



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:56 PM UTC

PDB ID : 6K5H / pdb_00006k5h
Title : Structural and catalytic analysis of two diverse uridine phosphorylases in the oomycete *Phytophthora capsici*.
Authors : Yang, C.C.; Zhang, X.G.
Deposited on : 2019-05-28
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

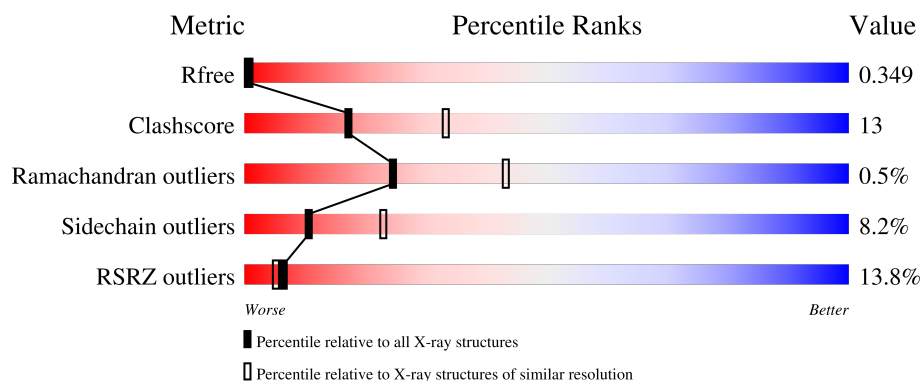
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	9% 71% 20% 7%
1	B	309	17% 61% 29% 7%
1	C	309	9% 69% 21% 7%
1	D	309	16% 66% 24% 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URA	A	401	-	X	-	-
2	URA	B	401	-	X	-	-
2	URA	C	401	-	X	-	-
2	URA	D	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17465 atoms, of which 8607 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	287	Total	C	H	N	O	S	0	0	0
			4291	1340	2144	375	420	12			
1	B	286	Total	C	H	N	O	S	0	0	0
			4273	1334	2133	374	421	11			
1	C	287	Total	C	H	N	O	S	0	0	0
			4277	1337	2136	372	420	12			
1	D	288	Total	C	H	N	O	S	0	0	0
			4297	1342	2145	376	423	11			

There are 52 discrepancies between the modelled and reference sequences:

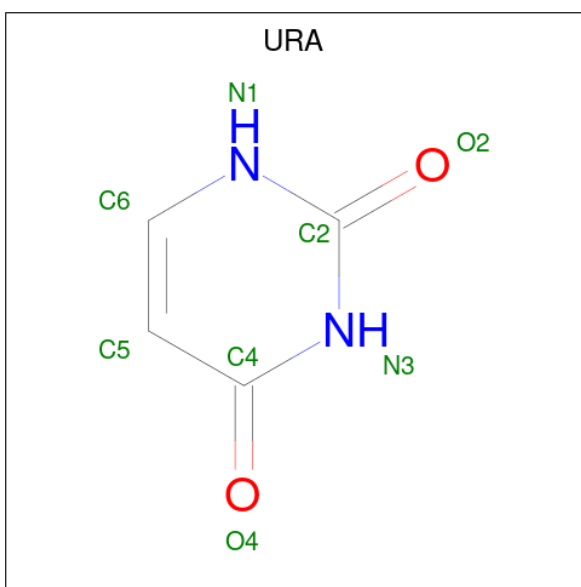
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A0A410UCT3
A	0	GLY	-	expression tag	UNP A0A410UCT3
A	297	ALA	-	expression tag	UNP A0A410UCT3
A	298	ALA	-	expression tag	UNP A0A410UCT3
A	299	ALA	-	expression tag	UNP A0A410UCT3
A	300	LEU	-	expression tag	UNP A0A410UCT3
A	301	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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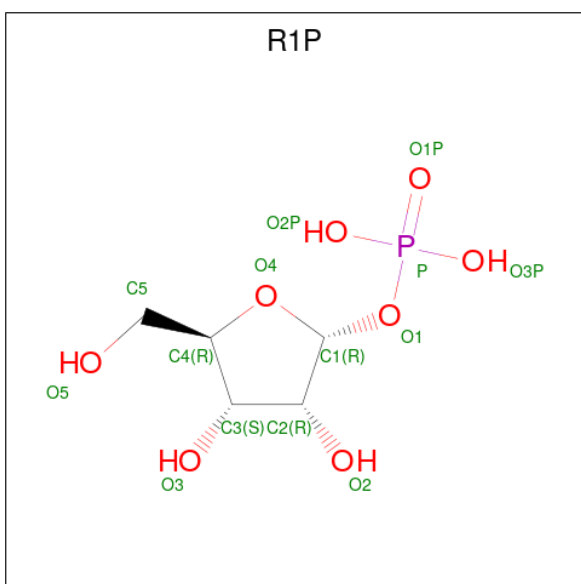
Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP A0A410UCT3
B	304	HIS	-	expression tag	UNP A0A410UCT3
B	305	HIS	-	expression tag	UNP A0A410UCT3
B	306	HIS	-	expression tag	UNP A0A410UCT3
B	307	HIS	-	expression tag	UNP A0A410UCT3
C	-1	MET	-	expression tag	UNP A0A410UCT3
C	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 URACIL (CCD ID: URA) (formula: C₄H₄N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	B	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	C	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	D	1	Total	C	H	N	O	0	0
			12	4	4	2	2		

- Molecule 3 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
3	A	1	Total	C	H	O	P	0	0
			22	5	8	8	1		
3	B	1	Total	C	H	O	P	0	0
			22	5	8	8	1		
3	C	1	Total	C	H	O	P	0	0
			22	5	8	8	1		
3	D	1	Total	C	H	O	P	0	0
			23	5	9	8	1		

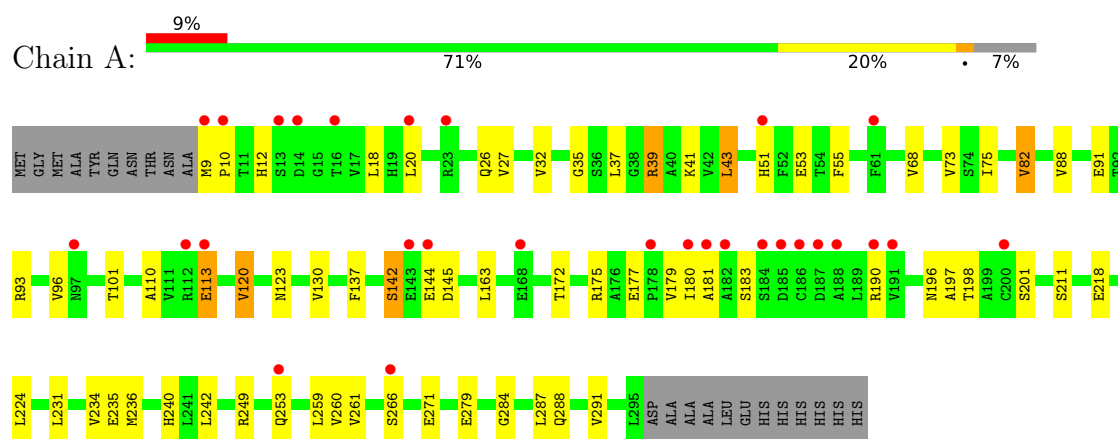
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	50	Total	O	0	0
			50	50		
4	C	44	Total	O	0	0
			44	44		
4	D	55	Total	O	0	0
			55	55		

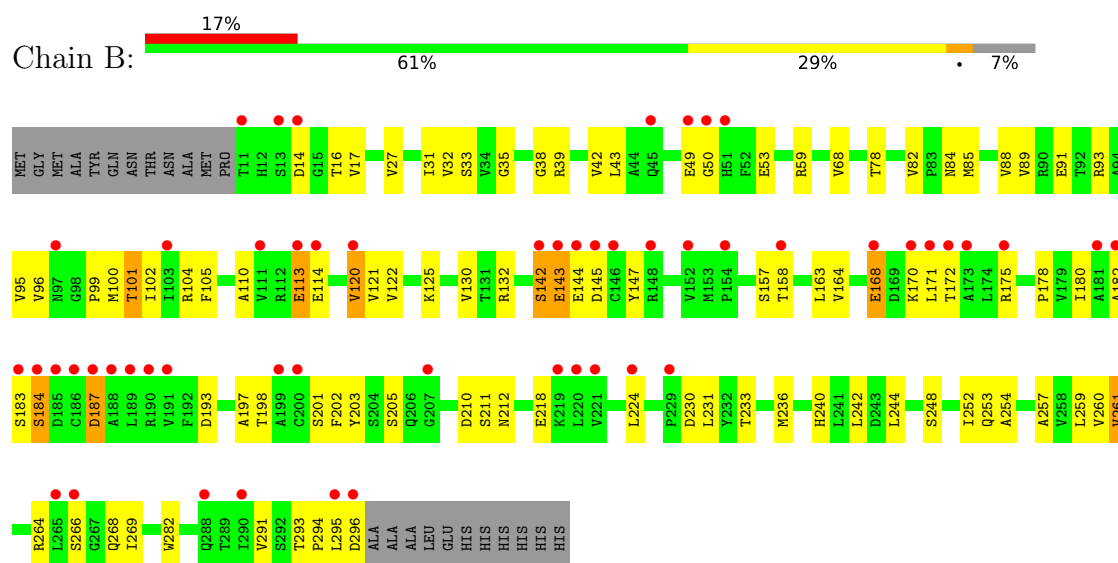
3 Residue-property plots [i](#)

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

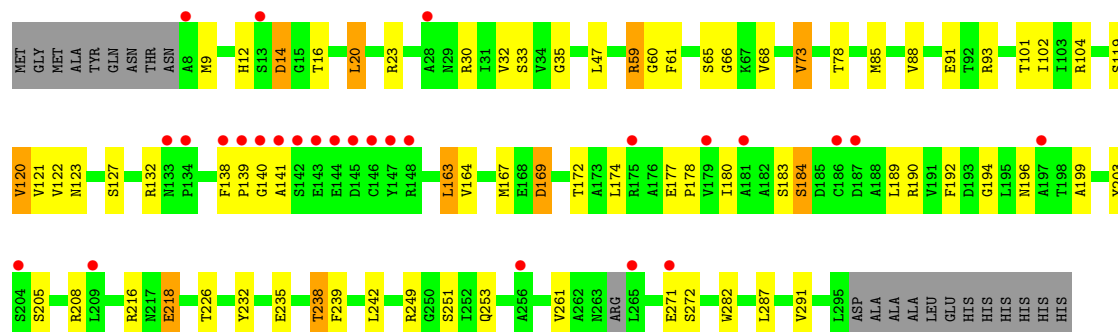


• Molecule 1: Uridine phosphorylase

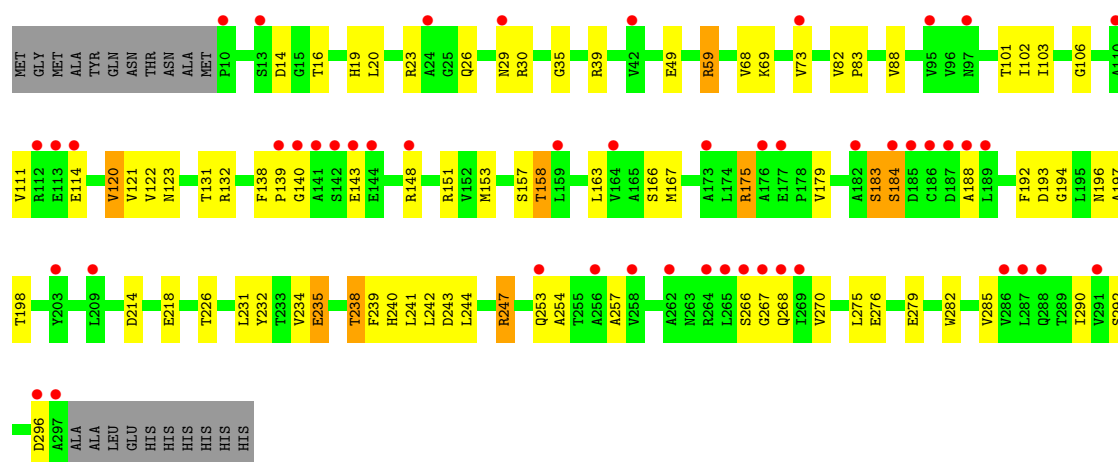


• Molecule 1: Uridine phosphorylase





● 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	66.97Å 97.69Å 188.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 2.50 48.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.84-2.50) 99.0 (48.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.256 , 0.349 0.256 , 0.349	Depositor DCC
R_{free} test set	2174 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 51.4	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	17465	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 66.65 % 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 5.8392e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.63	0/2181	0.76	0/2961
1	B	0.67	0/2173	0.81	0/2950
1	C	0.61	0/2174	0.77	0/2951
1	D	0.67	0/2186	0.80	0/2968
All	All	0.65	0/8714	0.79	0/11830

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	SER	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	2147	2144	2144	45	0
1	B	2140	2133	2132	74	0
1	C	2141	2136	2135	46	0
1	D	2152	2145	2145	51	0
2	A	8	4	3	0	0
2	B	8	4	3	0	0
2	C	8	4	3	0	0
2	D	8	4	3	0	0
3	A	14	8	0	4	0
3	B	14	8	0	1	0
3	C	14	8	0	2	0
3	D	14	9	0	2	0
4	A	41	0	0	4	0
4	B	50	0	0	6	0
4	C	44	0	0	6	0
4	D	55	0	0	9	0
All	All	8858	8607	8568	217	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 13.

