



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:22 AM UTC

PDB ID : 3QQS / pdb_00003qqs
Title : Anthranilate phosphoribosyltransferase (TRPD) from Mycobacterium tuberculosis (complex with inhibitor ACS172)
Authors : Castell, A.; Short, F.L.; Lott, J.S.; TB Structural Genomics Consortium (TB-SGC)
Deposited on : 2011-02-16
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

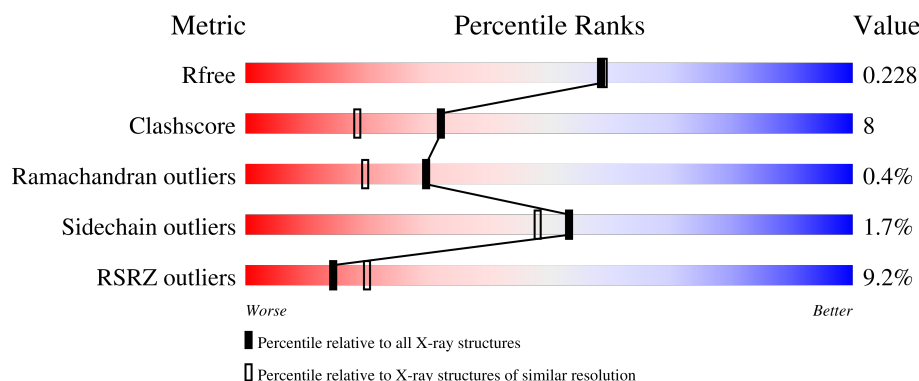
1 Overall quality at a glance

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	377	3% 82% 9% 8%
1	B	377	2% 81% 11% 8%
1	C	377	16% 71% 19% 9%
1	D	377	12% 73% 14% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10712 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2505	1566	465	465	9			
1	B	346	Total	C	N	O	S	0	0	0
			2505	1566	465	465	9			
1	C	343	Total	C	N	O	S	0	0	0
			2482	1552	461	460	9			
1	D	330	Total	C	N	O	S	0	0	0
			2406	1508	448	441	9			

There are 32 discrepancies between the modelled and reference sequences:

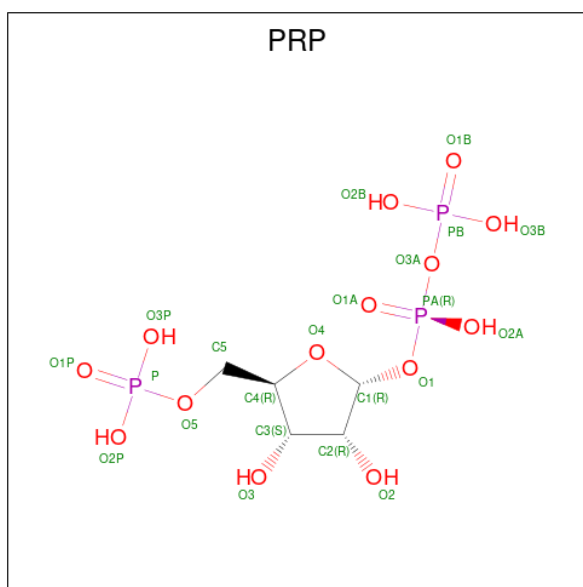
Chain	Residue	Modelled	Actual	Comment	Reference
A	371	LEU	-	expression tag	UNP P66992
A	372	GLU	-	expression tag	UNP P66992
A	373	HIS	-	expression tag	UNP P66992
A	374	HIS	-	expression tag	UNP P66992
A	375	HIS	-	expression tag	UNP P66992
A	376	HIS	-	expression tag	UNP P66992
A	377	HIS	-	expression tag	UNP P66992
A	378	HIS	-	expression tag	UNP P66992
B	371	LEU	-	expression tag	UNP P66992
B	372	GLU	-	expression tag	UNP P66992
B	373	HIS	-	expression tag	UNP P66992
B	374	HIS	-	expression tag	UNP P66992
B	375	HIS	-	expression tag	UNP P66992
B	376	HIS	-	expression tag	UNP P66992
B	377	HIS	-	expression tag	UNP P66992
B	378	HIS	-	expression tag	UNP P66992
C	371	LEU	-	expression tag	UNP P66992
C	372	GLU	-	expression tag	UNP P66992
C	373	HIS	-	expression tag	UNP P66992
C	374	HIS	-	expression tag	UNP P66992
C	375	HIS	-	expression tag	UNP P66992

