD1	1:A:3:TYR:C	2.92	0.48
1:A:261:VAL:HG21	6:A:505:HOH:O	2.14	0.48
1:B:103:ILE:HG23	1:B:290:ILE:HD12	1.96	0.48
1:C:130:VAL:HG21	1:C:224:LEU:HD11	1.95	0.48
1:A:5:ASN:CB	1:D:97:ASN:OD1	2.59	0.47
1:A:107:THR:HG21	6:A:623:HOH:O	2.14	0.47
1:B:100:MET:HG3	1:B:252:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:O	1:A:144:GLU:HB2	2.14	0.47
1:A:122:VAL:HB	1:A:164:VAL:HG22	1.95	0.47
1:B:197:ALA:O	1:B:234:VAL:HA	2.15	0.47
1:C:82:VAL:HG13	1:C:240:HIS:HB2	1.97	0.47
1:D:103:ILE:HG13	1:D:290:ILE:HD12	1.97	0.47
1:B:32:VAL:HG12	6:B:505:HOH:O	2.15	0.47
1:A:5:ASN:HB2	1:D:97:ASN:CG	2.39	0.47
1:B:48:ASP:C	1:B:49:GLU:O	2.55	0.47
1:B:93:ARG:HE	1:B:252:ILE:HD11	1.79	0.46
1:D:82:VAL:HG21	1:D:129:MET:HE1	1.98	0.46
1:A:11:THR:CG2	1:A:15:GLY:HA2	2.46	0.46
1:B:32:VAL:CG1	6:B:505:HOH:O	2.62	0.46
1:C:122:VAL:O	1:C:193:ASP:HA	2.16	0.46
1:A:27:VAL:HG13	1:A:96:VAL:CG2	2.46	0.46
1:C:101:THR:HG23	1:C:159:LEU:HD21	1.97	0.46
1:D:230:ASP:HB2	6:D:507:HOH:O	2.16	0.46
1:C:175:ARG:NH2	1:C:189:LEU:O	2.49	0.46
1:B:39:ARG:HH22	1:B:106:GLY:C	2.24	0.46
1:B:93:ARG:HD3	1:B:93:ARG:C	2.40	0.46
1:C:122:VAL:HB	1:C:164:VAL:HG22	1.98	0.46
1:C:142:SER:HA	1:C:144:GLU:HB2	1.98	0.45
1:D:107:THR:OG1	4:D:401:R1P:C1	2.63	0.45
1:A:271:GLU:HG3	6:A:610:HOH:O	2.15	0.45
1:D:249:ARG:O	1:D:249:ARG:HD3	2.14	0.45
1:B:145:ASP:HB2	1:B:148:ARG:HE	1.82	0.45
1:B:178:PRO:O	1:B:181:ALA:HB3	2.16	0.45
1:C:82:VAL:HG13	1:C:240:HIS:CB	2.46	0.45
1:A:8:ALA:O	1:A:10:PRO:HD3	2.16	0.45
1:D:93:ARG:O	1:D:93:ARG:CD	2.65	0.45
1:B:102:ILE:O	1:B:254:ALA:HA	2.16	0.45
1:B:190:ARG:HB2	1:B:192:PHE:CE1	2.51	0.45
1:D:16:THR:CA	6:D:506:HOH:O	2.61	0.45
1:D:263:ASN:HB3	1:D:266:SER:OG	2.17	0.45
1:B:287:LEU:O	1:B:291:VAL:HG23	2.16	0.45
1:B:93:ARG:NH2	1:B:251:SER:HB2	2.32	0.45
1:B:101:THR:HG23	1:B:159:LEU:HD11	1.99	0.45
1:C:104:ARG:CG	1:C:104:ARG:HH11	2.30	0.45
1:D:34:VAL:HB	1:D:39:ARG:HD2	1.99	0.45
1:D:120:VAL:CG1	1:D:167:MET:CE	2.95	0.45
1:A:4:GLN:HB2	1:A:11:THR:O	2.17	0.45
1:A:11:THR:CG2	1:A:12:HIS:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ARG:HD2	6:D:575:HOH:O	2.17	0.44
1:A:137:PHE:CZ	1:A:146:CYS:HB3	2.53	0.44
1:C:27:VAL:HG13	1:C:96:VAL:HG22	1.99	0.44
1:C:198:THR:HG23	1:C:236:MET:HA	2.00	0.44
1:B:263:ASN:HB3	1:B:266:SER:HB2	2.00	0.44
1:D:93:ARG:HD3	1:D:93:ARG:C	2.42	0.44
1:D:30:ARG:HB3	1:D:290:ILE:HG12	1.99	0.44
1:D:103:ILE:CD1	1:D:290:ILE:HD12	2.48	0.44
1:A:288:GLN:HG2	1:A:289:THR:N	2.33	0.44
1:D:39:ARG:NH2	1:D:107:THR:CG2	2.81	0.44
1:A:8:ALA:HB2	1:D:249:ARG:HH22	1.79	0.44
1:A:204:SER:HB2	6:A:507:HOH:O	2.17	0.44
1:A:82:VAL:HG13	1:A:240:HIS:CG	2.53	0.44
1:B:71:VAL:HB	1:B:291:VAL:HG13	2.00	0.44
1:D:270:VAL:HG22	1:D:274:VAL:HG13	1.99	0.43
1:A:11:THR:HG22	1:A:12:HIS:O	2.18	0.43
1:A:166:SER:O	1:A:170:LYS:HD3	2.18	0.43
1:C:25:GLY:N	6:C:508:HOH:O	2.51	0.43
1:C:190:ARG:HB2	6:C:533:HOH:O	2.18	0.43
1:D:180:ILE:O	1:D:180:ILE:CG2	2.66	0.43
1:A:107:THR:OG1	3:A:402:THM:O4'	2.36	0.43
1:D:59:ARG:NH2	6:D:514:HOH:O	2.50	0.43
1:D:120:VAL:CG1	1:D:167:MET:HE3	2.46	0.43
1:A:39:ARG:NH2	1:A:107:THR:CG2	2.78	0.43
1:B:27:VAL:CG2	1:B:63:THR:HG21	2.32	0.43
1:B:33:SER:C	6:B:505:HOH:O	2.60	0.43
1:D:21:GLY:CA	6:D:501:HOH:O	2.65	0.43
1:B:100:MET:CG	1:B:252:ILE:HD12	2.48	0.43
1:B:66:GLY:O	1:B:72:PRO:HA	2.19	0.43
1:B:252:ILE:O	6:B:507:HOH:O	2.21	0.43
1:D:93:ARG:HD3	1:D:93:ARG:HA	1.95	0.43
1:A:68:VAL:HB	1:A:291:VAL:HG21	2.00	0.42
1:A:218:GLU:CD	1:A:218:GLU:H	2.26	0.42
1:D:145:ASP:HB2	1:D:148:ARG:HH11	1.84	0.42
1:A:3:TYR:HE1	1:B:269:ILE:HG22	1.85	0.42
1:A:177:GLU:O	1:A:178:PRO:C	2.63	0.42
1:A:112:ARG:HD3	1:A:114:GLU:OE2	2.19	0.42
1:C:235:GLU:HB2	6:C:570:HOH:O	2.19	0.42
1:A:3:TYR:C	1:A:4:GLN:HG2	2.44	0.42
1:C:104:ARG:HH11	1:C:104:ARG:HG3	1.84	0.42
1:C:185:ASP:C	1:C:187:ASP:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:PHE:CD1	1:D:239:PHE:C	2.97	0.42
1:C:112:ARG:NH1	1:C:114:GLU:OE2	2.51	0.42
1:B:219:LYS:HG2	1:B:223:ASP:CG	2.45	0.41
1:C:122:VAL:HG21	1:C:164:VAL:HG22	2.03	0.41
1:B:93:ARG:NH2	1:B:251:SER:O	2.53	0.41
1:C:124:GLY:O	6:C:511:HOH:O	2.21	0.41
1:C:141:ALA:O	1:C:142:SER:CB	2.65	0.41
1:C:185:ASP:C	1:C:187:ASP:H	2.29	0.41
1:A:3:TYR:CD2	1:A:18:LEU:CD1	3.01	0.40
1:A:29:ASN:HB3	6:A:512:HOH:O	2.20	0.40
1:A:249:ARG:HH11	1:A:249:ARG:HG2	1.86	0.40
1:C:49:GLU:OE1	1:C:49:GLU:CA	2.69	0.40
1:A:270:VAL:HG22	1:A:271:GLU:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:647:HOH:O	6:C:659:HOH:O[1_545]	2.12	0.08
1:A:161:LYS:HZ1	1:B:181:ALA:O[1_455]	1.59	0.01

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	292/309 (94%)	278 (95%)	10 (3%)	4 (1%)	9	3
1	B	278/309 (90%)	268 (96%)	10 (4%)	0	100	100
1	C	292/309 (94%)	272 (93%)	17 (6%)	3 (1%)	12	5
1	D	278/309 (90%)	270 (97%)	7 (2%)	1 (0%)	30	21
All	All	1140/1236 (92%)	1088 (95%)	44 (4%)	8 (1%)	18	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	THR
1	A	144	GLU
1	C	142	SER
1	C	6	THR
1	D	141	ALA
1	A	143	GLU
1	C	184	SER

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	242/253 (96%)	235 (97%)	7 (3%)	37	29
1	B	231/253 (91%)	223 (96%)	8 (4%)	32	22
1	C	242/253 (96%)	231 (96%)	11 (4%)	24	14
1	D	231/253 (91%)	218 (94%)	13 (6%)	19	8
All	All	946/1012 (94%)	907 (96%)	39 (4%)	27	17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	11	THR
1	A	59	ARG
1	A	168	GLU
1	A	235	GLU
1	A	271	GLU
1	A	288	GLN
1	B	16	THR
1	B	17	VAL
1	B	103	ILE
1	B	159	LEU
1	B	186	CYS