All (217) 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)
3:A:402:R1P:C1	3:A:402:R1P:O4	1.64	1.23
1:D:188:ALA:O	4:D:501:HOH:O	1.88	0.91
1:B:39:ARG:NH2	4:B:501:HOH:O	2.03	0.90
1:A:20:LEU:HD21	1:A:88:VAL:HA	1.54	0.89
1:B:130:VAL:HG21	1:B:224:LEU:HD11	1.54	0.89
3:A:402:R1P:O1P	4:A:501:HOH:O	1.93	0.87
1:B:180:ILE:O	1:B:183:SER:OG	1.96	0.83
1:A:82:VAL:HG22	1:A:240:HIS:HB2	1.65	0.79
1:C:101:THR:HG22	1:C:253:GLN:HG3	1.65	0.78
1:A:172:THR:OG1	1:A:175:ARG:NH1	2.18	0.77
1:B:184:SER:N	4:B:502:HOH:O	2.09	0.77
1:A:180:ILE:O	1:A:183:SER:OG	2.03	0.77
3:D:402:R1P:O2P	3:D:402:R1P:O3	2.03	0.77
1:A:27:VAL:O	4:A:502:HOH:O	2.02	0.76
1:D:121:VAL:HG22	1:D:192:PHE:HB2	1.68	0.76
1:A:130:VAL:HG21	1:A:224:LEU:HD11	1.67	0.75
3:A:402:R1P:O5	1:D:19:HIS:NE2	2.21	0.73
1:C:20:LEU:HD21	1:C:88:VAL:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLU:OE2	4:D:502:HOH:O	2.07	0.72
1:B:78:THR:HG23	1:B:88:VAL:HG21	1.72	0.72
1:D:35:GLY:O	4:D:503:HOH:O	2.08	0.71
1:B:84:ASN:N	4:B:504:HOH:O	2.11	0.71
1:B:120:VAL:HG13	1:B:259:LEU:HD23	1.73	0.70
1:B:158:THR:OG1	4:B:503:HOH:O	2.10	0.68
1:A:177:GLU:OE2	4:A:503:HOH:O	2.11	0.68
1:D:270:VAL:HG11	1:D:275:LEU:HD22	1.74	0.68
1:C:101:THR:HG22	1:C:253:GLN:CG	2.24	0.68
1:D:270:VAL:CG1	1:D:275:LEU:HD22	2.25	0.67
1:D:20:LEU:HD21	1:D:88:VAL:HA	1.76	0.67
1:D:122:VAL:HG22	1:D:257:ALA:HB2	1.76	0.67
1:A:93:ARG:NH2	1:A:96:VAL:O	2.26	0.66
3:D:402:R1P:O1P	4:D:504:HOH:O	2.13	0.66
1:D:266:SER:O	1:D:268:GLN:N	2.29	0.66
1:C:138:PHE:O	1:C:140:GLY:N	2.29	0.66
1:A:287:LEU:O	1:A:291:VAL:HG22	1.95	0.65
1:C:20:LEU:HD22	1:C:91:GLU:HB2	1.78	0.65
1:C:60:GLY:O	4:C:502:HOH:O	2.15	0.64
1:D:175:ARG:NH1	4:D:506:HOH:O	2.25	0.64
1:B:122:VAL:HB	1:B:164:VAL:HG22	1.80	0.64
1:D:183:SER:OG	1:D:184:SER:N	2.28	0.64
1:B:122:VAL:HG11	1:B:164:VAL:HG23	1.80	0.63
1:B:82:VAL:HG22	1:B:240:HIS:HB2	1.81	0.63
1:A:68:VAL:HG23	1:A:73:VAL:HG11	1.81	0.62
1:C:123:ASN:ND2	4:C:504:HOH:O	2.30	0.61
1:B:113:GLU:CD	1:B:113:GLU:H	2.08	0.61
1:B:230:ASP:OD2	4:B:506:HOH:O	2.16	0.60
1:A:10:PRO:HD3	4:D:545:HOH:O	2.00	0.60
1:B:27:VAL:HG13	1:B:96:VAL:CG2	2.32	0.60
1:B:122:VAL:CB	1:B:164:VAL:HG22	2.33	0.59
1:A:120:VAL:HG13	1:A:259:LEU:HD23	1.86	0.58
1:B:121:VAL:HG21	1:B:233:THR:CG2	2.34	0.57
1:B:142:SER:O	1:B:144:GLU:HG2	2.04	0.57
1:C:172:THR:HG23	4:C:508:HOH:O	2.03	0.57
1:D:101:THR:HG22	1:D:253:GLN:HB2	1.86	0.57
1:C:16:THR:HG22	1:C:23:ARG:HB3	1.85	0.57
1:B:122:VAL:O	1:B:193:ASP:HA	2.05	0.57
1:A:179:VAL:O	1:A:183:SER:HB3	2.05	0.56
1:B:121:VAL:HG21	1:B:233:THR:HG23	1.86	0.56
1:B:85:MET:O	1:B:89:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:HIS:NE2	1:D:244:LEU:HD11	2.20	0.56
1:D:197:ALA:HB3	1:D:234:VAL:HG22	1.88	0.56
1:C:32:VAL:HG21	1:C:287:LEU:HD23	1.86	0.55
1:A:113:GLU:CD	1:A:113:GLU:H	2.13	0.55
1:A:20:LEU:HD22	1:A:91:GLU:HB2	1.87	0.55
1:B:78:THR:HG23	1:B:88:VAL:CG2	2.35	0.55
1:A:26:GLN:HB3	1:A:55:PHE:CZ	2.43	0.54
1:B:122:VAL:HG11	1:B:164:VAL:CG2	2.37	0.54
1:C:216:ARG:HA	1:C:218:GLU:OE2	2.06	0.54
1:D:123:ASN:ND2	1:D:196:ASN:HB2	2.22	0.54
1:A:123:ASN:CG	1:A:196:ASN:HB2	2.32	0.54
1:B:203:TYR:CZ	1:C:9:MET:HE1	2.43	0.54
1:C:132:ARG:NH2	4:C:506:HOH:O	2.37	0.53
1:C:14:ASP:HB3	1:C:16:THR:HG23	1.89	0.53
1:A:180:ILE:HA	1:A:183:SER:OG	2.09	0.53
1:D:120:VAL:HG11	1:D:167:MET:HE1	1.89	0.53
1:D:282:TRP:CE3	1:D:285:VAL:HG21	2.43	0.53
1:C:121:VAL:HG22	1:C:192:PHE:HB2	1.91	0.53
1:D:101:THR:HA	1:D:253:GLN:O	2.08	0.53
1:D:138:PHE:O	1:D:140:GLY:N	2.42	0.52
1:B:130:VAL:CG2	1:B:224:LEU:HD11	2.33	0.52
1:B:198:THR:HG23	1:B:236:MET:C	2.34	0.52
1:B:248:SER:HB2	1:B:252:ILE:HD12	1.90	0.52
1:D:30:ARG:O	1:D:73:VAL:HA	2.10	0.52
1:B:32:VAL:HG11	1:B:43:LEU:HD21	1.91	0.52
1:A:39:ARG:HD3	1:A:279:GLU:HG2	1.92	0.51
1:B:248:SER:CB	1:B:252:ILE:HD12	2.40	0.51
1:A:32:VAL:HG11	1:A:43:LEU:HD21	1.93	0.51
1:B:197:ALA:HB2	1:B:231:LEU:HD11	1.93	0.51
1:D:158:THR:OG1	4:D:505:HOH:O	2.16	0.51
1:B:121:VAL:HB	1:B:233:THR:HG21	1.93	0.51
1:A:175:ARG:O	1:A:181:ALA:HB2	2.12	0.50
1:A:197:ALA:HB2	1:A:231:LEU:HD11	1.92	0.50
1:B:27:VAL:CG2	1:B:31:ILE:HD11	2.40	0.50
1:B:201:SER:C	1:B:236:MET:HE3	2.37	0.50
1:D:82:VAL:HB	1:D:83:PRO:HD3	1.92	0.50
1:C:33:SER:OG	1:C:85:MET:HE1	2.11	0.50
1:D:153:MET:HE3	1:D:243:ASP:CG	2.37	0.49
1:B:110:ALA:HB2	1:B:260:VAL:HG11	1.95	0.49
1:B:172:THR:HA	1:B:175:ARG:CZ	2.43	0.49
1:C:194:GLY:HA3	1:C:232:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:VAL:O	1:C:261:VAL:CG1	2.61	0.48
1:B:172:THR:HA	1:B:175:ARG:NH1	2.27	0.48
1:A:179:VAL:O	1:A:179:VAL:HG12	2.14	0.48
1:B:32:VAL:HG11	1:B:43:LEU:CD2	2.43	0.48
1:C:120:VAL:HG22	1:C:282:TRP:NE1	2.28	0.48
1:B:68:VAL:HB	1:B:291:VAL:HG11	1.95	0.48
1:A:43:LEU:HG	1:A:287:LEU:HD11	1.96	0.48
1:C:189:LEU:O	1:C:190:ARG:HG2	2.14	0.48
1:D:197:ALA:O	1:D:234:VAL:HA	2.14	0.47
1:B:101:THR:CG2	1:B:295:LEU:HD23	2.44	0.47
1:B:171:LEU:O	1:B:175:ARG:HD3	2.14	0.47
1:C:16:THR:HG23	1:C:23:ARG:HE	1.78	0.47
1:B:93:ARG:NH2	1:B:96:VAL:O	2.45	0.47
1:C:16:THR:CG2	1:C:23:ARG:HE	2.26	0.47
1:C:123:ASN:CG	1:C:196:ASN:HB2	2.40	0.47
1:D:39:ARG:HD2	1:D:279:GLU:HG3	1.97	0.47
1:A:68:VAL:HB	1:A:291:VAL:HG11	1.96	0.47
1:A:82:VAL:HG22	1:A:240:HIS:CB	2.42	0.47
1:C:104:ARG:HD3	1:C:238:THR:OG1	2.16	0.46
1:B:102:ILE:O	1:B:254:ALA:HA	2.15	0.46
1:B:101:THR:HB	1:B:253:GLN:HG3	1.97	0.46
1:B:114:GLU:O	1:B:114:GLU:HG2	2.15	0.46
1:B:91:GLU:O	1:B:95:VAL:HG22	2.16	0.46
1:B:264:ARG:HG3	1:B:264:ARG:HH11	1.80	0.46
1:C:14:ASP:CB	1:C:16:THR:HG23	2.46	0.46
1:C:127:SER:HA	1:C:196:ASN:O	2.16	0.46
1:C:167:MET:HA	1:C:282:TRP:CZ3	2.51	0.46
1:B:38:GLY:O	1:B:42:VAL:HG23	2.16	0.45
1:D:238:THR:O	1:D:239:PHE:C	2.59	0.45
1:D:103:ILE:HG13	1:D:290:ILE:HD12	1.98	0.45
1:D:266:SER:C	1:D:268:GLN:H	2.24	0.45
1:A:12:HIS:CE1	1:A:18:LEU:HA	2.52	0.45
1:B:184:SER:OG	4:B:502:HOH:O	2.20	0.45
1:A:198:THR:HG23	1:A:236:MET:C	2.41	0.44
1:D:132:ARG:NH2	4:D:512:HOH:O	2.38	0.44
1:C:249:ARG:NH2	4:C:510:HOH:O	2.44	0.44
1:A:53:GLU:HG3	1:B:53:GLU:HG3	1.99	0.44
1:B:101:THR:HA	1:B:253:GLN:O	2.17	0.44
1:B:178:PRO:O	1:B:182:ALA:HB3	2.17	0.44
1:C:35:GLY:HA3	3:C:402:R1P:O3P	2.18	0.44
1:D:19:HIS:HD2	1:D:59:ARG:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:O	1:A:144:GLU:HG2	2.18	0.44
1:C:30:ARG:O	1:C:73:VAL:HA	2.17	0.44
1:B:132:ARG:HG3	1:B:147:TYR:CE1	2.53	0.44
1:C:78:THR:HG23	1:C:88:VAL:HG21	2.00	0.44
1:D:198:THR:HA	1:D:235:GLU:O	2.17	0.44
1:A:43:LEU:HD23	1:A:75:ILE:HG12	1.99	0.44
1:C:59:ARG:HD2	4:C:517:HOH:O	2.17	0.44
1:A:110:ALA:HB2	1:A:260:VAL:HG11	1.99	0.44
1:B:89:VAL:HB	1:B:244:LEU:HD12	1.99	0.44
1:B:143:GLU:O	1:B:143:GLU:HG2	2.18	0.44
1:A:32:VAL:HG11	1:A:43:LEU:CD2	2.48	0.43
1:B:210:ASP:OD1	1:B:212:ASN:HB2	2.18	0.43
1:B:31:ILE:HD12	1:B:100:MET:CE	2.49	0.43
1:D:194:GLY:HA3	1:D:232:TYR:CD1	2.53	0.43
1:C:238:THR:O	1:C:239:PHE:C	2.62	0.43
1:C:93:ARG:NH1	1:C:251:SER:HB2	2.34	0.43
1:A:68:VAL:HG21	1:A:287:LEU:HB3	2.01	0.43
1:B:202:PHE:O	1:B:202:PHE:CD1	2.72	0.43
1:C:33:SER:O	1:C:104:ARG:HA	2.17	0.43
3:C:402:R1P:O3	3:C:402:R1P:O1	2.37	0.43
1:B:193:ASP:C	1:B:193:ASP:OD1	2.61	0.43
1:C:20:LEU:HD12	1:C:61:PHE:CD2	2.54	0.43
1:C:140:GLY:O	1:C:141:ALA:C	2.62	0.43
1:B:180:ILE:HA	1:B:183:SER:OG	2.19	0.42
1:C:203:TYR:HA	1:C:208:ARG:HB2	2.01	0.42
1:A:37:LEU:HG	1:A:41:LYS:HE3	2.01	0.42
1:B:14:ASP:HB2	1:B:16:THR:HG23	2.00	0.42
1:A:197:ALA:O	1:A:234:VAL:HA	2.20	0.42
1:B:49:GLU:O	1:B:50:GLY:C	2.62	0.42
1:B:143:GLU:O	1:B:143:GLU:CG	2.68	0.42
1:B:168:GLU:C	1:B:170:LYS:N	2.78	0.42
1:B:261:VAL:O	1:B:269:ILE:HG23	2.20	0.42
1:D:14:ASP:HB2	1:D:16:THR:H	1.83	0.42
1:A:35:GLY:HA3	3:A:402:R1P:O3P	2.19	0.42
1:D:282:TRP:CZ3	1:D:285:VAL:HG21	2.55	0.42
1:B:282:TRP:CE3	1:B:282:TRP:HA	2.54	0.42
1:D:120:VAL:HG11	1:D:167:MET:CE	2.49	0.42
1:D:49:GLU:OE1	1:D:49:GLU:HA	2.18	0.42
1:A:284:GLY:O	1:A:288:GLN:HG2	2.20	0.42
1:B:105:PHE:HA	1:B:257:ALA:O	2.20	0.42
1:B:187:ASP:OD1	1:B:187:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:O	1:D:69:LYS:C	2.63	0.42
1:D:114:GLU:O	1:D:114:GLU:HG2	2.19	0.42
1:D:20:LEU:CD2	1:D:88:VAL:HA	2.47	0.41
1:D:29:ASN:OD1	1:D:29:ASN:C	2.63	0.41
1:D:151:ARG:HD2	4:D:507:HOH:O	2.20	0.41
1:D:193:ASP:C	1:D:193:ASP:OD1	2.62	0.41
1:B:125:LYS:HG2	1:B:193:ASP:OD1	2.19	0.41
1:C:47:LEU:HD13	1:C:66:GLY:HA3	2.02	0.41
1:A:137:PHE:HB3	1:D:247:ARG:HD2	2.02	0.41
1:B:293:THR:HA	1:B:294:PRO:HD3	1.89	0.41
1:C:169:ASP:OD1	1:C:169:ASP:C	2.62	0.41
1:B:33:SER:O	1:B:104:ARG:HA	2.21	0.41
1:B:266:SER:C	1:B:268:GLN:H	2.28	0.41
1:C:174:LEU:HD12	1:C:180:ILE:HG13	2.03	0.41
1:C:177:GLU:O	1:C:178:PRO:C	2.64	0.41
1:D:23:ARG:HG2	1:D:26:GLN:NE2	2.36	0.41
1:D:102:ILE:O	1:D:254:ALA:HA	2.20	0.41
1:A:197:ALA:HB2	1:A:231:LEU:CD1	2.50	0.41
1:B:17:VAL:HG21	1:B:91:GLU:HB3	2.03	0.41
1:B:99:PRO:HB2	1:B:295:LEU:HB3	2.02	0.41
1:B:168:GLU:C	1:B:170:LYS:H	2.28	0.41
1:D:197:ALA:HB2	1:D:231:LEU:HD11	2.03	0.41
1:A:175:ARG:O	4:A:504:HOH:O	2.22	0.41
1:C:122:VAL:HG22	1:C:163:LEU:HD13	2.03	0.41
1:D:39:ARG:NH2	1:D:106:GLY:HA2	2.36	0.41
1:C:199:ALA:HB1	1:C:205:SER:HB2	2.03	0.41
1:D:102:ILE:HG21	1:D:241:LEU:HD11	2.02	0.41
1:D:266:SER:C	1:D:268:GLN:N	2.79	0.41
1:A:101:THR:HA	1:A:253:GLN:O	2.21	0.41
1:A:26:GLN:HG2	1:A:55:PHE:CZ	2.56	0.40
1:A:197:ALA:CB	1:A:231:LEU:HD11	2.51	0.40
1:A:249:ARG:NH2	1:D:214:ASP:HA	2.36	0.40
1:B:35:GLY:HA3	3:B:402:R1P:O1P	2.21	0.40
1:C:68:VAL:HB	1:C:291:VAL:HG11	2.02	0.40
1:C:174:LEU:CD1	1:C:180:ILE:HG13	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	285/309 (92%)	267 (94%)	18 (6%)	0	100	100
1	B	284/309 (92%)	262 (92%)	21 (7%)	1 (0%)	30	49
1	C	283/309 (92%)	273 (96%)	7 (2%)	3 (1%)	11	22
1	D	286/309 (93%)	268 (94%)	16 (6%)	2 (1%)	18	34
All	All	1138/1236 (92%)	1070 (94%)	62 (5%)	6 (0%)	24	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	267	GLY
1	C	139	PRO
1	C	14	ASP
1	D	139	PRO
1	B	143	GLU
1	C	12	HIS