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Chain	Residue	Modelled	Actual	Comment	Reference
C	376	HIS	-	expression tag	UNP P66992
C	377	HIS	-	expression tag	UNP P66992
C	378	HIS	-	expression tag	UNP P66992
D	371	LEU	-	expression tag	UNP P66992
D	372	GLU	-	expression tag	UNP P66992
D	373	HIS	-	expression tag	UNP P66992
D	374	HIS	-	expression tag	UNP P66992
D	375	HIS	-	expression tag	UNP P66992
D	376	HIS	-	expression tag	UNP P66992
D	377	HIS	-	expression tag	UNP P66992
D	378	HIS	-	expression tag	UNP P66992

- Molecule 2 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (CCD ID: PRP) (formula: $C_5H_{13}O_{14}P_3$).

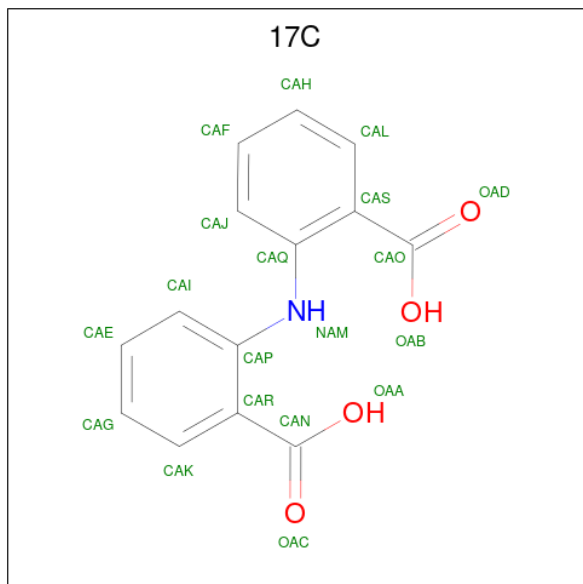


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			22	5	14	3		
2	B	1	Total	C	O	P	0	0
			22	5	14	3		
2	C	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

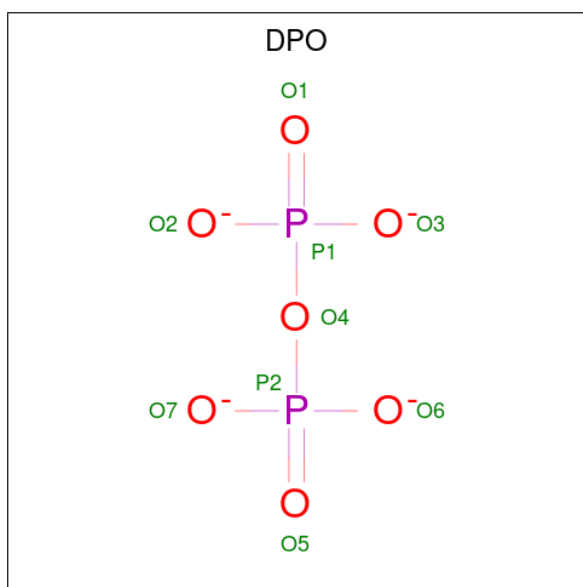
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 2,2'-iminodibenzoic acid (CCD ID: 17C) (formula: C₁₄H₁₁NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 19 14 1 4	0	0
4	B	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	D	1	Total C N O 19 14 1 4	0	0
4	D	1	Total C N O 19 14 1 4	0	0