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Mol	Chain	Res	Type
1	B	210	ASP
1	B	235	GLU
1	B	276	GLU
1	C	5	ASN
1	C	13	SER
1	C	59	ARG
1	C	73	VAL
1	C	93	ARG
1	C	175	ARG
1	C	179	VAL
1	C	185	ASP
1	C	235	GLU
1	C	279	GLU
1	C	288	GLN
1	D	16	THR
1	D	17	VAL
1	D	18	LEU
1	D	20	LEU
1	D	49	GLU
1	D	100	MET
1	D	144	GLU
1	D	177	GLU
1	D	186	CYS
1	D	210	ASP
1	D	235	GLU
1	D	272	SER
1	D	290	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	133	ASN
1	B	84	ASN
1	C	45	GLN
1	C	51	HIS
1	C	253	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
5	TDR	D	402	-	9,9,9	4.90	6 (66%)	12,12,12	2.99	5 (41%)
4	R1P	D	401	-	13,14,14	5.26	8 (61%)	21,21,21	3.93	8 (38%)
3	THM	C	402	-	18,18,18	5.26	13 (72%)	26,26,26	1.85	6 (23%)
2	PO4	A	401	-	4,4,4	1.36	0	6,6,6	0.89	0
3	THM	A	402	-	18,18,18	5.30	14 (77%)	26,26,26	2.14	9 (34%)
5	TDR	B	402	-	9,9,9	5.32	7 (77%)	12,12,12	3.07	7 (58%)
2	PO4	C	401	-	4,4,4	2.04	1 (25%)	6,6,6	0.58	0
4	R1P	B	401	-	13,14,14	5.51	7 (53%)	21,21,21	4.23	9 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TDR	D	402	-	-	-	0/1/1/1
4	R1P	D	401	-	-	0/6/23/23	0/1/1/1
3	THM	C	402	-	-	0/6/18/18	0/2/2/2
5	TDR	B	402	-	-	-	0/1/1/1
3	THM	A	402	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	R1P	B	401	-	-	0/6/23/23	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	R1P	O4-C1	16.39	1.70	1.41
4	D	401	R1P	O4-C1	15.91	1.69	1.41
3	A	402	THM	C2'-C3'	-11.91	1.22	1.52
3	C	402	THM	C2'-C3'	-11.21	1.24	1.52
3	C	402	THM	C6-C5	9.07	1.49	1.34
3	A	402	THM	C6-C5	8.83	1.49	1.34
5	B	402	TDR	C2-N1	8.63	1.47	1.36
5	D	402	TDR	C2-N1	8.35	1.47	1.36
5	B	402	TDR	C6-C5	7.99	1.44	1.34
3	A	402	THM	C2-N1	7.86	1.50	1.38
3	C	402	THM	O4'-C4'	-7.43	1.28	1.45
5	D	402	TDR	C6-C5	7.35	1.44	1.34
3	C	402	THM	C2-N1	7.16	1.49	1.38
3	A	402	THM	O4'-C4'	-6.92	1.29	1.45
3	A	402	THM	C2-N3	6.88	1.49	1.38
4	B	401	R1P	C1-C2	-6.62	1.44	1.52
3	C	402	THM	C2-N3	6.53	1.49	1.38
5	B	402	TDR	C2-N3	6.53	1.48	1.37
4	D	401	R1P	C1-C2	-6.40	1.44	1.52
5	B	402	TDR	C6-N1	6.27	1.46	1.36
5	D	402	TDR	C2-N3	5.58	1.46	1.37
3	C	402	THM	C1'-N1	-5.47	1.34	1.48
5	D	402	TDR	C6-N1	5.35	1.45	1.36
3	C	402	THM	O3'-C3'	5.28	1.54	1.43
3	A	402	THM	C1'-N1	-5.15	1.35	1.48
3	A	402	THM	C3'-C4'	4.90	1.65	1.53
3	C	402	THM	C6-N1	4.73	1.46	1.38
3	A	402	THM	O3'-C3'	4.71	1.53	1.43
4	B	401	R1P	O4-C4	-4.69	1.34	1.45
3	C	402	THM	C3'-C4'	4.66	1.65	1.53
3	C	402	THM	O4'-C1'	4.53	1.52	1.42
4	B	401	R1P	O3-C3	-4.50	1.31	1.43
4	D	401	R1P	O4-C4	-4.17	1.35	1.45
3	A	402	THM	O4'-C1'	4.06	1.51	1.42
5	B	402	TDR	C4-N3	4.01	1.46	1.38
4	D	401	R1P	C3-C4	3.79	1.62	1.53
4	B	401	R1P	C3-C4	3.75	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	402	TDR	C4-N3	3.73	1.45	1.38
5	D	402	TDR	O4-C4	-3.58	1.16	1.23
4	B	401	R1P	C3-C2	3.45	1.62	1.53
3	A	402	THM	C6-N1	3.42	1.43	1.38
3	A	402	THM	C4-N3	3.37	1.45	1.38
5	B	402	TDR	O4-C4	-3.09	1.17	1.23
4	B	401	R1P	O2-C2	3.04	1.50	1.43
2	C	401	PO4	P-O4	-3.03	1.45	1.54
4	D	401	R1P	C3-C2	2.94	1.61	1.53
4	D	401	R1P	O3-C3	-2.93	1.35	1.43
4	D	401	R1P	O2-C2	2.69	1.49	1.43
5	B	402	TDR	C4-C5	2.67	1.49	1.44
4	D	401	R1P	P-O2P	-2.66	1.44	1.54
3	C	402	THM	O4-C4	-2.18	1.19	1.23
3	A	402	THM	C2'-C1'	2.12	1.58	1.52
3	C	402	THM	C4-N3	2.10	1.42	1.38
3	A	402	THM	C4-C5	2.09	1.48	1.44
3	A	402	THM	O4-C4	-2.08	1.19	1.23
3	C	402	THM	C4-C5	2.07	1.48	1.44

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	R1P	O4-C1-O1	13.16	134.24	109.16
4	D	401	R1P	O4-C1-O1	11.52	131.11	109.16
4	D	401	R1P	O4-C1-C2	-8.62	94.02	104.98
4	B	401	R1P	O4-C1-C2	-7.75	95.13	104.98
4	D	401	R1P	O1-C1-C2	7.70	119.15	106.65
4	B	401	R1P	O4-C4-C5	6.24	122.41	109.22
5	D	402	TDR	O4-C4-C5	-5.87	118.20	124.92
3	A	402	THM	C5-C4-N3	5.06	119.72	115.32
4	B	401	R1P	O3P-P-O1	5.03	125.44	105.85
5	D	402	TDR	C5-C4-N3	4.94	119.62	115.32
3	A	402	THM	C4-N3-C2	-4.87	120.96	127.34
5	B	402	TDR	C5-C4-N3	4.84	119.53	115.32
3	C	402	THM	C5-C4-N3	4.72	119.43	115.32
4	B	401	R1P	O1-C1-C2	4.58	114.08	106.65
5	B	402	TDR	N1-C2-N3	4.57	119.98	115.17
5	B	402	TDR	C4-N3-C2	-4.45	120.25	126.37
5	B	402	TDR	O4-C4-C5	-4.24	120.06	124.92
5	B	402	TDR	C6-N1-C2	-4.20	118.79	122.69
5	D	402	TDR	C4-N3-C2	-4.12	120.69	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	THM	O4-C4-C5	-4.03	120.31	124.92
4	B	401	R1P	C1-C2-C3	3.94	107.20	102.29
4	D	401	R1P	O4-C4-C5	3.87	117.39	109.22
4	D	401	R1P	O2P-P-O1	3.54	119.62	105.85
5	D	402	TDR	N1-C2-N3	3.49	118.85	115.17
3	C	402	THM	C4-N3-C2	-3.25	123.08	127.34
4	B	401	R1P	C1-O4-C4	3.16	117.80	105.76
5	D	402	TDR	C6-N1-C2	-3.15	119.77	122.69
4	B	401	R1P	C5-C4-C3	-3.07	107.86	115.10
4	D	401	R1P	C1-C2-C3	2.91	105.91	102.29
4	D	401	R1P	C5-C4-C3	-2.88	108.29	115.10
3	C	402	THM	O4-C4-C5	-2.83	121.68	124.92
3	C	402	THM	C5-C6-N1	-2.76	120.32	123.31
3	A	402	THM	O4'-C1'-C2'	-2.73	101.14	106.25
3	A	402	THM	C5-C6-N1	-2.70	120.38	123.31
3	A	402	THM	N3-C2-N1	2.60	118.27	114.89
4	B	401	R1P	O4-C4-C3	-2.57	100.05	105.15
3	A	402	THM	C6-C5-C4	2.55	120.12	118.02
3	C	402	THM	C5M-C5-C6	-2.49	119.47	122.85
3	A	402	THM	O4'-C4'-C5'	2.40	114.28	109.22
5	B	402	TDR	O2-C2-N1	-2.18	120.53	122.79
3	A	402	THM	C5M-C5-C6	-2.18	119.91	122.85
5	B	402	TDR	CM5-C5-C6	-2.14	121.03	123.23
3	C	402	THM	C5M-C5-C4	2.07	120.99	118.78
4	D	401	R1P	C1-O4-C4	2.02	113.46	105.76

There are no chirality outliers.

There are no torsion outliers.