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	237/253 (94%)	218 (92%)	19 (8%)	11	24
1	B	236/253 (93%)	219 (93%)	17 (7%)	13	28
1	C	236/253 (93%)	217 (92%)	19 (8%)	11	23
1	D	237/253 (94%)	214 (90%)	23 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	946/1012 (94%)	868 (92%)	78 (8%)	10	23

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	39	ARG
1	A	43	LEU
1	A	51	HIS
1	A	82	VAL
1	A	113	GLU
1	A	120	VAL
1	A	142	SER
1	A	145	ASP
1	A	163	LEU
1	A	190	ARG
1	A	201	SER
1	A	211	SER
1	A	218	GLU
1	A	235	GLU
1	A	242	LEU
1	A	261	VAL
1	A	266	SER
1	A	271	GLU
1	B	59	ARG
1	B	101	THR
1	B	113	GLU
1	B	120	VAL
1	B	142	SER
1	B	145	ASP
1	B	157	SER
1	B	163	LEU
1	B	168	GLU
1	B	184	SER
1	B	187	ASP
1	B	205	SER
1	B	211	SER
1	B	218	GLU
1	B	242	LEU
1	B	261	VAL
1	B	296	ASP
1	C	20	LEU

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Mol	Chain	Res	Type
1	C	59	ARG
1	C	65	SER
1	C	73	VAL
1	C	102	ILE
1	C	119	SER
1	C	120	VAL
1	C	163	LEU
1	C	164	VAL
1	C	169	ASP
1	C	183	SER
1	C	184	SER
1	C	218	GLU
1	C	226	THR
1	C	235	GLU
1	C	238	THR
1	C	242	LEU
1	C	271	GLU
1	C	272	SER
1	D	59	ARG
1	D	111	VAL
1	D	120	VAL
1	D	131	THR
1	D	143	GLU
1	D	148	ARG
1	D	157	SER
1	D	158	THR
1	D	163	LEU
1	D	166	SER
1	D	175	ARG
1	D	179	VAL
1	D	183	SER
1	D	184	SER
1	D	218	GLU
1	D	226	THR
1	D	235	GLU
1	D	238	THR
1	D	242	LEU
1	D	247	ARG
1	D	276	GLU
1	D	292	SER
1	D	296	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	ASN

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$
2	URA	B	401	-	8,8,8	5.76	7 (87%)	10,10,10	3.15	5 (50%)
3	R1P	B	402	-	13,14,14	4.92	7 (53%)	21,21,21	1.62	3 (14%)
3	R1P	C	402	-	13,14,14	5.22	5 (38%)	21,21,21	2.47	7 (33%)
2	URA	C	401	-	8,8,8	4.80	6 (75%)	10,10,10	3.12	6 (60%)
2	URA	A	401	-	8,8,8	5.50	7 (87%)	10,10,10	2.85	5 (50%)
2	URA	D	401	-	8,8,8	4.60	8 (100%)	10,10,10	3.04	5 (50%)
3	R1P	D	402	-	13,14,14	5.33	6 (46%)	21,21,21	1.51	4 (19%)
3	R1P	A	402	-	13,14,14	5.43	6 (46%)	21,21,21	1.20	2 (9%)