- Molecule 5 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			9	7	2		

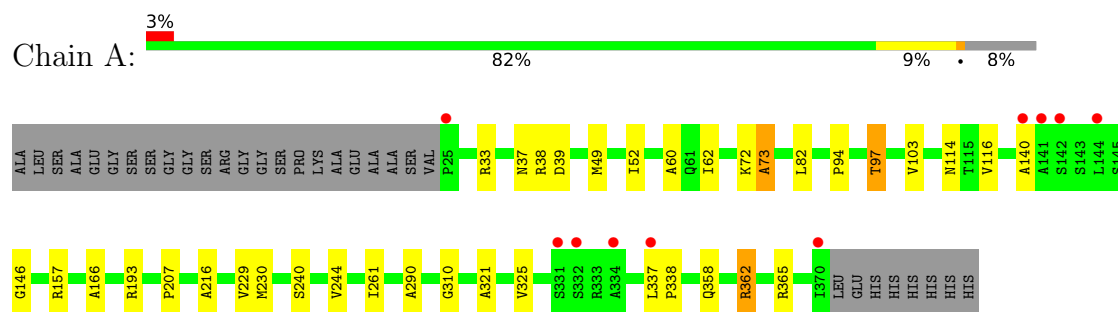
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	B	176	Total	O	0	0
			176	176		
6	C	111	Total	O	0	0
			111	111		
6	D	123	Total	O	0	0
			123	123		

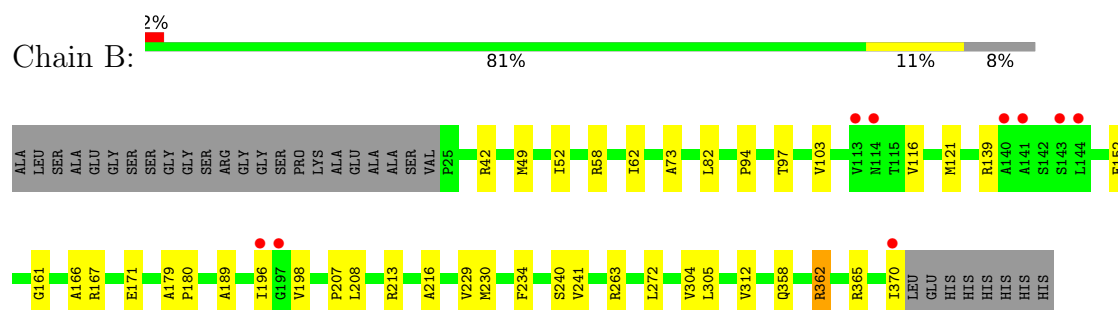
3 Residue-property plots [i](#)

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.

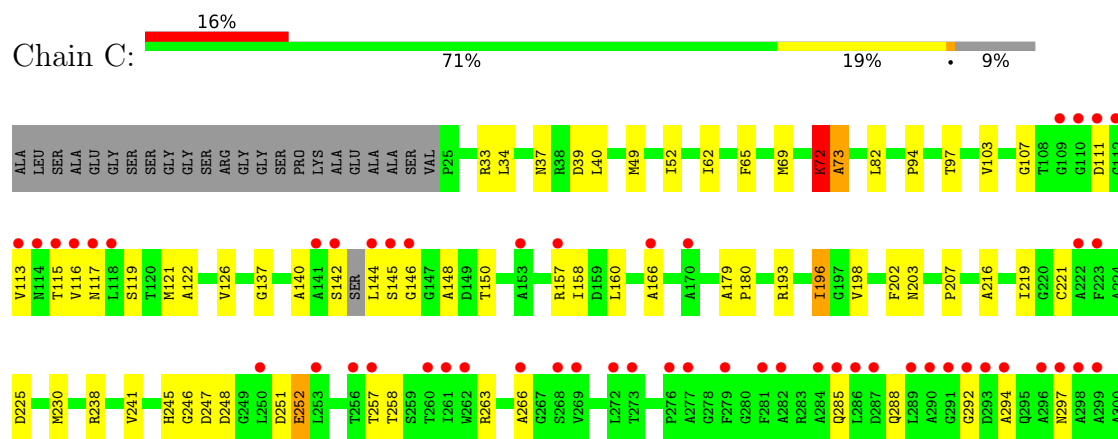
- Molecule 1: Anthranilate phosphoribosyltransferase