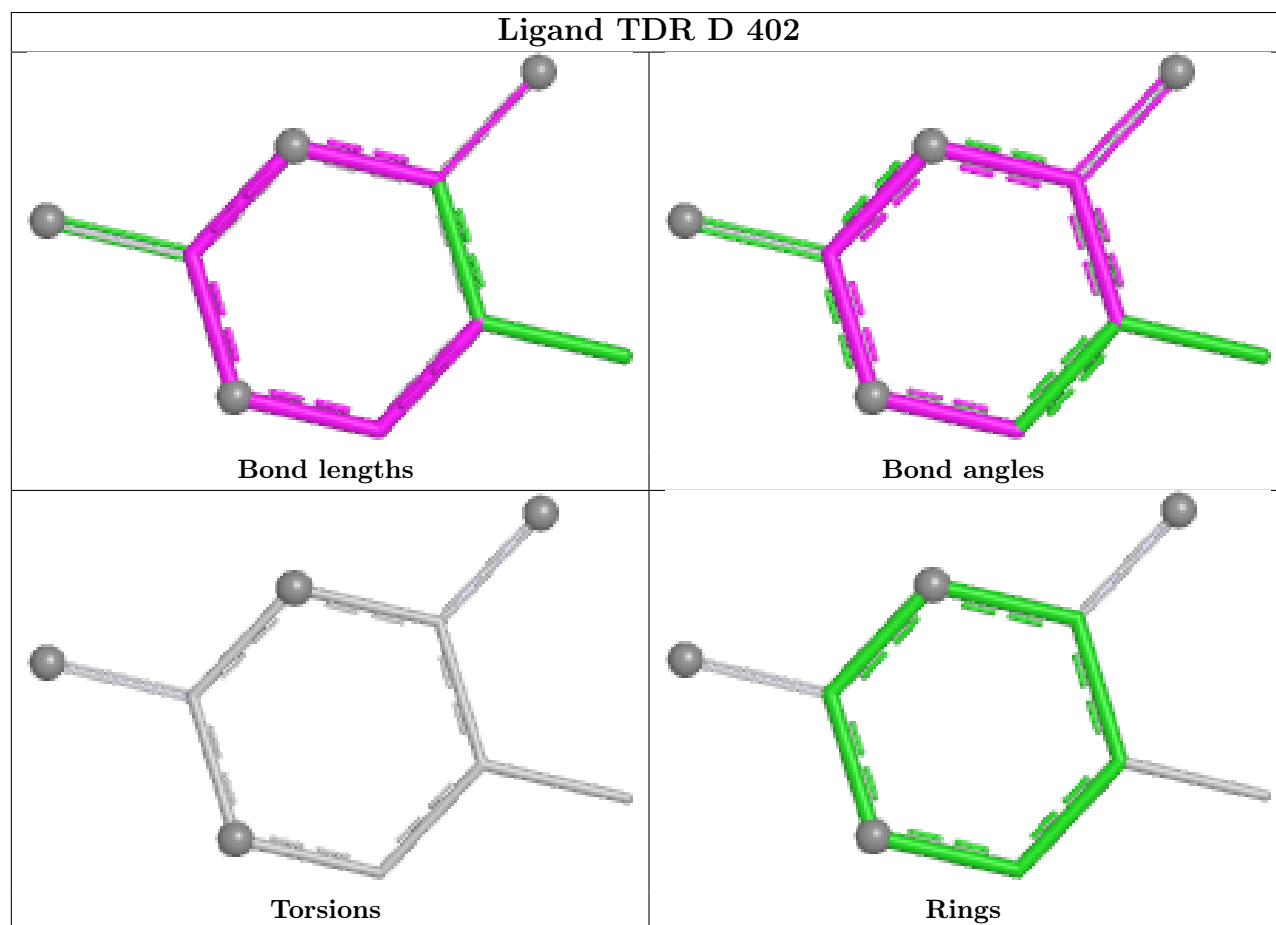
There are no ring outliers.

5 monomers are involved in 8 short contacts:

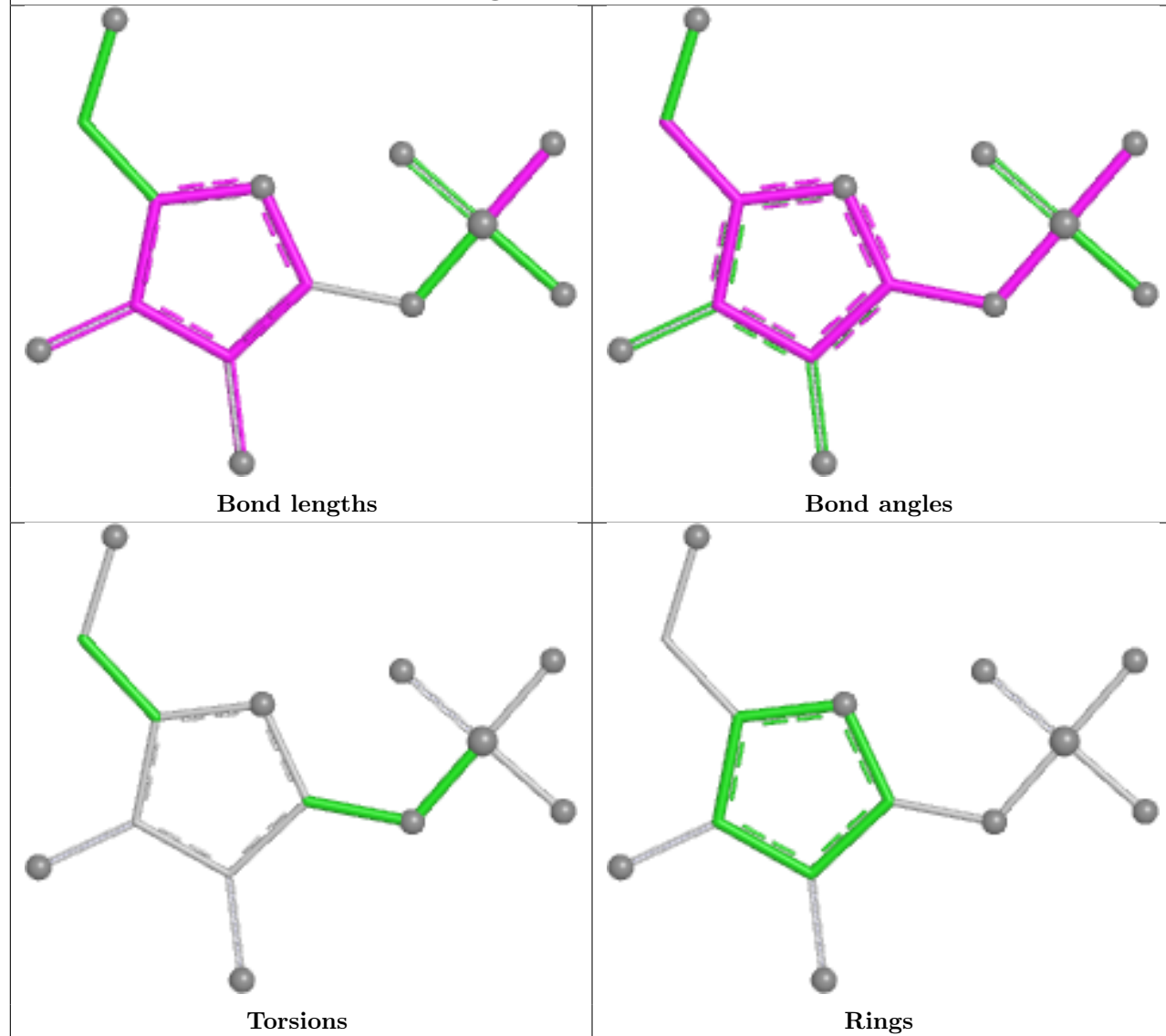
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	R1P	3	0
3	C	402	THM	1	0
2	A	401	PO4	1	0
3	A	402	THM	1	0
4	B	401	R1P	2	0

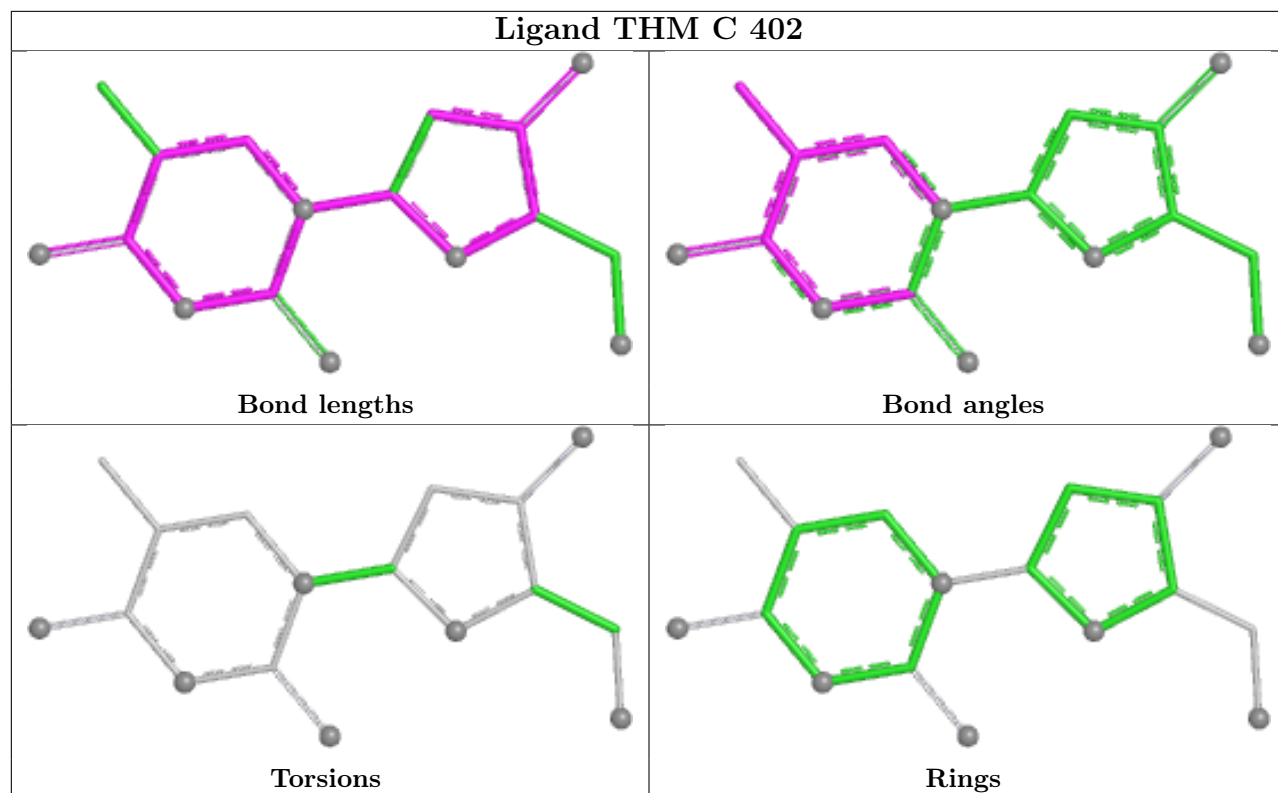
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