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	URA	B	401	-	-	-	0/1/1/1
3	R1P	C	402	-	-	1/6/23/23	0/1/1/1
3	R1P	B	402	-	-	0/6/23/23	0/1/1/1
2	URA	C	401	-	-	-	0/1/1/1
2	URA	A	401	-	-	-	0/1/1/1
2	URA	D	401	-	-	-	0/1/1/1
3	R1P	D	402	-	-	0/6/23/23	0/1/1/1
3	R1P	A	402	-	-	2/6/23/23	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	R1P	C1-C2	-13.23	1.36	1.52
3	A	402	R1P	O4-C1	12.81	1.64	1.41
3	C	402	R1P	C1-C2	-12.69	1.36	1.52
3	A	402	R1P	C1-C2	-12.25	1.37	1.52
3	C	402	R1P	O4-C1	11.83	1.62	1.41
3	B	402	R1P	O4-C1	11.28	1.61	1.41
3	D	402	R1P	O4-C1	10.88	1.60	1.41
3	B	402	R1P	C1-C2	-10.87	1.39	1.52
2	A	401	URA	C2-N1	9.78	1.49	1.36
2	B	401	URA	C2-N1	9.48	1.49	1.36
2	C	401	URA	C2-N1	9.03	1.48	1.36
2	B	401	URA	C2-N3	8.26	1.51	1.37
2	A	401	URA	C2-N3	7.65	1.50	1.37
2	D	401	URA	C2-N1	7.47	1.46	1.36
2	B	401	URA	C6-N1	7.41	1.47	1.36
2	A	401	URA	C6-N1	6.58	1.45	1.36
2	C	401	URA	C2-N3	6.43	1.48	1.37
2	D	401	URA	C2-N3	6.06	1.47	1.37
3	A	402	R1P	O4-C4	-5.91	1.31	1.45
3	D	402	R1P	P-O1	5.86	1.69	1.59
3	B	402	R1P	O4-C4	-5.51	1.32	1.45
2	D	401	URA	C6-N1	5.44	1.44	1.36
3	D	402	R1P	O4-C4	-4.83	1.34	1.45
3	C	402	R1P	O4-C4	-4.62	1.34	1.45
2	C	401	URA	C6-N1	4.52	1.42	1.36
3	B	402	R1P	P-O1	4.39	1.67	1.59
2	C	401	URA	C4-N3	4.16	1.45	1.38
2	B	401	URA	C6-C5	4.09	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	URA	C4-N3	3.90	1.45	1.38
2	D	401	URA	C4-N3	3.87	1.45	1.38
3	C	402	R1P	P-O1	3.73	1.66	1.59
2	A	401	URA	C6-C5	3.67	1.43	1.35
3	A	402	R1P	P-O1	3.61	1.65	1.59
2	B	401	URA	O4-C4	-3.61	1.17	1.24
2	B	401	URA	C4-N3	3.61	1.44	1.38
2	C	401	URA	C6-C5	3.38	1.42	1.35
2	A	401	URA	O4-C4	-3.28	1.18	1.24
2	D	401	URA	C6-C5	3.19	1.42	1.35
3	C	402	R1P	C3-C4	3.04	1.60	1.53
2	B	401	URA	C5-C4	3.04	1.50	1.43
2	C	401	URA	O4-C4	-3.01	1.18	1.24
3	D	402	R1P	C3-C4	2.99	1.60	1.53
2	D	401	URA	O4-C4	-2.92	1.18	1.24
2	D	401	URA	C5-C4	2.80	1.49	1.43
3	B	402	R1P	C3-C4	2.65	1.59	1.53
3	A	402	R1P	O3-C3	-2.63	1.36	1.43
3	A	402	R1P	C3-C4	2.55	1.59	1.53
3	B	402	R1P	O3-C3	-2.42	1.37	1.43
2	D	401	URA	O2-C2	-2.40	1.18	1.23
3	D	402	R1P	O2-C2	2.25	1.48	1.43
2	A	401	URA	C5-C4	2.16	1.48	1.43
3	B	402	R1P	O2-C2	2.07	1.48	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	URA	C4-N3-C2	-6.51	119.24	125.55
2	B	401	URA	C4-N3-C2	-6.22	119.52	125.55
2	C	401	URA	C4-N3-C2	-6.11	119.63	125.55
2	A	401	URA	C4-N3-C2	-5.84	119.89	125.55
3	C	402	R1P	O4-C1-C2	-5.64	97.80	104.98
3	B	402	R1P	O1-C1-C2	5.25	115.17	106.65
3	C	402	R1P	O1-C1-C2	5.01	114.78	106.65
2	A	401	URA	C5-C4-N3	4.78	121.50	114.80
2	B	401	URA	C5-C4-N3	4.18	120.65	114.80
2	D	401	URA	N1-C2-N3	4.12	119.52	115.17
2	B	401	URA	C6-N1-C2	-3.96	119.97	122.40
3	C	402	R1P	O3P-P-O1	3.95	121.26	105.85
2	C	401	URA	O4-C4-C5	-3.92	118.41	125.16
3	C	402	R1P	O3P-P-O1P	-3.63	96.71	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	URA	N1-C2-N3	3.59	118.96	115.17
3	C	402	R1P	O1-P-O1P	-3.59	96.54	109.33
2	D	401	URA	C5-C4-N3	3.51	119.71	114.80
2	C	401	URA	C5-C4-N3	3.50	119.70	114.80
2	C	401	URA	C6-N1-C2	-3.29	120.38	122.40
3	D	402	R1P	C1-C2-C3	3.27	106.36	102.29
2	A	401	URA	O4-C4-C5	-3.23	119.59	125.16
2	B	401	URA	O4-C4-C5	-3.14	119.75	125.16
2	C	401	URA	N1-C2-N3	3.10	118.44	115.17
2	D	401	URA	O4-C4-C5	-2.93	120.11	125.16
3	A	402	R1P	O1-C1-C2	2.87	111.31	106.65
3	A	402	R1P	O4-C1-O1	2.78	114.46	109.16
2	A	401	URA	C6-N1-C2	-2.78	120.70	122.40
3	B	402	R1P	C1-C2-C3	2.76	105.73	102.29
3	C	402	R1P	C1-C2-C3	-2.71	98.92	102.29
3	D	402	R1P	O1-C1-C2	2.66	110.96	106.65
2	D	401	URA	C6-N1-C2	-2.58	120.81	122.40
3	C	402	R1P	P-O1-C1	-2.41	117.07	123.54
2	C	401	URA	O2-C2-N1	-2.33	120.38	122.79
3	B	402	R1P	C2-C3-C4	-2.19	98.38	102.61
3	D	402	R1P	O4-C1-C2	2.07	107.61	104.98
2	A	401	URA	N1-C2-N3	2.07	117.35	115.17
3	D	402	R1P	C5-C4-C3	-2.00	110.36	115.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

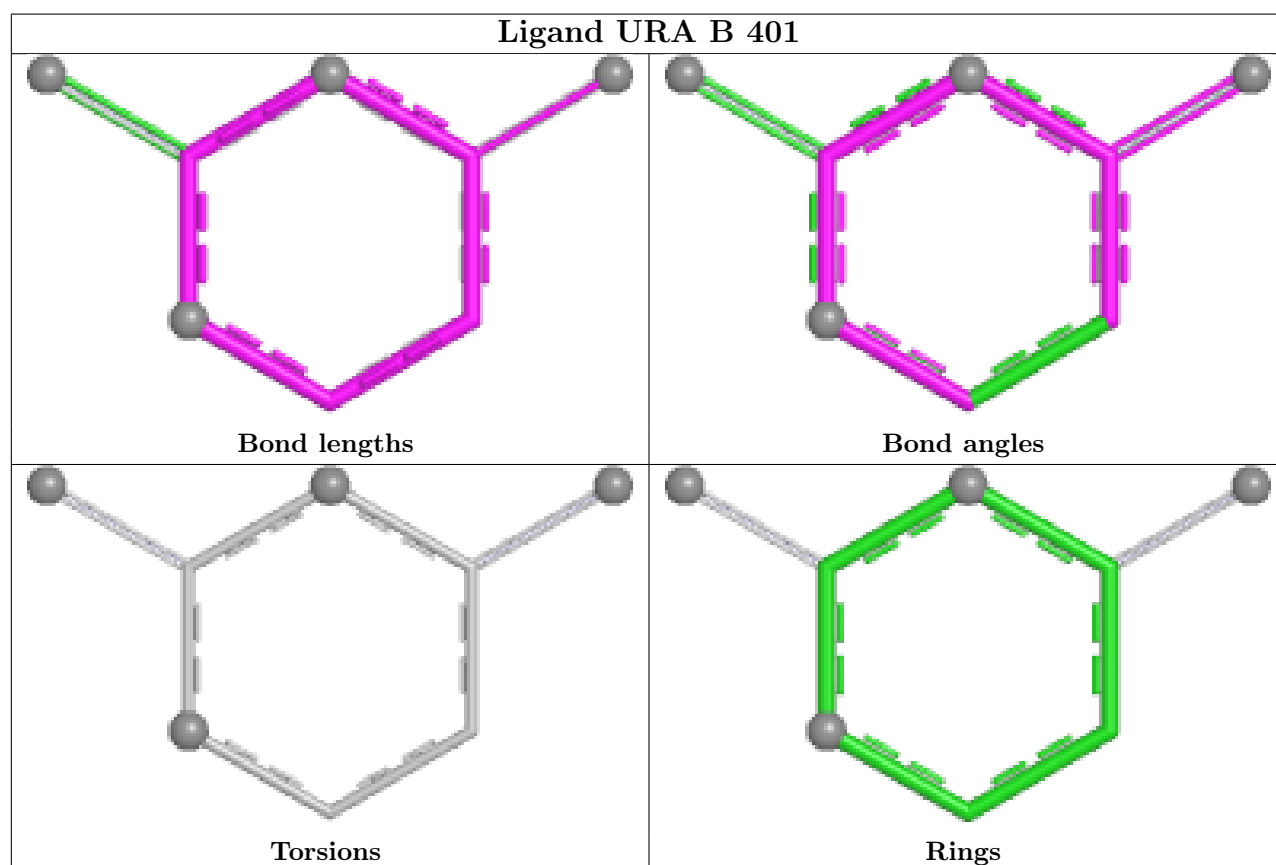
Mol	Chain	Res	Type	Atoms
3	A	402	R1P	C3-C4-C5-O5
3	A	402	R1P	O4-C4-C5-O5
3	C	402	R1P	C1-O1-P-O2P

There are no ring outliers.

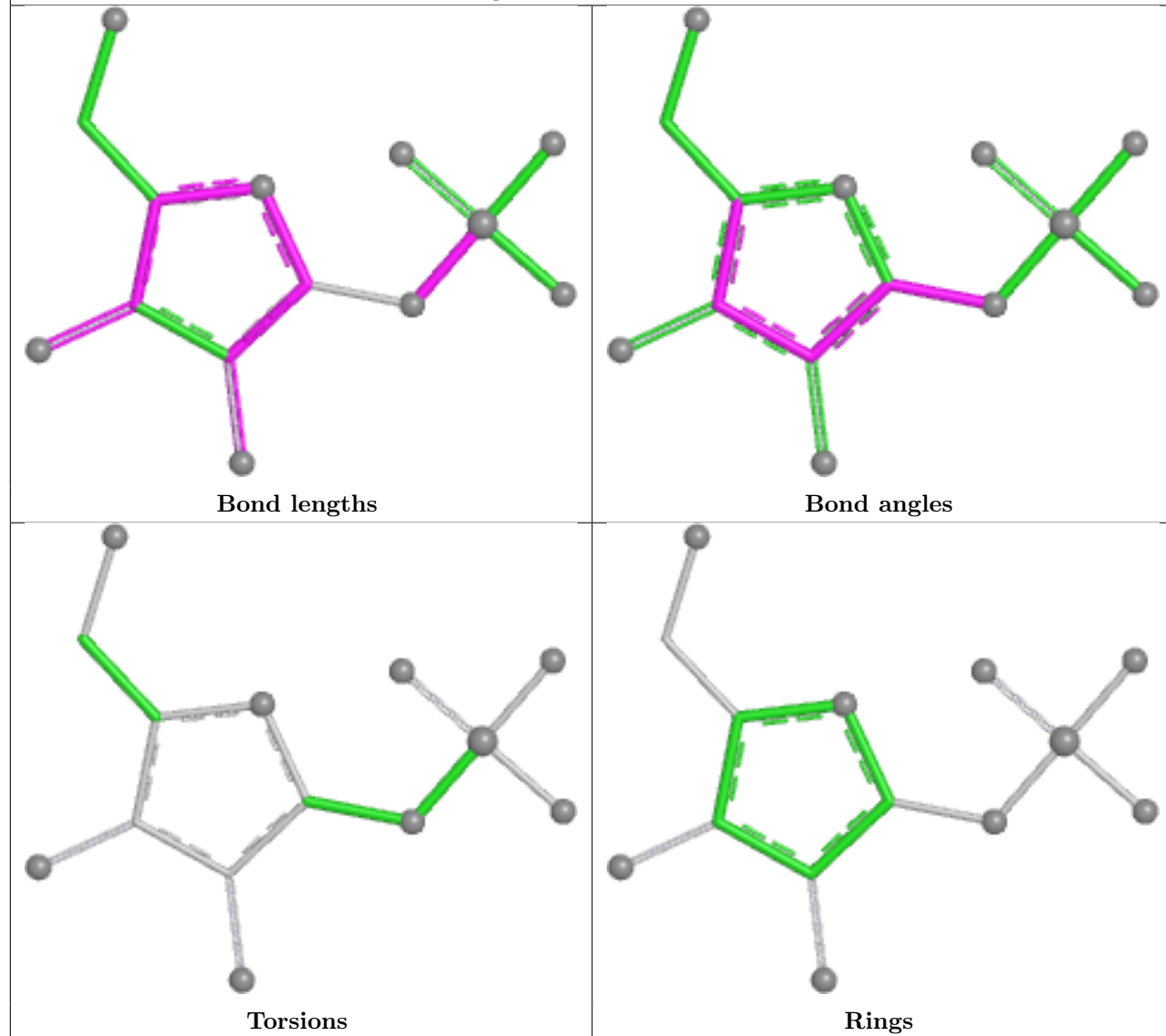
4 monomers are involved in 9 short contacts:

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

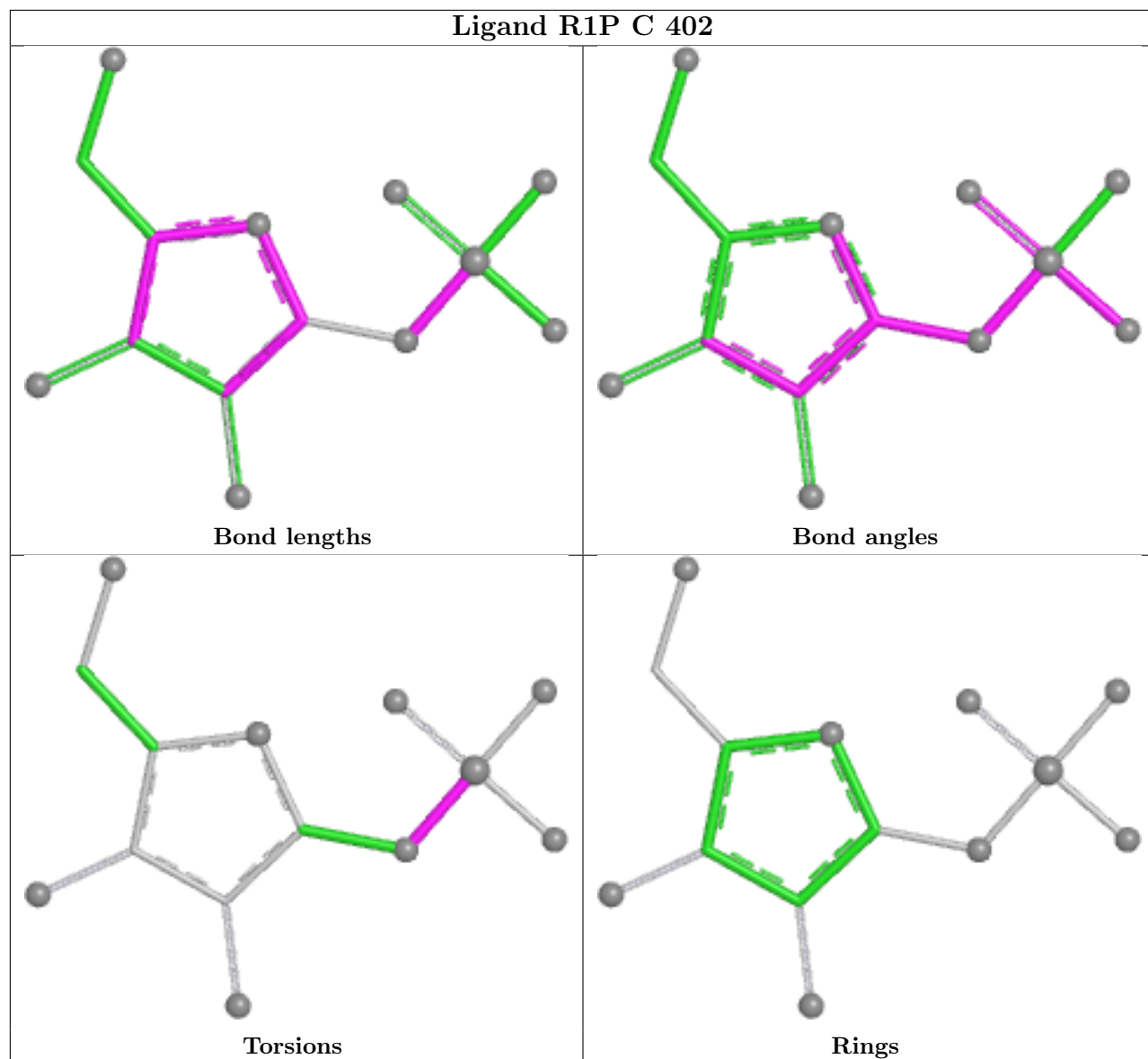
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

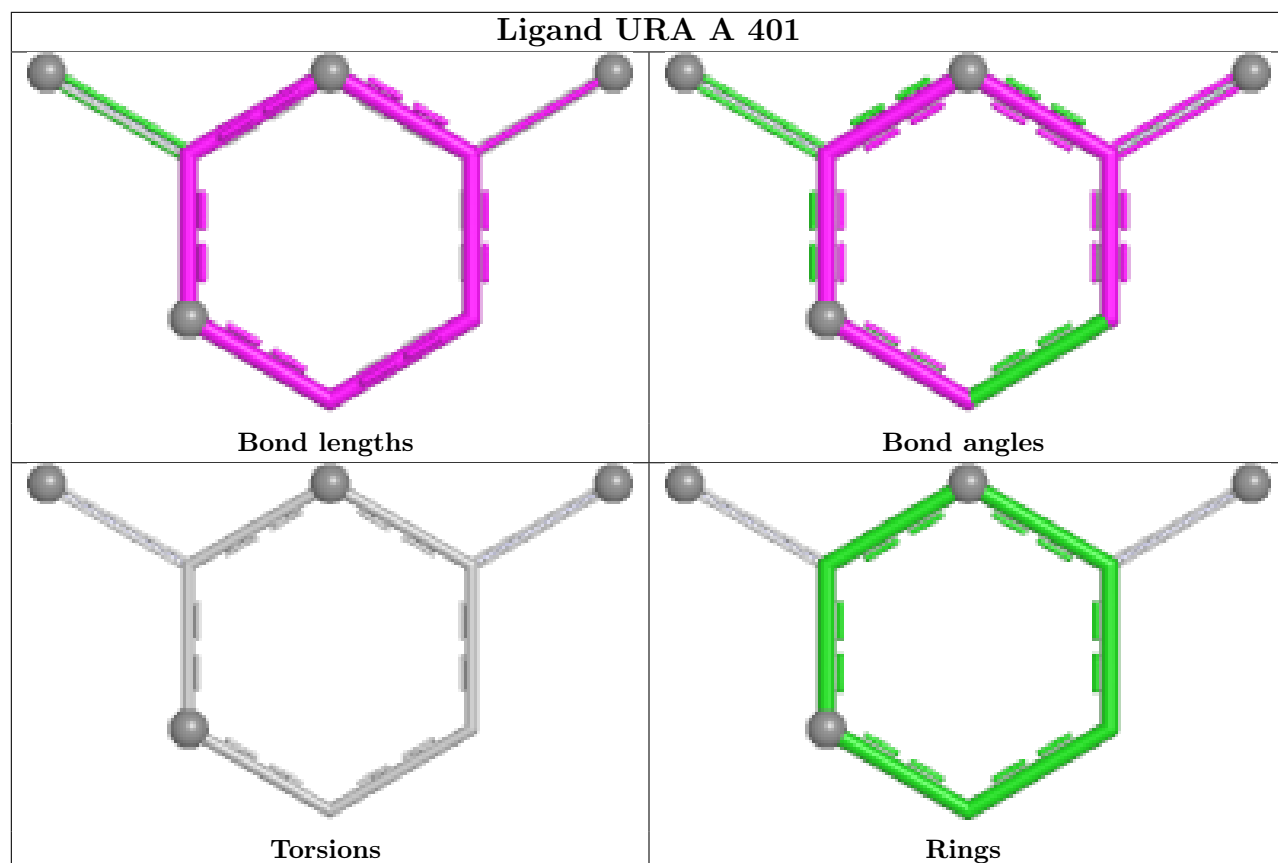
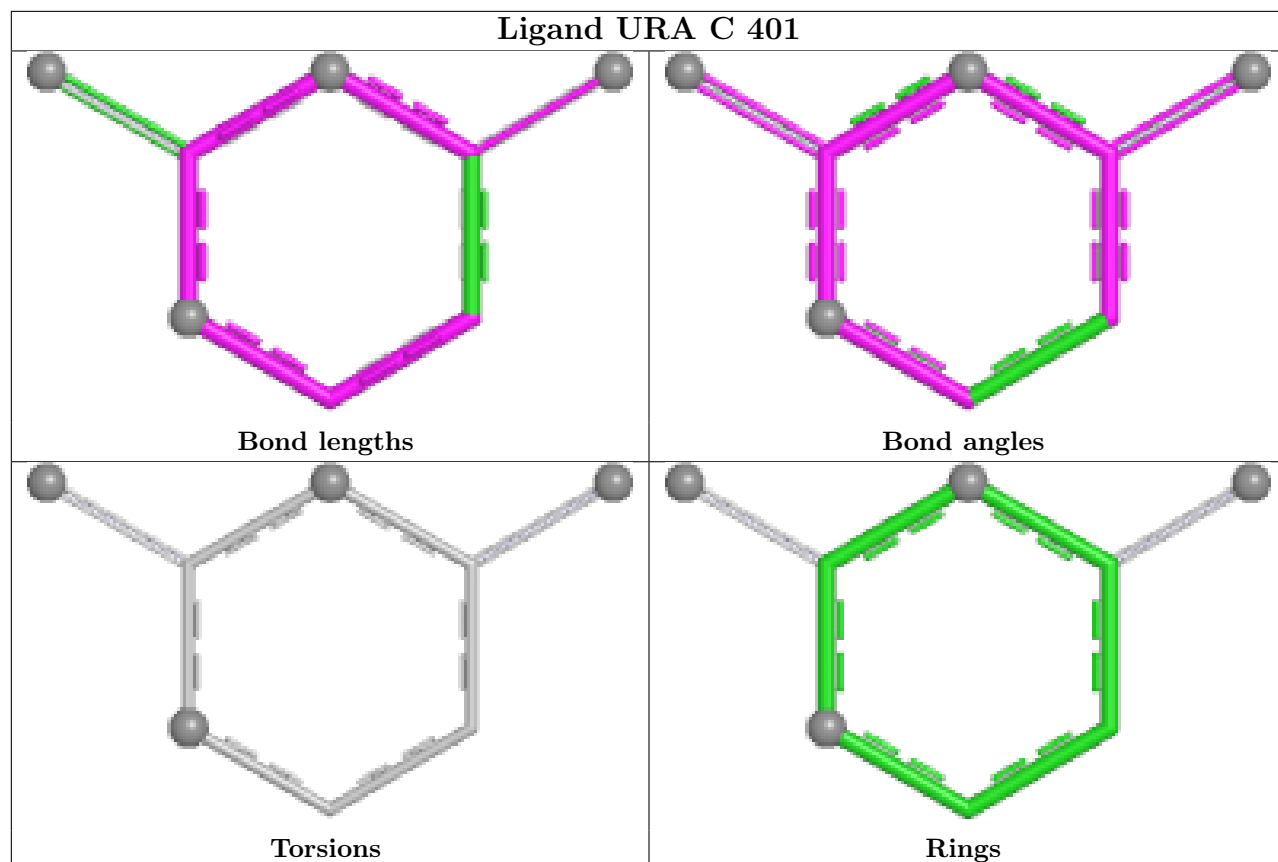