- Molecule 1: Anthranilate phosphoribosyltransferase

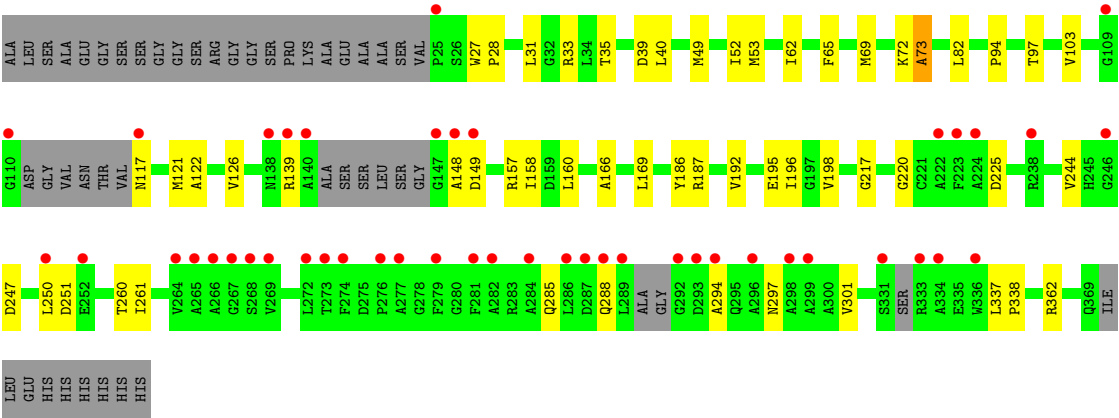


- Molecule 1: Anthranilate phosphoribosyltransferase





● Molecule 1: Anthranilate phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.93Å 78.21Å 101.70Å 90.00° 111.01° 90.00°	Depositor
Resolution (Å)	88.75 – 1.97 88.75 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.0 (88.75-1.97) 99.0 (88.75-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.259 (Not available) , 0.228	Depositor DCC
R_{free} test set	4846 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10712	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 81.25 % 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 3.7047e-07. 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: DPO, MG, 17C, PRP