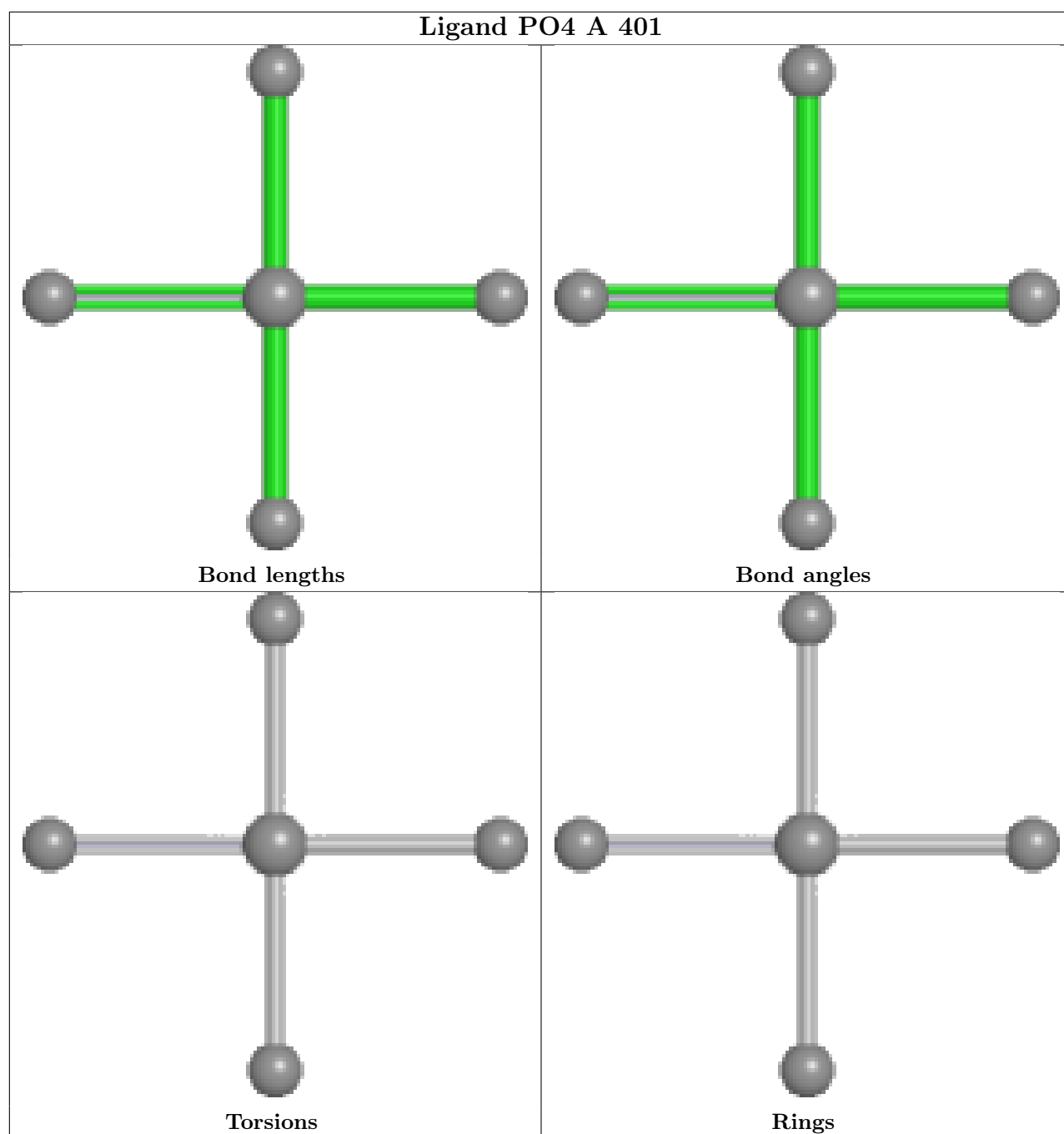
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

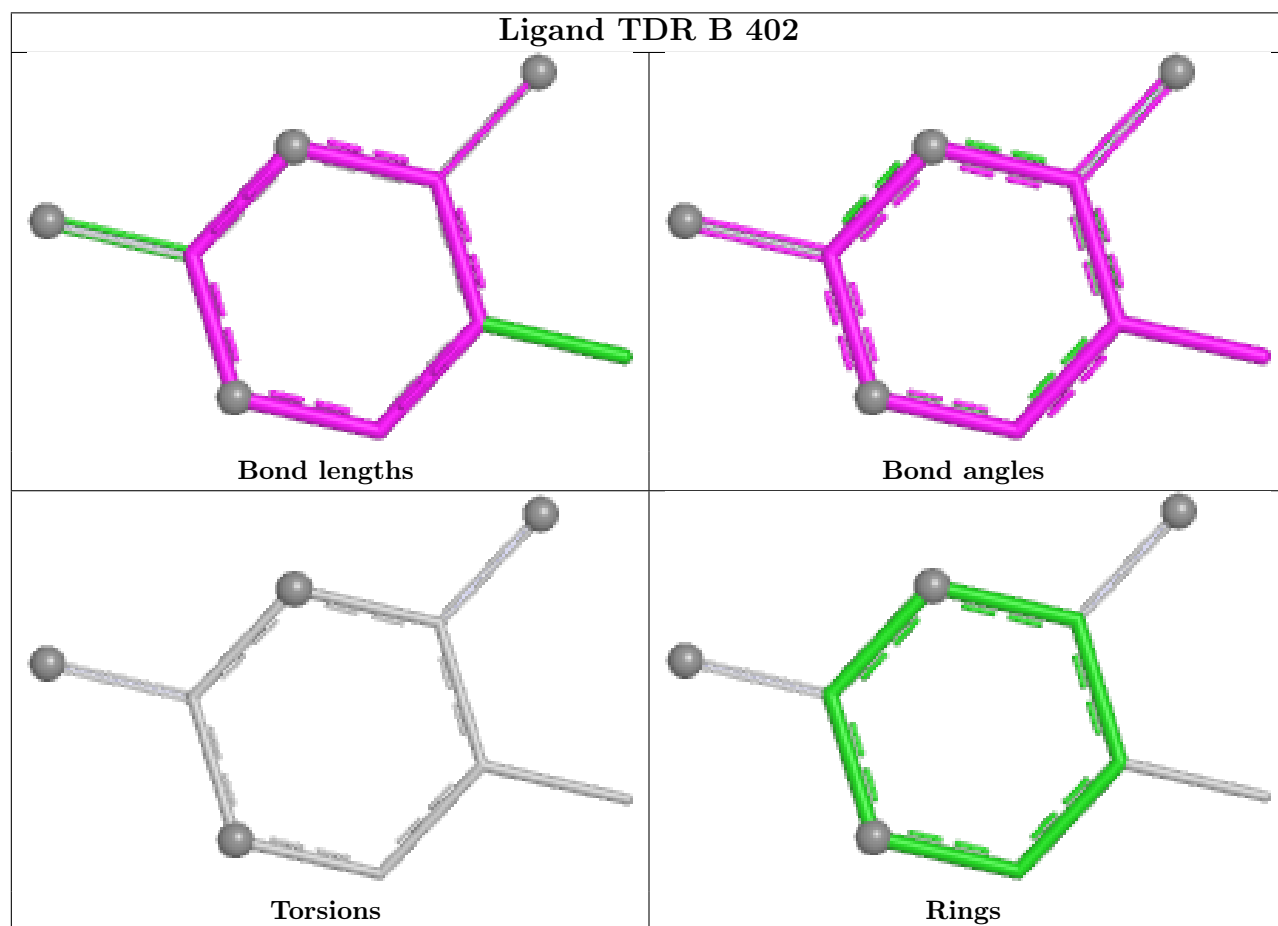
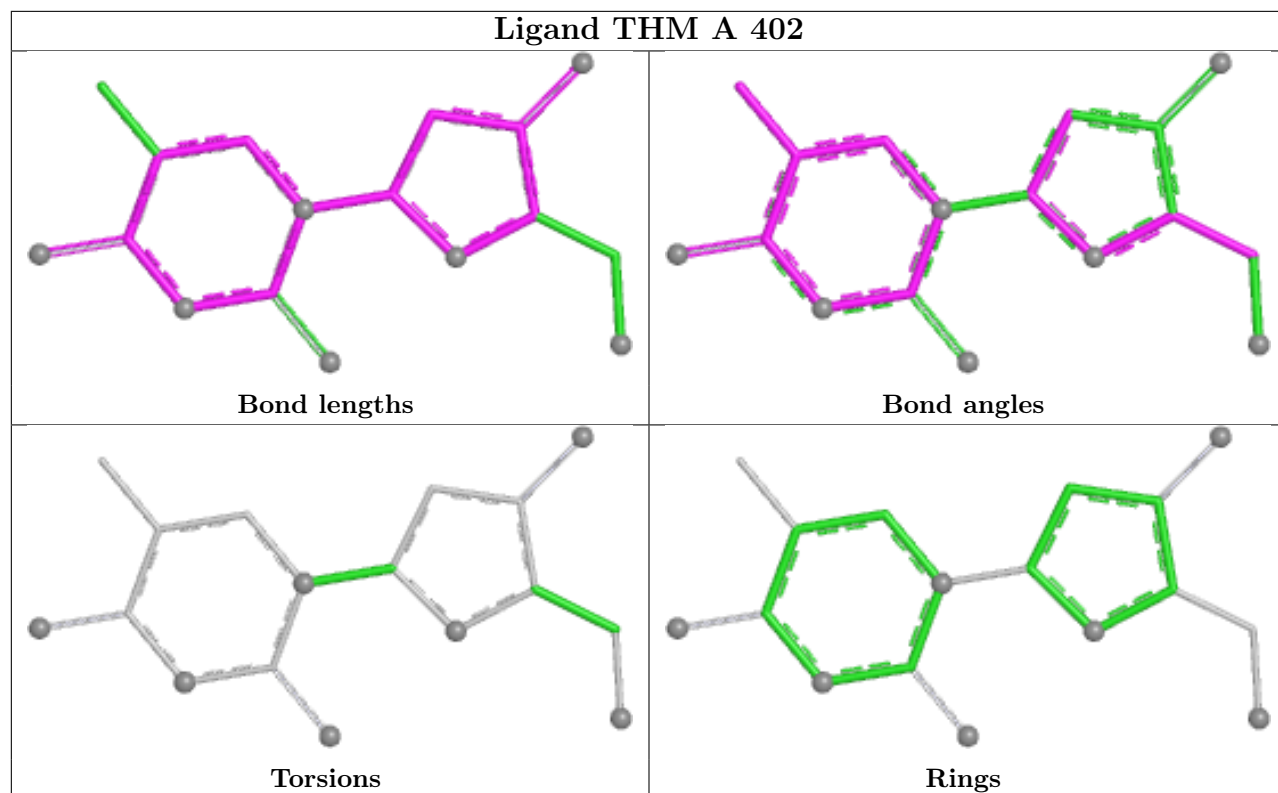