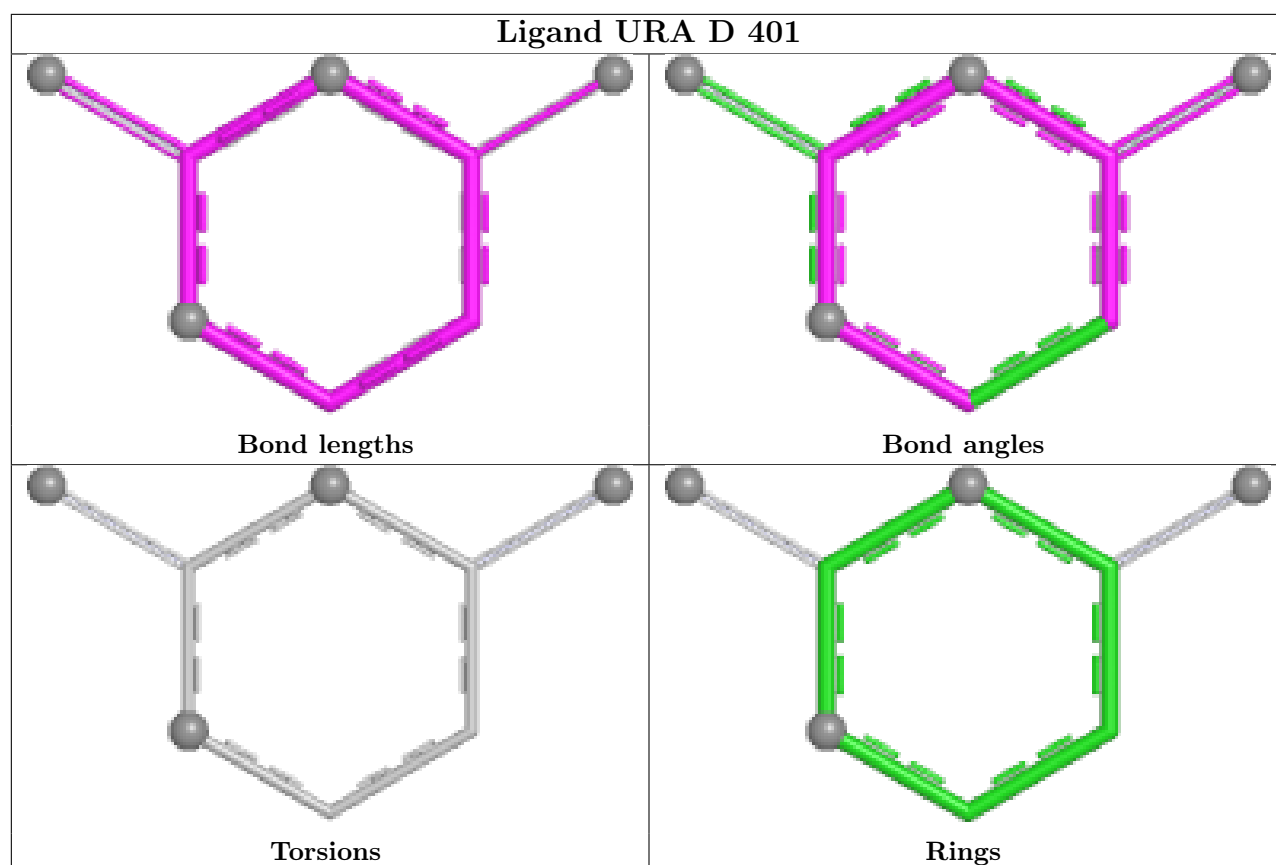
Ligand R1P B 402



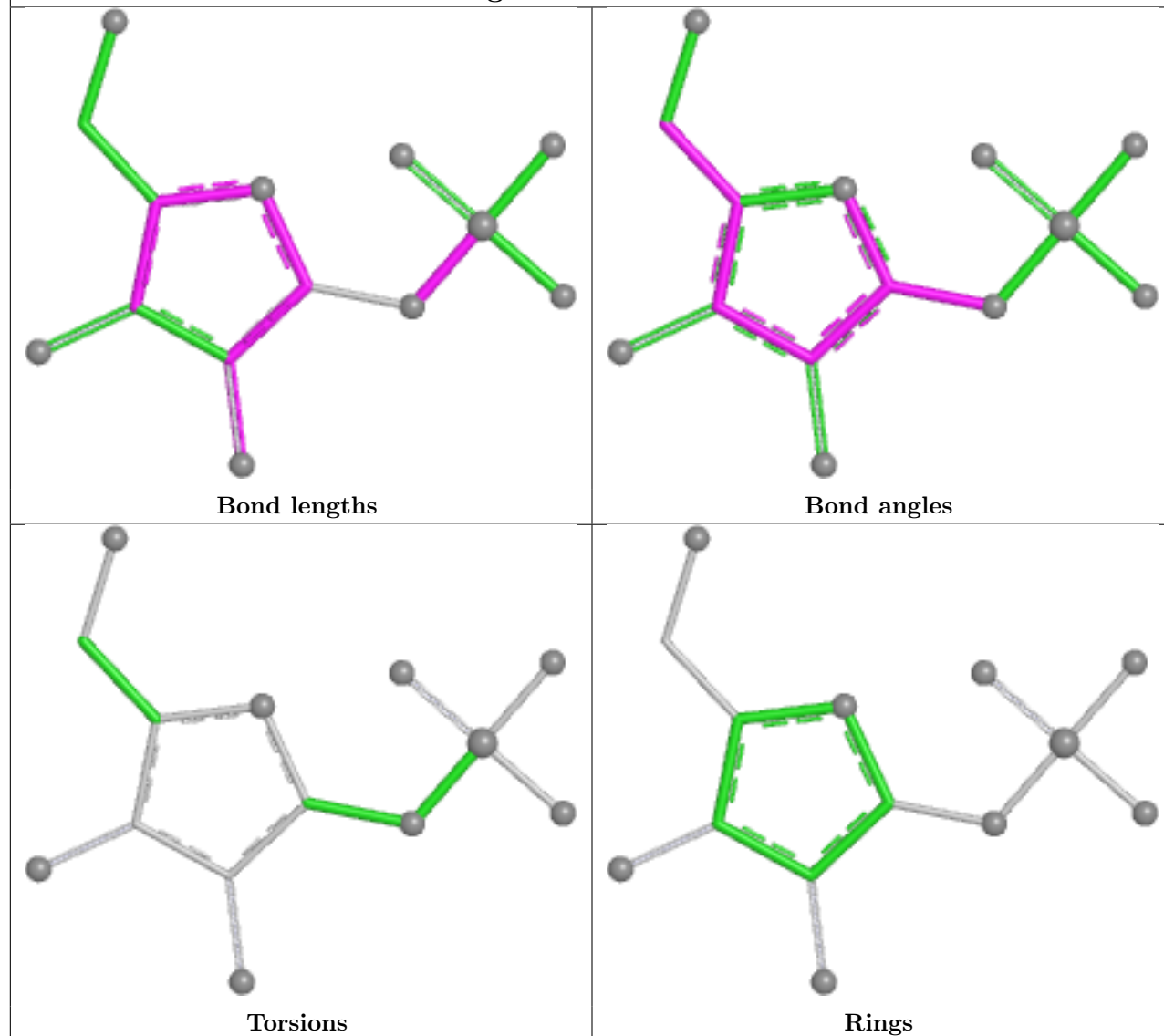
Ligand R1P C 402

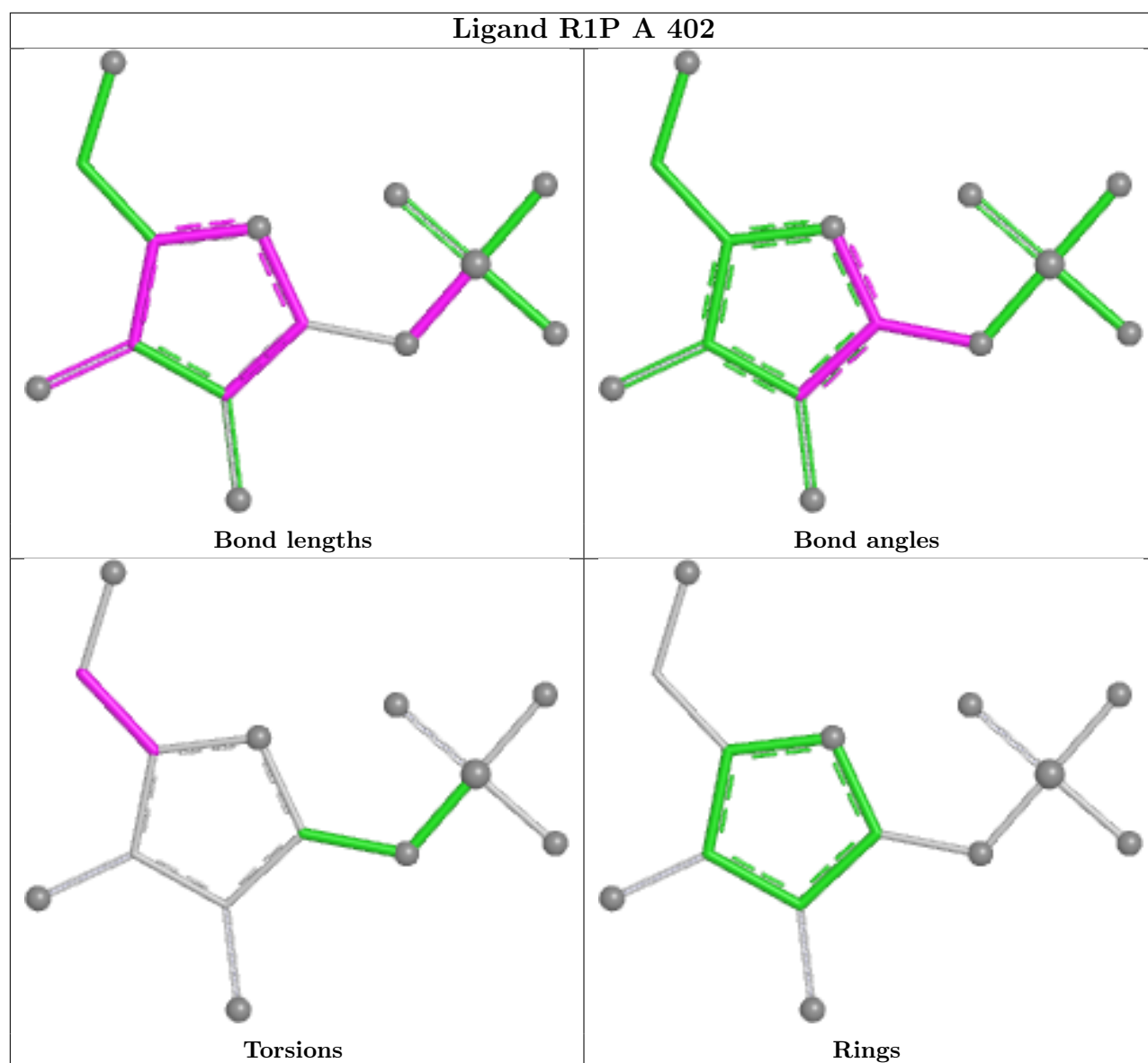






Ligand R1P D 402





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	287/309 (92%)	0.75	29 (10%)	12 10	23, 39, 73, 103	0
1	B	286/309 (92%)	1.14	53 (18%)	3 2	23, 39, 78, 125	0
1	C	287/309 (92%)	0.76	27 (9%)	14 12	20, 40, 70, 130	0
1	D	288/309 (93%)	1.12	49 (17%)	4 3	19, 41, 76, 115	0
All	All	1148/1236 (92%)	0.94	158 (13%)	6 5	19, 40, 75, 130	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	GLU	6.2
1	B	185	ASP	5.6
1	C	8	ALA	5.2
1	B	266	SER	5.0
1	D	297	ALA	4.9
1	B	97	ASN	4.9
1	C	139	PRO	4.6
1	A	182	ALA	4.5
1	C	133	ASN	4.4
1	D	141	ALA	4.4
1	B	296	ASP	4.4
1	B	184	SER	4.4
1	B	190	ARG	4.3
1	B	187	ASP	4.2
1	B	143	GLU	4.2
1	D	267	GLY	4.1
1	C	179	VAL	4.0
1	B	142	SER	3.9
1	B	189	LEU	3.9
1	B	182	ALA	3.9
1	D	97	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	103	ILE	3.9
1	A	188	ALA	3.8
1	A	10	PRO	3.8
1	A	185	ASP	3.8
1	C	148	ARG	3.7
1	D	114	GLU	3.7
1	D	291	VAL	3.6
1	D	288	GLN	3.6
1	A	184	SER	3.6
1	A	191	VAL	3.6
1	D	286	VAL	3.6
1	D	209	LEU	3.5
1	D	13	SER	3.5
1	A	9	MET	3.5
1	C	142	SER	3.5
1	C	143	GLU	3.4
1	D	143	GLU	3.4
1	D	262	ALA	3.4
1	D	144	GLU	3.4
1	C	141	ALA	3.4
1	D	269	ILE	3.4
1	D	142	SER	3.4
1	C	187	ASP	3.4
1	B	288	GLN	3.4
1	B	186	CYS	3.3
1	D	287	LEU	3.3
1	A	190	ARG	3.3
1	B	175	ARG	3.3
1	B	181	ALA	3.3
1	D	176	ALA	3.3
1	D	10	PRO	3.3
1	D	42	VAL	3.3
1	B	188	ALA	3.3
1	D	185	ASP	3.2
1	C	145	ASP	3.1
1	B	148	ARG	3.1
1	B	191	VAL	3.1
1	D	113	GLU	3.1
1	C	28	ALA	3.0
1	D	266	SER	3.0
1	A	143	GLU	3.0
1	B	113	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	144	GLU	3.0
1	B	290	ILE	3.0
1	C	147	TYR	3.0
1	C	175	ARG	3.0
1	D	189	LEU	2.9
1	D	29	ASN	2.9
1	D	73	VAL	2.8
1	B	220	LEU	2.8
1	C	271	GLU	2.8
1	D	253	GLN	2.8
1	B	145	ASP	2.8
1	D	184	SER	2.7
1	A	20	LEU	2.7
1	D	296	ASP	2.7
1	D	164	VAL	2.7
1	C	181	ALA	2.7
1	A	187	ASP	2.7
1	C	13	SER	2.7
1	A	168	GLU	2.7
1	B	45	GLN	2.6
1	B	265	LEU	2.6
1	B	295	LEU	2.6
1	D	268	GLN	2.6
1	A	178	PRO	2.5
1	B	199	ALA	2.5
1	D	182	ALA	2.5
1	B	50	GLY	2.5
1	C	138	PHE	2.5
1	B	51	HIS	2.5