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	0.82	1/2553 (0.0%)	0.97	2/3483 (0.1%)
1	B	0.81	0/2553	0.97	4/3483 (0.1%)
1	C	0.70	1/2529 (0.0%)	0.95	3/3449 (0.1%)
1	D	0.71	0/2450	0.96	0/3336
All	All	0.76	2/10085 (0.0%)	0.96	9/13751 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	VAL	C-O	-6.57	1.16	1.24
1	C	72	LYS	C-O	-5.60	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	CA-C-N	-5.23	114.57	119.85
1	B	213	ARG	C-N-CA	-5.23	114.57	119.85
1	C	310	GLY	CA-C-N	5.03	125.06	119.32
1	C	310	GLY	C-N-CA	5.03	125.06	119.32
1	A	310	GLY	CA-C-N	5.03	124.63	119.05
1	A	310	GLY	C-N-CA	5.03	124.63	119.05
1	C	137	GLY	N-CA-C	5.01	117.99	110.18
1	B	161	GLY	CA-C-N	5.00	124.44	119.24
1	B	161	GLY	C-N-CA	5.00	124.44	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2500	21	0
1	B	2505	0	2500	26	0
1	C	2482	0	2476	61	0
1	D	2406	0	2401	37	0
2	A	22	0	8	0	0
2	B	22	0	8	0	0
2	C	22	0	8	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
4	A	19	0	9	4	0
4	B	19	0	9	2	0
4	C	57	0	27	5	0
4	D	38	0	18	10	0
5	D	9	0	0	0	0
6	A	191	0	0	3	0
6	B	176	0	0	3	0
6	C	111	0	0	3	0
6	D	123	0	0	1	0
All	All	10712	0	9964	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:MET:HE3	1:C:82:LEU:HD22	1.44	1.00
1:D:49:MET:HE2	1:D:82:LEU:HD22	1.55	0.89
1:A:362:ARG:HG3	1:A:365:ARG:NH2	1.92	0.85
1:C:65:PHE:CZ	1:C:69:MET:HE3	2.17	0.78
1:C:193:ARG:HD2	6:C:532:HOH:O	1.83	0.77
1:C:97:THR:HG23	1:C:166:ALA:HB1	1.67	0.76
1:C:117:ASN:ND2	1:C:150:THR:OG1	2.19	0.75
4:D:403:17C:CAJ	4:D:403:17C:HAI	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG12	1:B:216:ALA:HB3	1.71	0.72
1:A:358:GLN:O	1:A:362:ARG:HD3	1.93	0.69
1:B:229:VAL:HG23	6:B:532:HOH:O	1.91	0.69
4:D:402:17C:CAI	4:D:402:17C:HAJ	2.21	0.69
1:A:103:VAL:HG12	1:A:216:ALA:HB3	1.75	0.68
1:D:285:GLN:HB2	1:D:288:GLN:HB2	1.75	0.68
1:C:49:MET:CE	1:C:82:LEU:HD22	2.23	0.68
1:A:229:VAL:HG23	6:A:524:HOH:O	1.92	0.67
4:D:402:17C:CAJ	4:D:402:17C:HAI	2.24	0.66
1:C:342:GLU:HA	1:C:345:ARG:NH1	2.12	0.65
1:C:40:LEU:HD11	1:C:69:MET:HE1	1.78	0.65
1:C:116:VAL:HA	1:C:297:ASN:ND2	2.12	0.65
4:D:402:17C:HAJ	4:D:402:17C:HAI	1.79	0.64
1:C:225:ASP:HB3	6:C:605:HOH:O	1.98	0.62
1:C:207:PRO:HG2	1:C:230:MET:HE1	1.81	0.62
1:C:97:THR:CG2	1:C:166:ALA:HB1	2.31	0.61
1:B:94:PRO:O	1:B:97:THR:HG22	2.01	0.61
1:C:238:ARG:NH2	1:C:266:ALA:O	2.33	0.61
4:D:403:17C:CAJ	4:D:403:17C:CAI	2.78	0.61
1:D:121:MET:HG2	1:D:301:VAL:HG22	1.84	0.60
4:A:404:17C:HAJ	4:A:404:17C:HAI	1.84	0.59
1:B:116:VAL:HG22	1:B:121:MET:CE	2.33	0.59
1:C:246:GLY:C	1:C:248:ASP:H	2.09	0.58
1:C:148:ALA:HB1	1:C:158:ILE:HD12	1.85	0.58
4:A:404:17C:HAI	4:A:404:17C:CAJ	2.33	0.57
1:B:358:GLN:O	1:B:362:ARG:HD3	2.04	0.57
1:D:117:ASN:HB3	1:D:297:ASN:ND2	2.19	0.57
4:C:405:17C:HAI	4:C:405:17C:HAJ	1.87	0.57
1:D:94:PRO:HG2	1:D:97:THR:HG21	1.87	0.57
4:D:402:17C:CAI	4:D:402:17C:CAJ	2.77	0.57