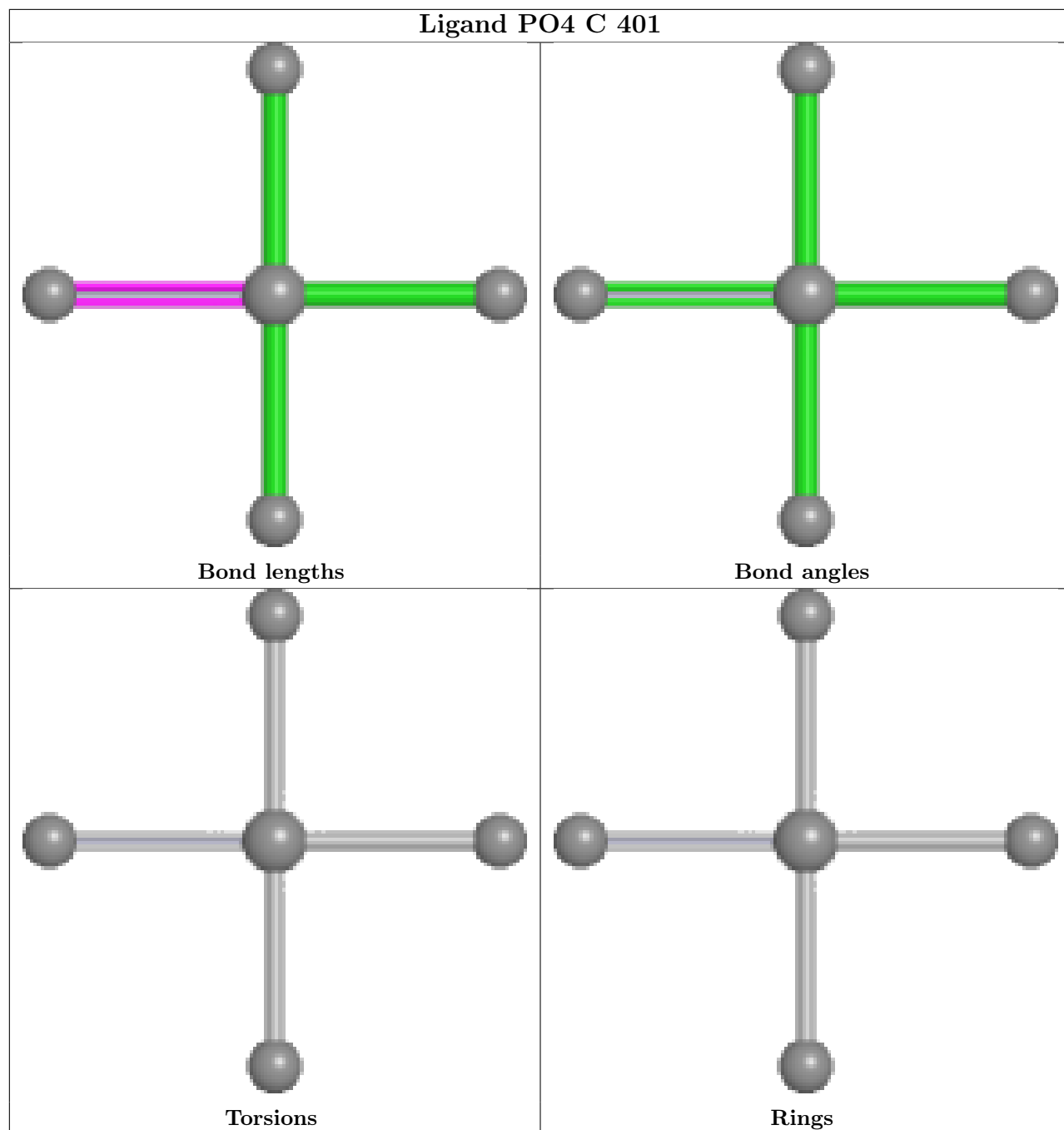
Ligand R1P D 401

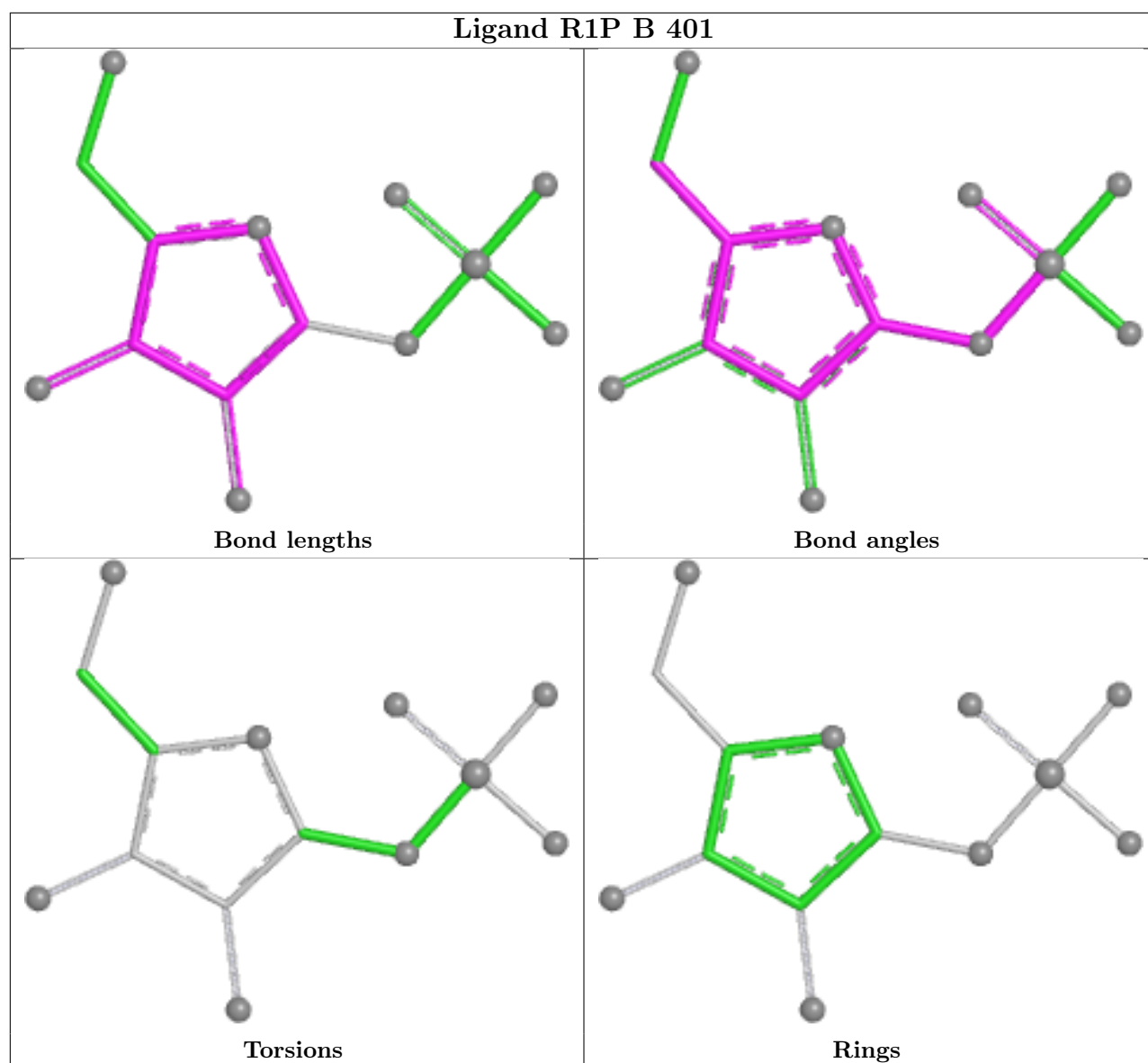












5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/309 (95%)	1.20	53 (18%) 3 3	14, 27, 66, 97	0
1	B	280/309 (90%)	1.66	99 (35%) 1 0	17, 30, 64, 122	0
1	C	294/309 (95%)	1.49	74 (25%) 1 1	15, 26, 70, 100	0
1	D	280/309 (90%)	1.41	59 (21%) 2 2	17, 31, 62, 106	0
All	All	1148/1236 (92%)	1.44	285 (24%) 2 1	14, 28, 66, 122	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	ALA	10.0
1	A	3	TYR	9.8
1	D	182	ALA	8.8
1	A	8	ALA	7.7
1	D	186	CYS	7.3
1	A	188	ALA	7.2
1	B	182	ALA	7.2
1	A	2	ALA	6.9
1	A	7	ASN	6.9
1	D	139	PRO	6.9
1	A	6	THR	6.8
1	B	186	CYS	6.7
1	C	143	GLU	6.5
1	C	142	SER	6.3
1	C	6	THR	6.3
1	A	185	ASP	6.2
1	C	186	CYS	6.1
1	B	269	ILE	5.9
1	D	183	SER	5.8
1	B	189	LEU	5.8
1	C	188	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	112	ARG	5.8
1	C	179	VAL	5.6
1	D	185	ASP	5.3
1	D	141	ALA	5.3
1	C	5	ASN	5.2
1	B	50	GLY	5.2
1	C	2	ALA	5.0
1	B	181	ALA	4.9
1	C	282	TRP	4.8
1	A	142	SER	4.8
1	A	211	SER	4.8
1	C	185	ASP	4.7
1	B	183	SER	4.7
1	A	144	GLU	4.7
1	D	138	PHE	4.7
1	C	266	SER	4.6
1	C	187	ASP	4.6
1	B	184	SER	4.5
1	B	210	ASP	4.5
1	A	4	GLN	4.5
1	A	5	ASN	4.5
1	B	141	ALA	4.5
1	C	181	ALA	4.5
1	C	265	LEU	4.5
1	D	184	SER	4.3
1	B	188	ALA	4.3
1	A	181	ALA	4.3
1	B	185	ASP	4.3
1	B	107	THR	4.2
1	A	176	ALA	4.2
1	C	171	LEU	4.2
1	D	142	SER	4.2
1	D	171	LEU	4.2
1	B	171	LEU	4.1
1	C	189	LEU	4.1
1	C	144	GLU	4.1
1	C	182	ALA	4.1
1	C	295	LEU	4.1
1	B	42	VAL	4.0
1	C	173	ALA	4.0
1	B	114	GLU	4.0
1	C	8	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	184	SER	4.0
1	A	9	MET	4.0
1	A	187	ASP	3.9
1	D	189	LEU	3.9
1	C	136	ALA	3.9
1	A	179	VAL	3.9
1	A	12	HIS	3.9
1	B	187	ASP	3.9
1	C	176	ALA	3.8
1	C	211	SER	3.7
1	B	261	VAL	3.7
1	B	266	SER	3.7
1	A	189	LEU	3.6
1	C	183	SER	3.6
1	C	288	GLN	3.6
1	A	182	ALA	3.6
1	B	142	SER	3.6
1	C	184	SER	3.6
1	C	7	ASN	3.6
1	C	175	ARG	3.6
1	D	258	VAL	3.5
1	C	141	ALA	3.5
1	B	103	ILE	3.5
1	B	68	VAL	3.5
1	B	159	LEU	3.5
1	B	267	GLY	3.5
1	C	192	PHE	3.4
1	A	209	LEU	3.4
1	A	13	SER	3.4
1	B	116	PRO	3.4
1	C	172	THR	3.4
1	D	209	LEU	3.4
1	B	294	PRO	3.4
1	D	137	PHE	3.4
1	B	139	PRO	3.4
1	C	114	GLU	3.3
1	D	145	ASP	3.3
1	D	36	SER	3.3
1	D	50	GLY	3.3
1	B	69	LYS	3.2
1	D	169	ASP	3.2
1	C	3	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	145	ASP	3.2
1	C	269	ILE	3.2
1	B	262	ALA	3.2
1	D	140	GLY	3.2
1	A	282	TRP	3.1
1	B	165	ALA	3.1
1	D	180	ILE	3.1
1	B	190	ARG	3.1
1	A	183	SER	3.1
1	B	176	ALA	3.1
1	D	25	GLY	3.1
1	B	265	LEU	3.0
1	B	51	HIS	3.0
1	C	13	SER	3.0
1	B	219	LYS	3.0
1	D	256	ALA	3.0
1	B	113	GLU	3.0
1	A	16	THR	3.0
1	B	286	VAL	2.9
1	B	291	VAL	2.9
1	B	20	LEU	2.9
1	D	148	ARG	2.9
1	B	143	GLU	2.9
1	D	133	ASN	2.9
1	B	249	ARG	2.9