1	D	188	ALA	2.5
1	B	11	THR	2.5
1	D	186	CYS	2.4
1	B	144	GLU	2.4
1	B	207	GLY	2.4
1	A	14	ASP	2.4
1	A	23	ARG	2.4
1	A	113	GLU	2.4
1	D	159	LEU	2.4
1	C	140	GLY	2.4
1	B	49	GLU	2.4
1	D	140	GLY	2.3
1	C	209	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	146	CYS	2.3
1	B	221	VAL	2.3
1	C	197	ALA	2.3
1	A	112	ARG	2.3
1	B	13	SER	2.3
1	B	183	SER	2.3
1	B	14	ASP	2.3
1	A	144	GLU	2.3
1	A	186	CYS	2.3
1	A	13	SER	2.3
1	B	120	VAL	2.3
1	A	97	ASN	2.2
1	D	256	ALA	2.2
1	D	187	ASP	2.2
1	D	258	VAL	2.2
1	D	264	ARG	2.2
1	D	139	PRO	2.2
1	A	51	HIS	2.2
1	A	180	ILE	2.2
1	C	204	SER	2.2
1	A	181	ALA	2.2
1	C	256	ALA	2.2
1	B	200	CYS	2.2
1	C	186	CYS	2.2
1	A	266	SER	2.2
1	A	253	GLN	2.1
1	D	110	ALA	2.1
1	A	200	CYS	2.1
1	B	154	PRO	2.1
1	A	16	THR	2.1
1	C	265	LEU	2.1
1	B	114	GLU	2.1
1	D	112	ARG	2.1
1	D	148	ARG	2.1
1	D	177	GLU	2.1
1	B	146	CYS	2.1
1	C	134	PRO	2.1
1	B	111	VAL	2.1
1	D	95	VAL	2.1
1	B	170	LYS	2.1
1	B	152	VAL	2.1
1	B	173	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	24	ALA	2.1
1	B	171	LEU	2.1
1	D	265	LEU	2.1
1	B	172	THR	2.1
1	D	173	ALA	2.0
1	B	224	LEU	2.0
1	B	158	THR	2.0
1	B	219	LYS	2.0
1	A	61	PHE	2.0
1	B	229	PRO	2.0
1	D	203	TYR	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](#)

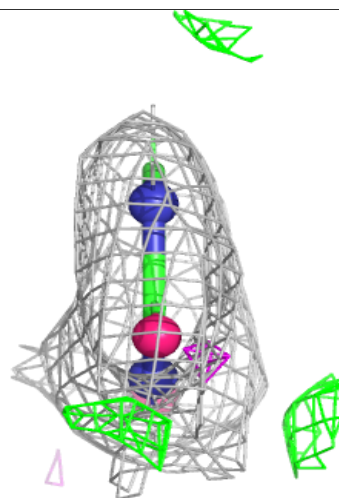
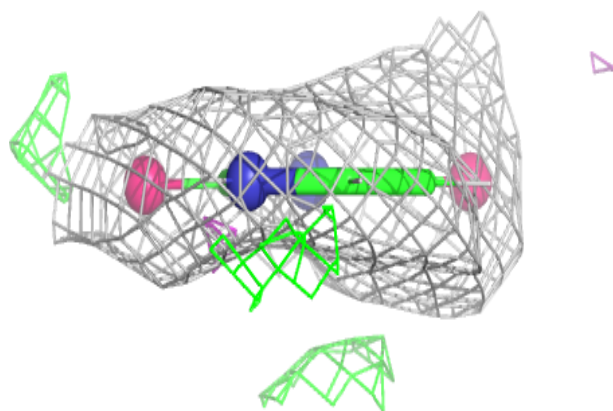
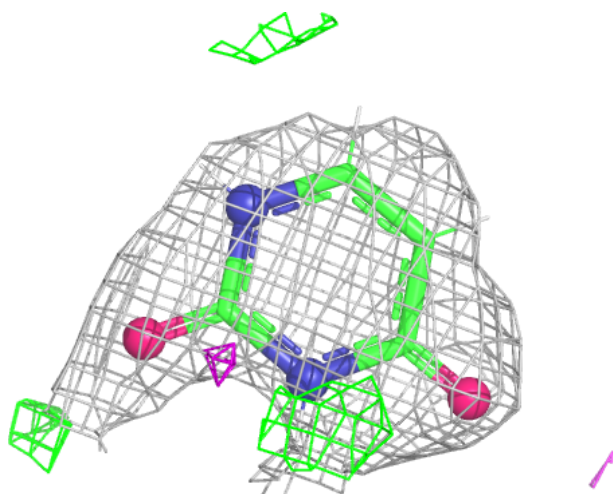
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	URA	B	401	8/8	0.86	0.18	28,35,42,44	0
2	URA	C	401	8/8	0.88	0.15	29,34,44,48	0
2	URA	A	401	8/8	0.89	0.13	28,37,44,47	0
3	R1P	C	402	14/14	0.90	0.11	24,37,45,49	0
2	URA	D	401	8/8	0.91	0.12	28,33,37,44	0
3	R1P	D	402	14/14	0.92	0.09	17,26,42,44	0
3	R1P	A	402	14/14	0.96	0.09	19,33,40,49	0
3	R1P	B	402	14/14	0.96	0.08	20,31,42,47	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.

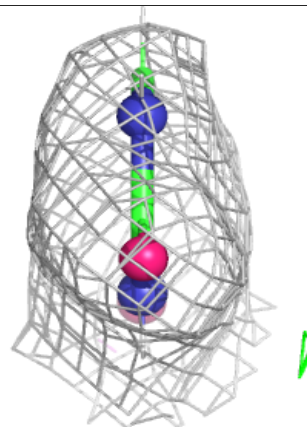
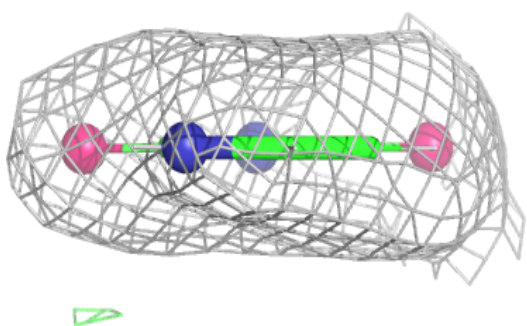
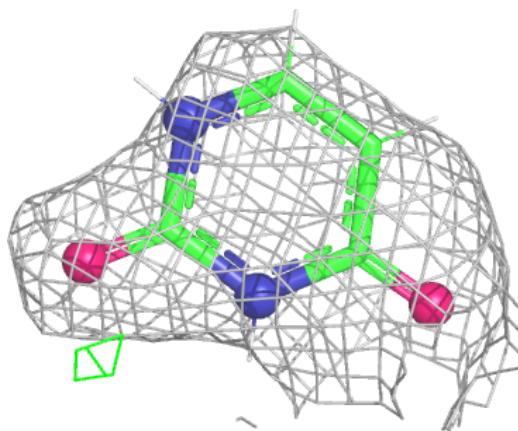
Electron density around URA B 401:

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



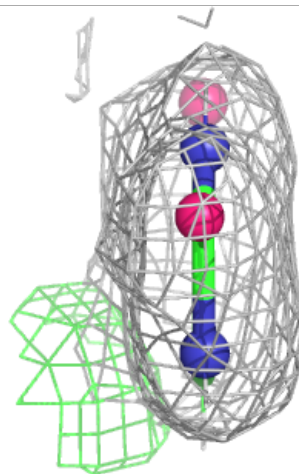
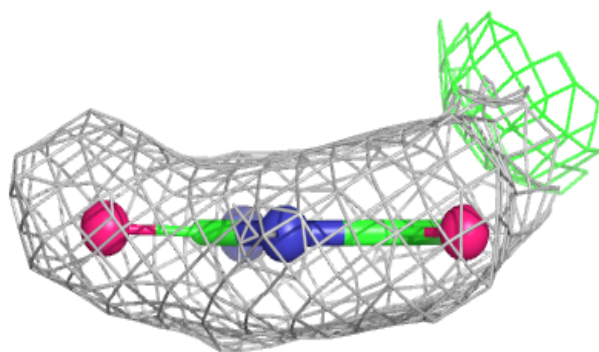
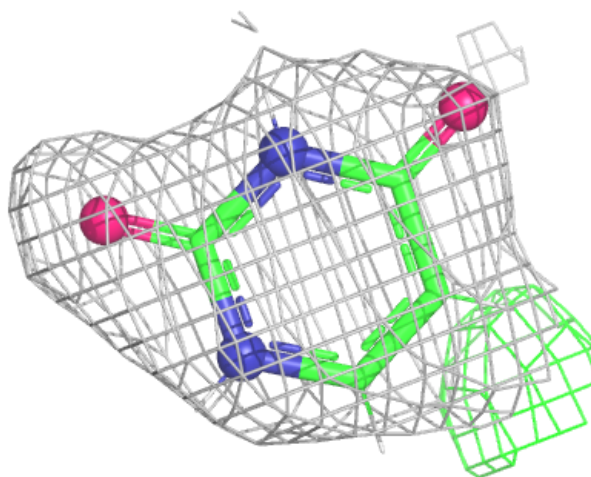
Electron density around URA C 401:

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



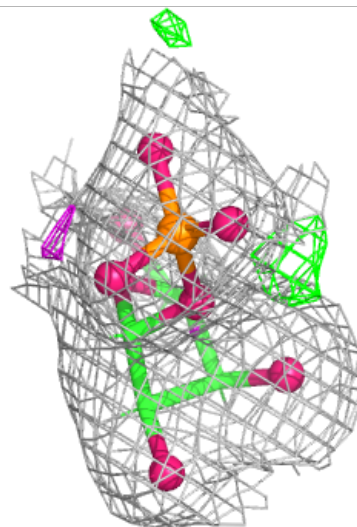
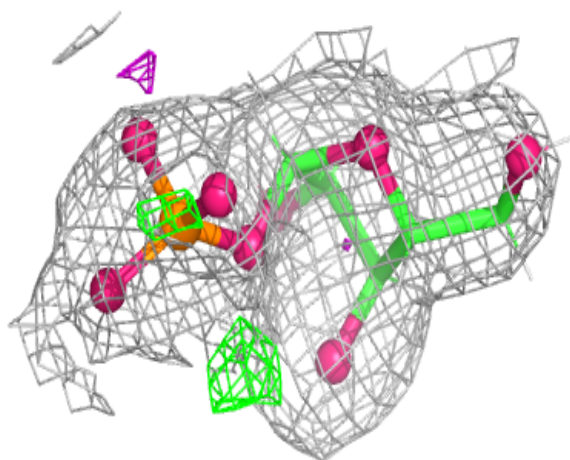
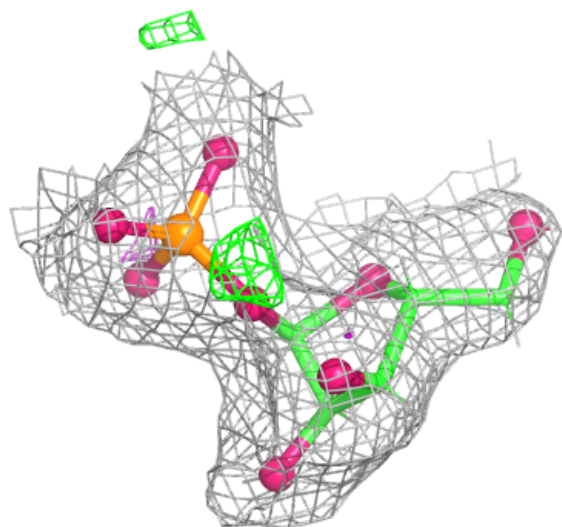
Electron density around URA A 401:

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



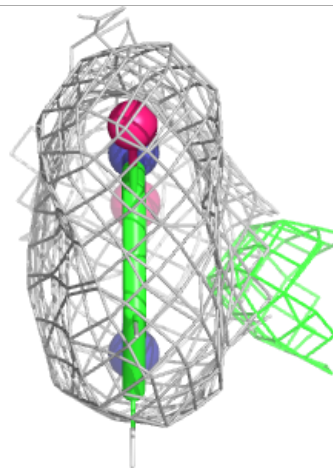
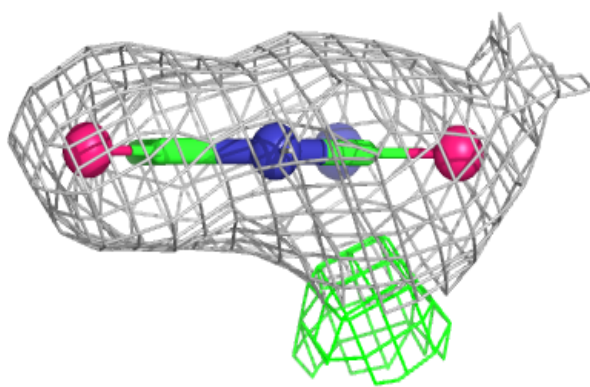
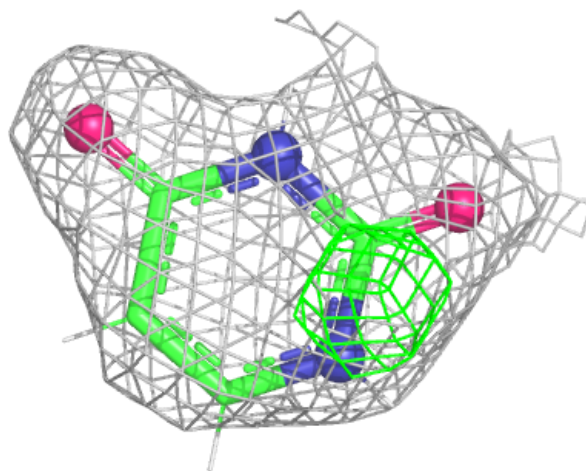
Electron density around R1P C 402:

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



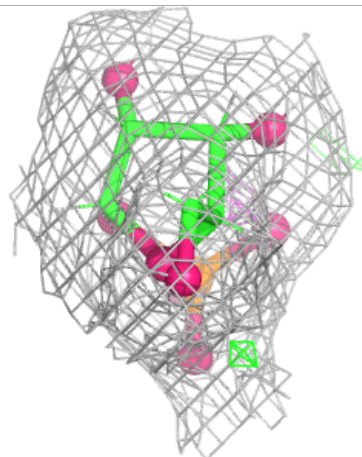
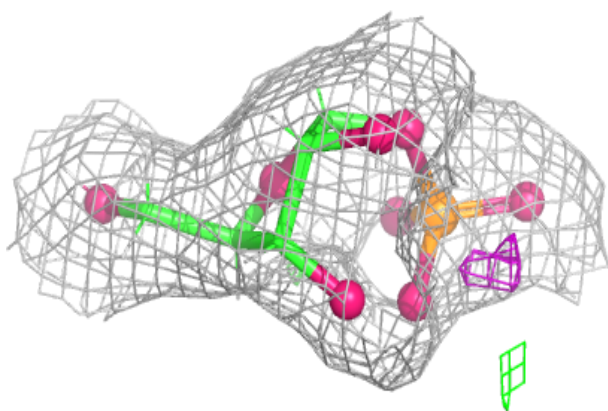
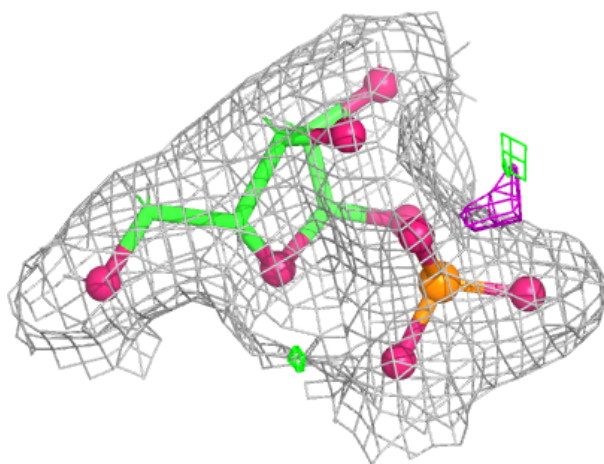
Electron density around URA D 401:

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



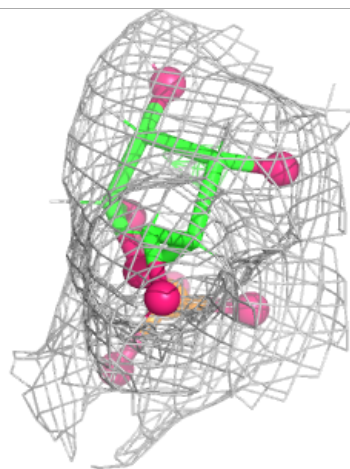
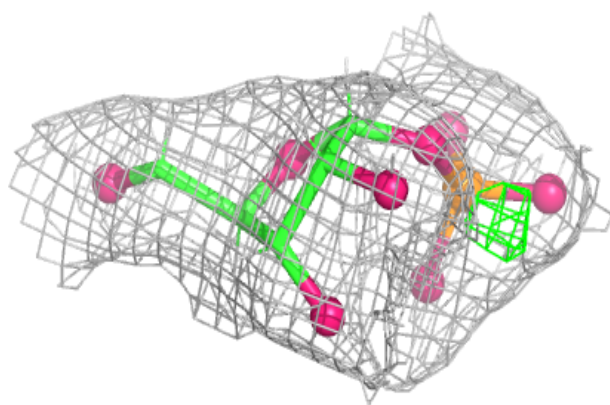
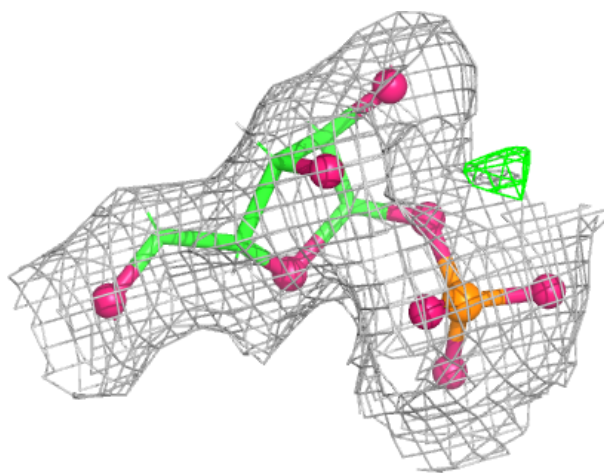
Electron density around R1P D 402:

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



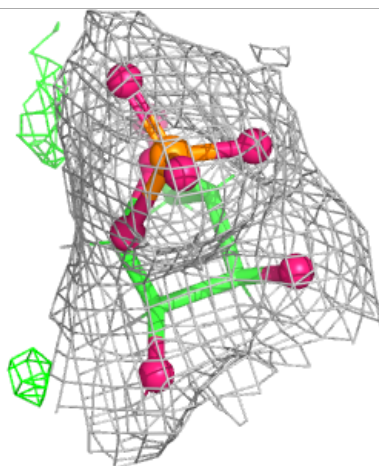
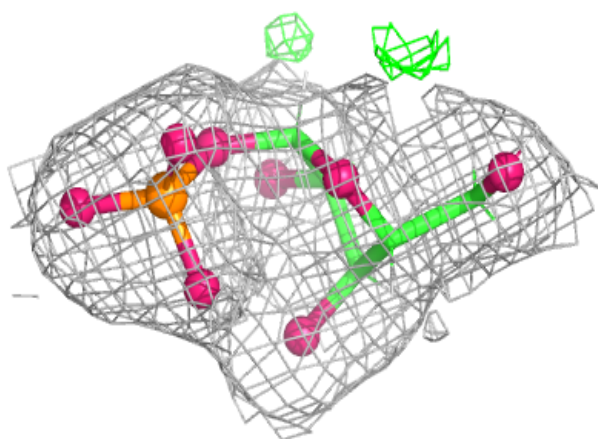
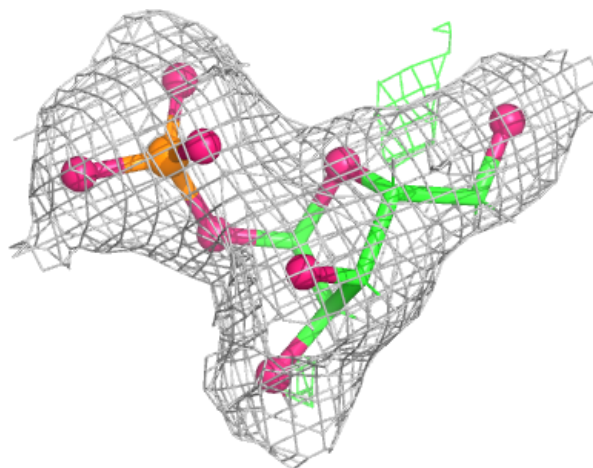
Electron density around R1P A 402:

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



Electron density around R1P 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.