1:B:116:VAL:HG22	1:B:121:MET:HE2	1.86	0.56
1:C:65:PHE:CE1	1:C:69:MET:HE3	2.40	0.56
4:C:405:17C:HAI	4:C:405:17C:CAJ	2.36	0.55
1:D:97:THR:HB	1:D:166:ALA:HB1	1.87	0.55
1:D:103:VAL:HG22	1:D:217:GLY:HA2	1.87	0.55
1:C:119:SER:HB2	2:C:401:PRP:PB	2.46	0.55
1:C:196:ILE:HG23	1:C:198:VAL:HG22	1.89	0.55
1:A:52:ILE:HG12	1:A:62:ILE:HG12	1.89	0.54
1:B:42:ARG:HD3	6:B:674:HOH:O	2.08	0.54
1:C:103:VAL:HG12	1:C:216:ALA:HB3	1.89	0.53
1:A:337:LEU:HB2	1:A:338:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ARG:HD3	1:D:39:ASP:O	2.09	0.53
1:D:196:ILE:HG22	1:D:198:VAL:HG22	1.90	0.53
1:B:216:ALA:HA	1:B:240:SER:O	2.09	0.53
1:D:157:ARG:HG2	1:D:160:LEU:HD21	1.89	0.53
1:B:196:ILE:HG22	1:B:198:VAL:HG22	1.89	0.53
4:B:404:17C:CAJ	4:B:404:17C:HAI	2.39	0.53
1:C:97:THR:CG2	1:C:166:ALA:CB	2.87	0.52
1:A:33:ARG:HD3	1:A:39:ASP:O	2.09	0.52
1:B:42:ARG:NH1	6:B:544:HOH:O	2.42	0.52
1:C:121:MET:CE	1:C:304:VAL:HB	2.39	0.52
1:C:116:VAL:HA	1:C:297:ASN:HD22	1.75	0.52
1:B:198:VAL:HG11	1:D:31:LEU:HB2	1.90	0.52
1:B:207:PRO:HB2	1:B:230:MET:HE1	1.92	0.52
1:D:65:PHE:CZ	1:D:69:MET:HE2	2.45	0.52
1:B:97:THR:OG1	1:B:166:ALA:HB1	2.11	0.51
1:D:186:TYR:CD2	4:D:403:17C:HAK	2.45	0.51
1:A:33:ARG:HG2	1:A:38:ARG:HB2	1.92	0.51
1:B:207:PRO:HB2	1:B:230:MET:CE	2.40	0.51
1:C:65:PHE:CE1	1:C:69:MET:CE	2.94	0.51
1:D:103:VAL:CG2	1:D:217:GLY:HA2	2.41	0.51
1:A:140:ALA:HB2	1:A:146:GLY:N	2.26	0.51
1:D:149:ASP:OD2	1:D:294:ALA:HB2	2.10	0.50
1:C:121:MET:HE1	1:C:304:VAL:HB	1.93	0.50
1:C:111:ASP:C	1:C:113:VAL:H	2.20	0.49
1:A:193:ARG:HG3	6:A:541:HOH:O	2.11	0.49
1:C:117:ASN:HB3	2:C:401:PRP:O3B	2.11	0.49
1:D:49:MET:CE	1:D:82:LEU:HB3	2.42	0.49
1:A:94:PRO:O	1:A:97:THR:HG22	2.12	0.49
1:D:121:MET:CG	1:D:301:VAL:HG22	2.42	0.49
4:B:404:17C:HAI	4:B:404:17C:HAJ	1.94	0.48
1:C:246:GLY:C	1:C:248:ASP:N	2.71	0.48
1:D:220:GLY:HA3	1:D:251:ASP:O	2.13	0.48
1:C:145:SER:OG	1:C:294:ALA:HA	2.13	0.48
1:C:221:CYS:O	1:C:245:HIS:HD2	1.95	0.48
1:A:97:THR:OG1	1:A:166:ALA:HB1	2.13	0.48
1:C:193:ARG:HD3	1:C:202:PHE:CB	2.44	0.48
1:B:49:MET:HE2	1:B:82:LEU:HD22	1.95	0.48
1:C:34:LEU:HD11	1:C:69:MET:HE2	1.94	0.48
1:B:52:ILE:HG12	1:B:62:ILE:HG12	1.96	0.48
1:A:321:ALA:O	1:A:325:VAL:HG23	2.14	0.48
1:C:119:SER:HB2	2:C:401:PRP:O3B	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASN:HB3	1:D:297:ASN:CG	2.38	0.48
1:D:337:LEU:HB2	1:D:338:PRO:HD3	1.95	0.48
1:C:122:ALA:O	1:C:126:VAL:HG23	2.14	0.48
1:C:113:VAL:HG12	1:C:115:THR:HG23	1.96	0.47
4:C:405:17C:HAJ	4:C:405:17C:CAI	2.44	0.47
4:D:403:17C:CAI	4:D:403:17C:HAJ	2.44	0.47
1:B:139:ARG:NH2	1:B:152:GLU:OE1	2.47	0.47
1:C:121:MET:HE3	1:C:301:VAL:HA	1.95	0.47
1:A:216:ALA:HA	1:A:240:SER:O	2.14	0.47
1:B:362:ARG:HG3	1:B:365:ARG:HH21	1.80	0.47
1:D:139:ARG:HD3	1:D:149:ASP:HB3	1.96	0.47
1:C:179:ALA:HB3	1:C:180:PRO:HD3	1.96	0.47
1:B:167:ARG:O	1:B:171:GLU:HG3	2.15	0.46
1:A:114:ASN:O	1:A:290:ALA:HA	2.15	0.46