1	D	210	ASP	2.9
1	B	49	GLU	2.9
1	B	293	THR	2.9
1	A	178	PRO	2.9
1	C	178	PRO	2.9
1	C	217	ASN	2.8
1	A	143	GLU	2.8
1	A	186	CYS	2.8
1	A	31	ILE	2.8
1	D	16	THR	2.8
1	C	4	GLN	2.8
1	B	191	VAL	2.8
1	C	148	ARG	2.8
1	D	134	PRO	2.8
1	D	188	ALA	2.8
1	C	169	ASP	2.8
1	D	187	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	157	SER	2.8
1	C	281	PHE	2.8
1	A	97	ASN	2.8
1	B	46	LEU	2.8
1	D	114	GLU	2.8
1	B	245	ALA	2.7
1	C	267	GLY	2.7
1	B	209	LEU	2.7
1	D	179	VAL	2.7
1	B	64	TYR	2.7
1	C	9	MET	2.7
1	B	244	LEU	2.7
1	B	295	LEU	2.7
1	C	174	LEU	2.7
1	B	290	ILE	2.7
1	B	258	VAL	2.7
1	B	70	GLY	2.7
1	B	232	TYR	2.7
1	A	210	ASP	2.7
1	B	138	PHE	2.7
1	B	117	PRO	2.7
1	B	73	VAL	2.7
1	B	275	LEU	2.6
1	D	291	VAL	2.6
1	A	58	ALA	2.6
1	B	40	ALA	2.6
1	B	166	SER	2.6
1	D	211	SER	2.6
1	D	251	SER	2.6
1	A	18	LEU	2.6
1	D	174	LEU	2.6
1	B	140	GLY	2.6
1	B	144	GLU	2.6
1	D	120	VAL	2.6
1	C	96	VAL	2.6
1	C	158	THR	2.6
1	A	147	TYR	2.5
1	B	192	PHE	2.5
1	B	268	GLN	2.5
1	B	284	GLY	2.5
1	C	221	VAL	2.5
1	B	118	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	28	ALA	2.5
1	B	124	GLY	2.5
1	C	220	LEU	2.5
1	A	148	ARG	2.5
1	B	112	ARG	2.5
1	D	221	VAL	2.5
1	A	20	LEU	2.4
1	B	253	GLN	2.4
1	B	272	SER	2.4
1	B	75	ILE	2.4
1	C	180	ILE	2.4
1	D	88	VAL	2.4
1	D	202	PHE	2.4
1	B	101	THR	2.4
1	C	28	ALA	2.4
1	A	112	ARG	2.4
1	C	151	ARG	2.4
1	B	234	VAL	2.4
1	C	95	VAL	2.4
1	C	228	HIS	2.4
1	A	203	TYR	2.4
1	C	10	PRO	2.4
1	C	229	PRO	2.4
1	C	140	GLY	2.3
1	D	27	VAL	2.3
1	D	42	VAL	2.3
1	B	47	LEU	2.3
1	B	72	PRO	2.3
1	D	178	PRO	2.3
1	C	49	GLU	2.3
1	D	146	CYS	2.3
1	A	11	THR	2.3
1	C	12	HIS	2.3
1	C	225	THR	2.3
1	D	172	THR	2.3
1	C	134	PRO	2.3
1	C	113	GLU	2.3
1	D	268	GLN	2.3
1	B	179	VAL	2.3
1	A	158	THR	2.3
1	A	61	PHE	2.2
1	A	194	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	211	SER	2.2
1	A	145	ASP	2.2
1	B	180	ILE	2.2
1	B	108	CYS	2.2
1	B	174	LEU	2.2
1	B	287	LEU	2.2
1	C	231	LEU	2.2
1	A	60	GLY	2.2
1	B	102	ILE	2.2
1	D	219	LYS	2.2
1	A	190	ARG	2.2
1	B	43	LEU	2.2
1	B	110	ALA	2.2
1	C	239	PHE	2.2
1	D	144	GLU	2.2
1	B	17	VAL	2.2
1	C	164	VAL	2.2
1	D	200	CYS	2.2
1	D	278	LEU	2.2
1	C	294	PRO	2.2
1	B	254	ALA	2.2
1	C	247	ARG	2.2
1	D	249	ARG	2.2
1	C	223	ASP	2.1
1	C	258	VAL	2.1
1	B	22	LEU	2.1
1	B	178	PRO	2.1
1	A	28	ALA	2.1
1	B	256	ALA	2.1
1	B	203	TYR	2.1
1	B	16	THR	2.1
1	A	140	GLY	2.1
1	B	88	VAL	2.1
1	D	284	GLY	2.1
1	A	273	GLU	2.1
1	D	218	GLU	2.1
1	B	173	ALA	2.1
1	D	94	ALA	2.1
1	A	266	SER	2.1
1	A	280	SER	2.1
1	D	49	GLU	2.1
1	D	143	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	145	ASP	2.1
1	B	97	ASN	2.0
1	D	97	ASN	2.0
1	A	10	PRO	2.0
1	B	285	VAL	2.0
1	B	278	LEU	2.0
1	A	94	ALA	2.0
1	C	75	ILE	2.0
1	D	252	ILE	2.0
1	B	158	THR	2.0
1	B	27	VAL	2.0
1	C	291	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