1:C:207:PRO:HB3	1:C:219:ILE:HG23	1.97	0.46
1:D:225:ASP:OD2	1:D:225:ASP:N	2.47	0.46
1:C:107:GLY:HA3	6:C:508:HOH:O	2.14	0.46
1:C:33:ARG:HD3	1:C:39:ASP:O	2.16	0.45
1:C:360:LEU:O	1:C:364:VAL:HG23	2.16	0.45
1:C:157:ARG:HG2	1:C:160:LEU:CD2	2.46	0.45
1:D:52:ILE:HG12	1:D:62:ILE:HG12	1.97	0.45
1:C:40:LEU:CD1	1:C:69:MET:HE1	2.44	0.45
1:C:52:ILE:HG12	1:C:62:ILE:HG12	1.99	0.45
1:D:33:ARG:HD2	1:D:40:LEU:HD23	1.97	0.45
1:D:148:ALA:HB1	1:D:158:ILE:HD12	1.97	0.45
1:A:193:ARG:NH1	6:A:514:HOH:O	2.49	0.45
1:D:244:VAL:HG12	1:D:261:ILE:HG12	1.99	0.45
1:C:97:THR:HG21	1:C:166:ALA:HB2	1.99	0.45
1:D:122:ALA:O	1:D:126:VAL:HG23	2.17	0.45
1:C:117:ASN:OD1	2:C:401:PRP:O1B	2.33	0.44
1:C:263:ARG:HD3	1:C:336:TRP:CZ3	2.52	0.44
1:C:33:ARG:HD2	1:C:40:LEU:HD23	2.00	0.44
1:D:72:LYS:O	1:D:73:ALA:HB3	2.17	0.44
1:C:140:ALA:HB2	1:C:146:GLY:N	2.33	0.44
4:C:405:17C:CAJ	4:C:405:17C:CAI	2.96	0.44
1:A:72:LYS:O	1:A:73:ALA:HB3	2.18	0.44
4:A:404:17C:HAJ	4:A:404:17C:CAI	2.47	0.43
1:C:157:ARG:HG2	1:C:160:LEU:HD21	2.00	0.43
4:A:404:17C:CAJ	4:A:404:17C:CAI	2.96	0.43
4:C:404:17C:CAJ	4:C:404:17C:HAI	2.49	0.43
1:B:208:LEU:HD23	1:B:234:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG12	1:A:261:ILE:HG12	2.01	0.43
1:C:97:THR:HG21	1:C:166:ALA:CB	2.49	0.43
4:D:403:17C:HAI	4:D:403:17C:HAJ	2.00	0.43
1:B:58:ARG:HG3	1:D:195:GLU:HG2	2.00	0.42
1:D:247:ASP:OD1	1:D:260:THR:HG23	2.19	0.42
1:C:94:PRO:O	1:C:97:THR:HB	2.19	0.42
1:C:285:GLN:HB2	1:C:288:GLN:HG3	2.02	0.42
1:D:187:ARG:HD2	4:D:402:17C:CAS	2.49	0.42
1:A:207:PRO:HB2	1:A:230:MET:CE	2.50	0.42
1:D:49:MET:O	1:D:53:MET:HG2	2.20	0.42
1:C:257:THR:HG23	1:C:258:THR:O	2.20	0.41
1:D:27:TRP:HB2	1:D:28:PRO:HD3	2.02	0.41
1:C:142:SER:C	1:C:144:LEU:HA	2.44	0.41
1:D:31:LEU:O	1:D:35:THR:HG23	2.21	0.41
1:C:193:ARG:HD3	1:C:202:PHE:HB3	2.01	0.41
1:D:288:GLN:HA	6:D:545:HOH:O	2.19	0.41
1:D:49:MET:HE3	1:D:82:LEU:HB3	2.03	0.41
1:B:304:VAL:HG21	1:B:312:VAL:HG12	2.03	0.41
1:A:60:ALA:O	1:C:196:ILE:HD11	2.21	0.41
1:B:179:ALA:HB3	1:B:180:PRO:HD3	2.02	0.41
1:C:148:ALA:HB1	1:C:158:ILE:CD1	2.49	0.40
1:D:62:ILE:HB	1:D:192:VAL:HG21	2.02	0.40
1:A:49:MET:HE2	1:A:82:LEU:HD22	2.02	0.40
1:B:263:ARG:CZ	1:B:272:LEU:HD11	2.51	0.40
1:C:72:LYS:O	1:C:73:ALA:HB3	2.20	0.40
1:C:251:ASP:C	1:C:252:GLU:HG2	2.45	0.40
1:B:52:ILE:HG21	1:B:189:ALA:HB2	2.03	0.40
1:B:116:VAL:HG22	1:B:121:MET:HE1	2.04	0.40
1:C:72:LYS:O	1:C:73:ALA:CB	2.69	0.40
1:C:193:ARG:NH1	1:C:203:ASN:CG	2.80	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	344/377 (91%)	338 (98%)	5 (2%)	1 (0%)	36	27
1	B	344/377 (91%)	335 (97%)	8 (2%)	1 (0%)	36	27
1	C	339/377 (90%)	324 (96%)	12 (4%)	3 (1%)	14	6
1	D	320/377 (85%)	309 (97%)	10 (3%)	1 (0%)	36	27
All	All	1347/1508 (89%)	1306 (97%)	35 (3%)	6 (0%)	30	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	ASP
1	A	73	ALA
1	B	73	ALA
1	C	73	ALA
1	D	73	ALA
1	C	292	GLY