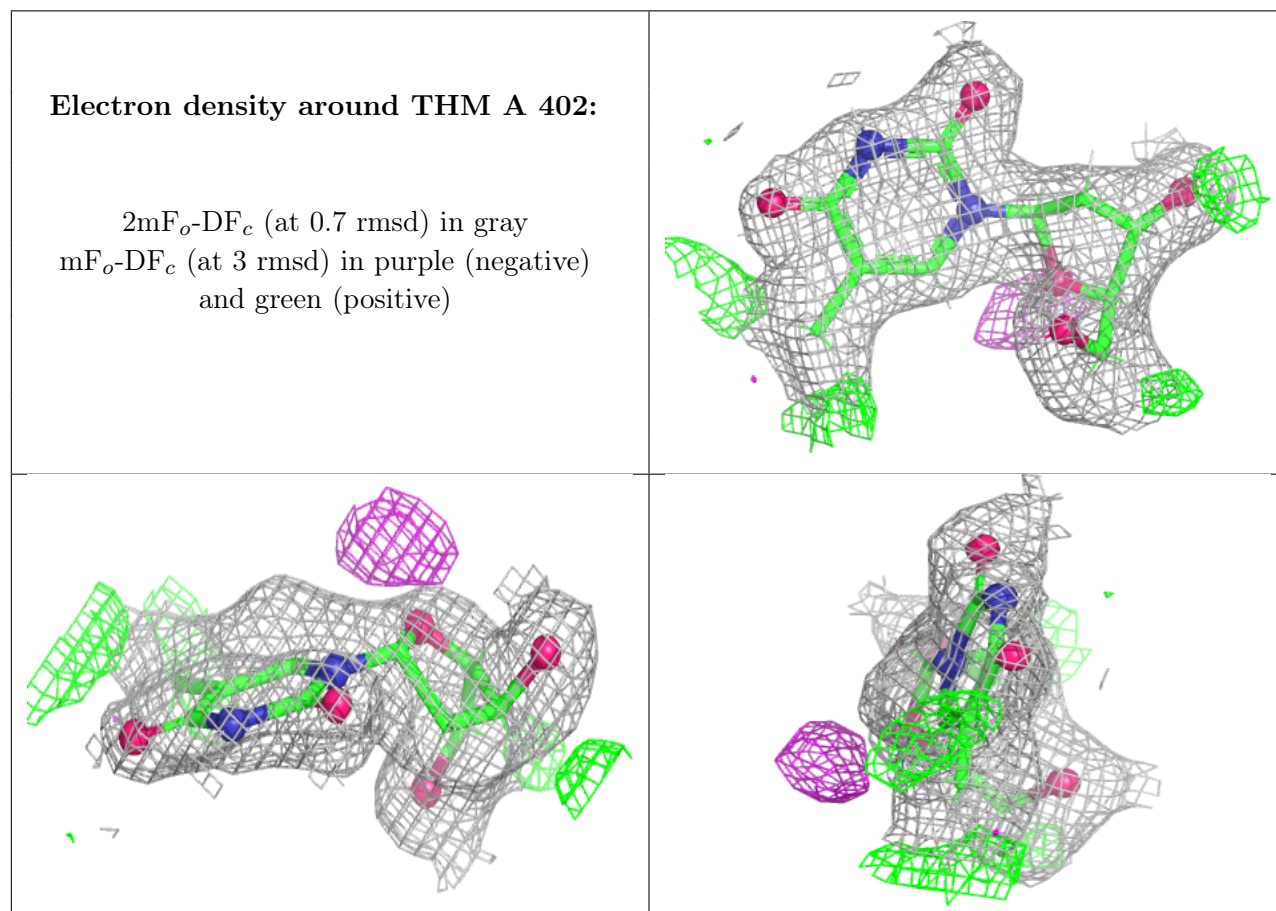
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	THM	A	402	17/17	0.82	0.12	20,30,36,37	0
3	THM	C	402	17/17	0.83	0.12	20,30,39,45	0
5	TDR	B	402	9/9	0.84	0.13	24,33,41,42	0
5	TDR	D	402	9/9	0.84	0.17	20,32,41,49	0
4	R1P	D	401	14/14	0.89	0.15	17,35,49,50	0
4	R1P	B	401	14/14	0.90	0.13	18,30,46,48	0
2	PO4	A	401	5/5	0.96	0.10	16,16,20,21	0
2	PO4	C	401	5/5	0.98	0.05	16,17,18,19	0

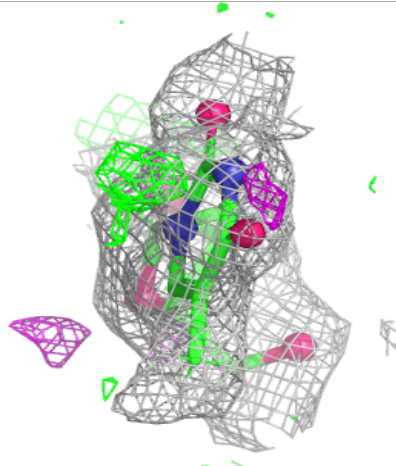
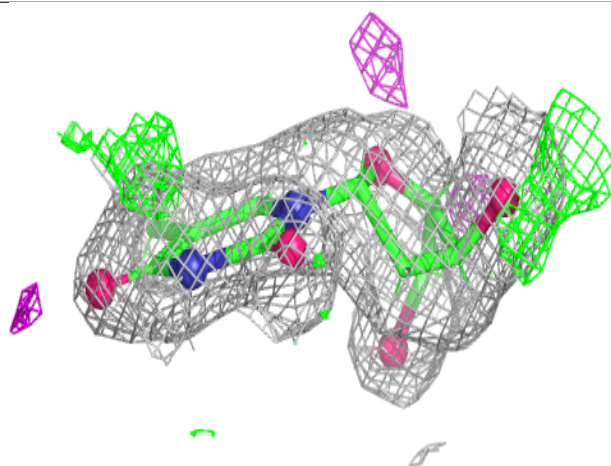
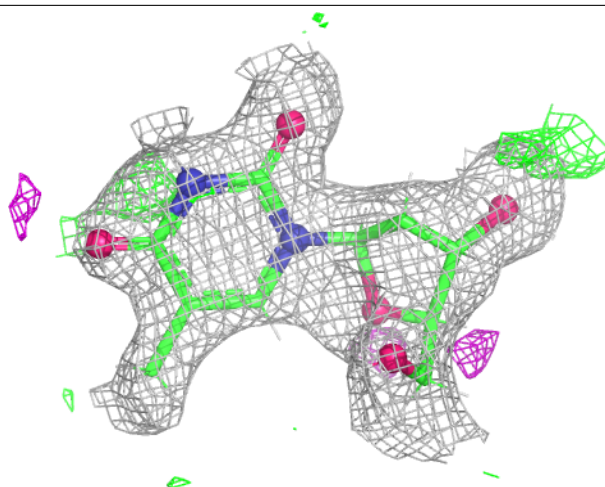
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



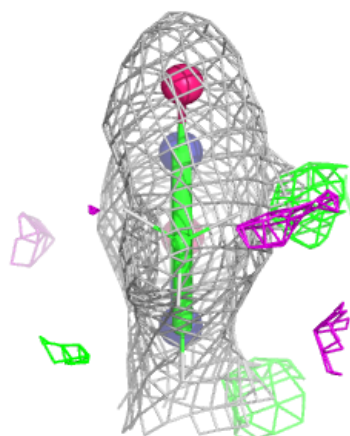
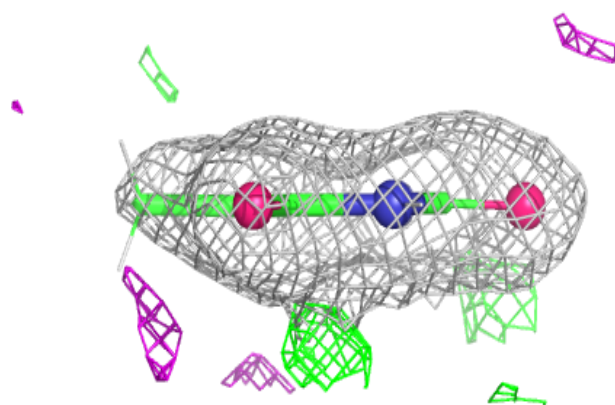
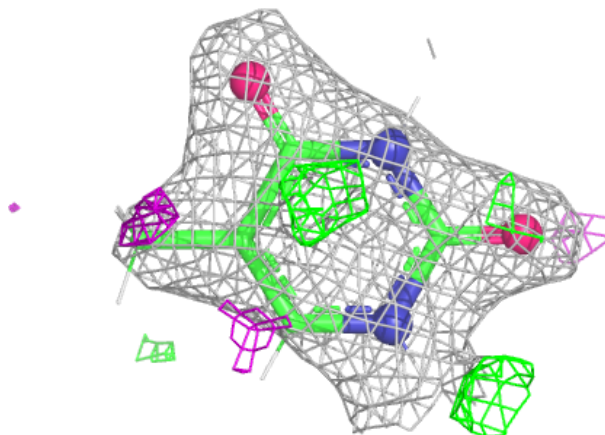
Electron density around THM C 402:

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



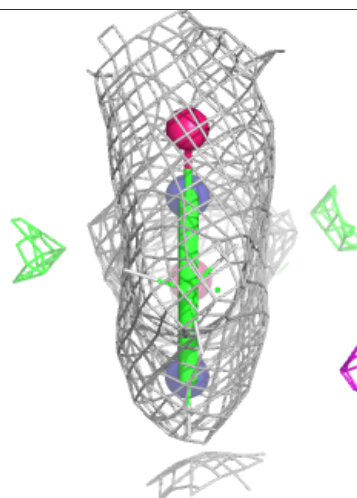
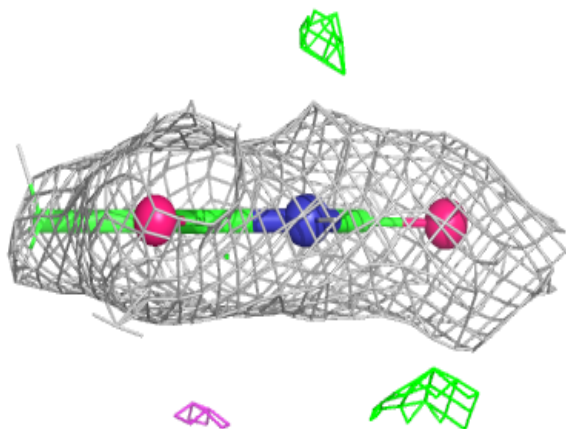
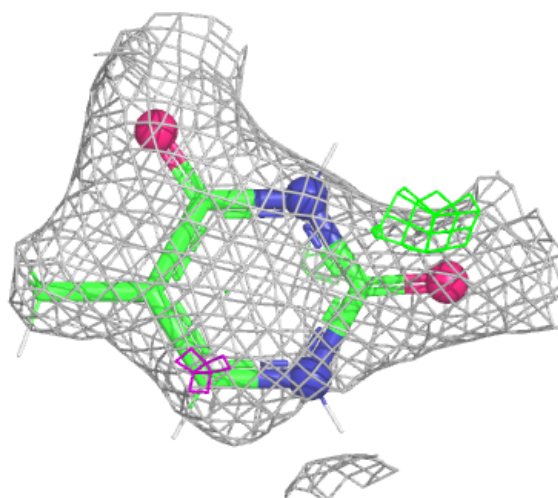
Electron density around TDR B 402:

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



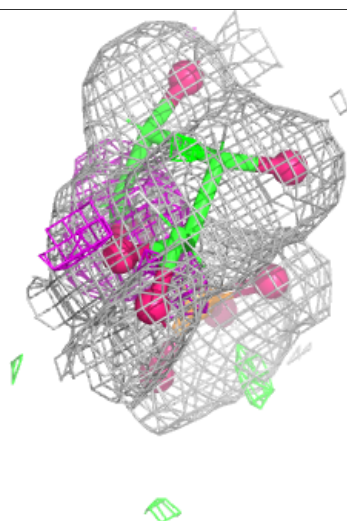
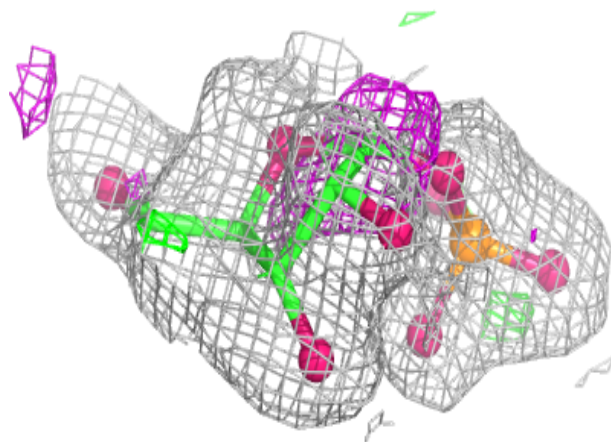
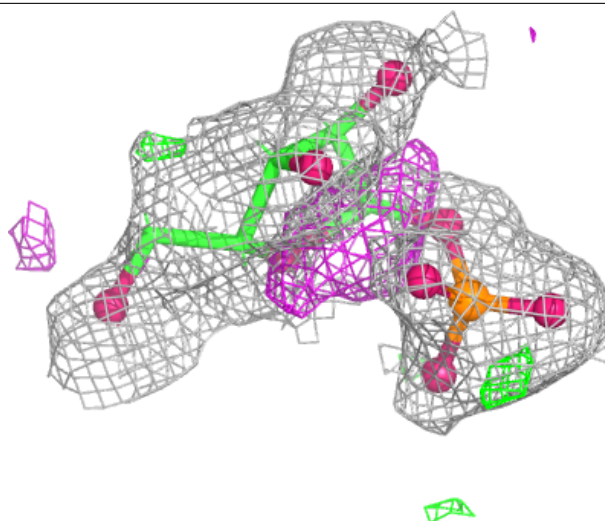
Electron density around TDR D 402:

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



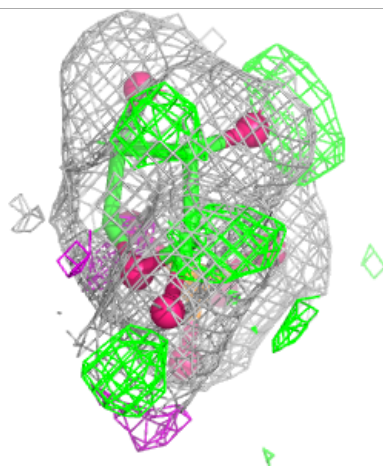
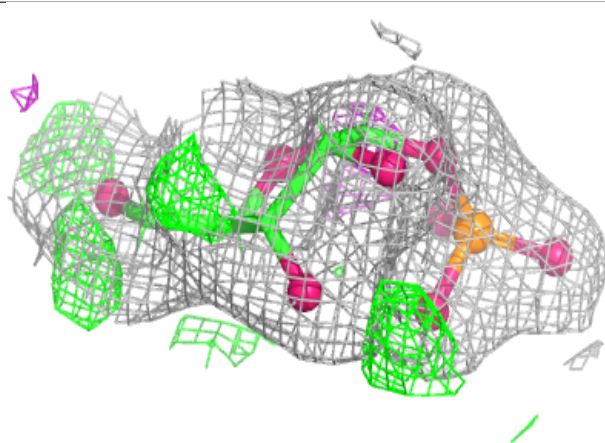
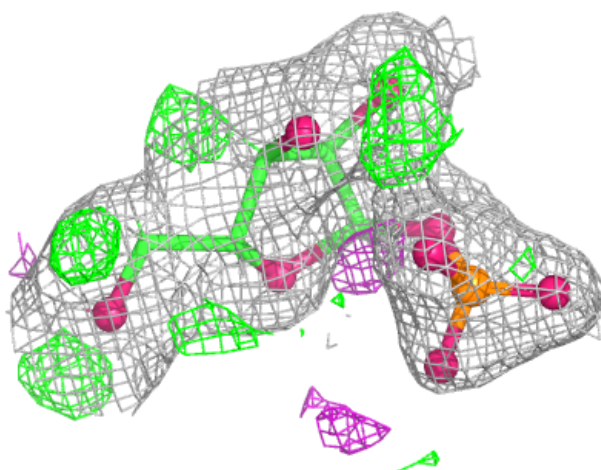
Electron density around R1P D 401:

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



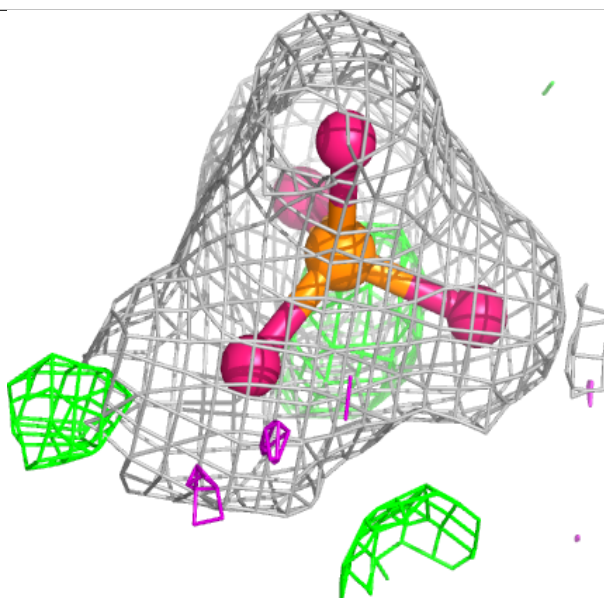
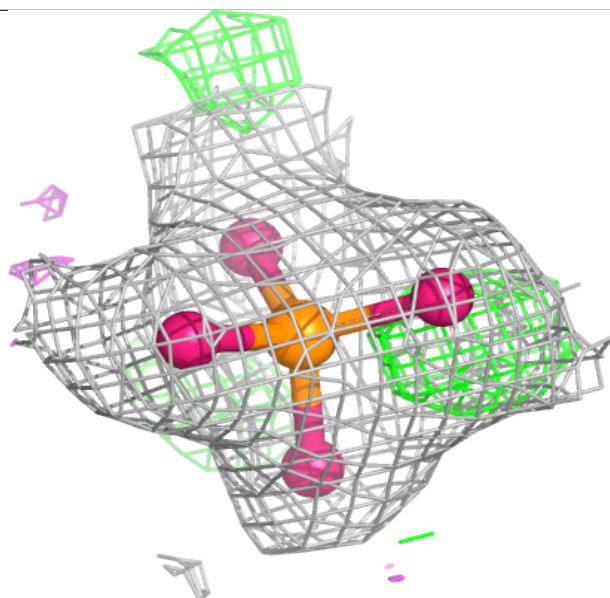
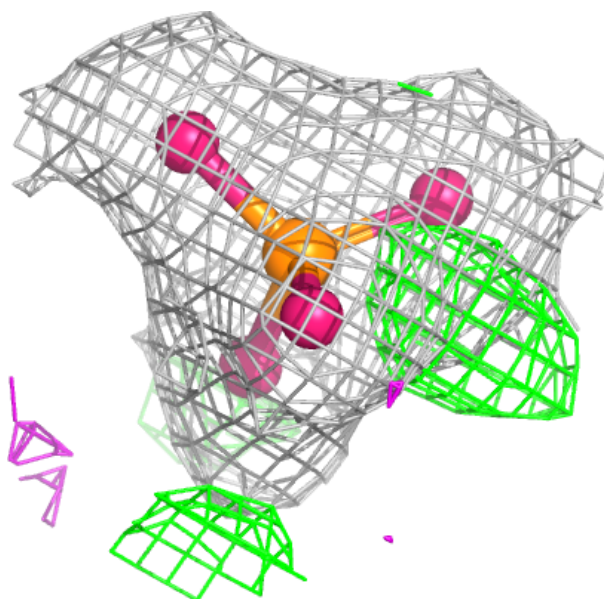
Electron density around R1P B 401:

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



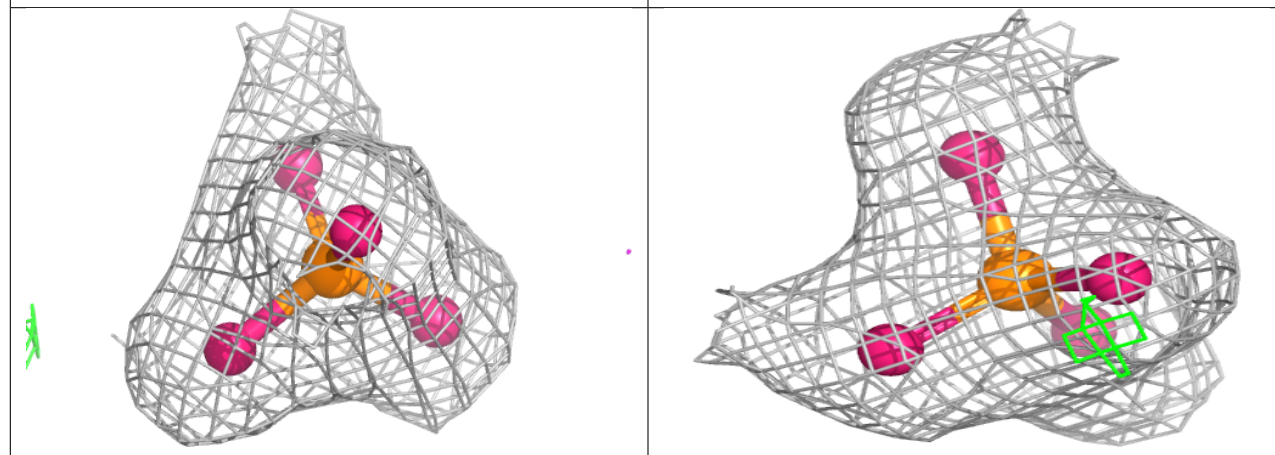
Electron density around PO4 A 401:

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



Electron density around PO4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.