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	243/264 (92%)	239 (98%)	4 (2%)	55	50
1	B	243/264 (92%)	239 (98%)	4 (2%)	55	50
1	C	240/264 (91%)	235 (98%)	5 (2%)	47	40
1	D	232/264 (88%)	229 (99%)	3 (1%)	61	57
All	All	958/1056 (91%)	942 (98%)	16 (2%)	53	48

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	97	THR

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Mol	Chain	Res	Type
1	A	157	ARG
1	A	362	ARG
1	B	241	VAL
1	B	305	LEU
1	B	362	ARG
1	B	370	ILE
1	C	37	ASN
1	C	72	LYS
1	C	196	ILE
1	C	241	VAL
1	C	252	GLU
1	D	169	LEU
1	D	250	LEU
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	114	ASN
1	A	358	GLN
1	B	285	GLN
1	B	358	GLN
1	C	56	ASN
1	C	117	ASN
1	C	245	HIS
1	C	297	ASN
1	D	56	ASN
1	D	297	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 ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	17C	C	404	-	20,20,20	1.11	0	27,27,27	1.03	1 (3%)
4	17C	A	404	-	20,20,20	0.91	0	27,27,27	0.97	1 (3%)
4	17C	D	402	-	20,20,20	1.05	1 (5%)	27,27,27	0.85	1 (3%)
2	PRP	B	401	3	20,22,22	1.96	6 (30%)	32,35,35	2.61	8 (25%)
4	17C	B	404	-	20,20,20	1.03	1 (5%)	27,27,27	1.00	1 (3%)
4	17C	C	405	-	20,20,20	1.23	2 (10%)	27,27,27	1.06	1 (3%)
2	PRP	A	401	3	20,22,22	1.86	5 (25%)	32,35,35	3.02	10 (31%)
4	17C	C	403	-	20,20,20	1.01	1 (5%)	27,27,27	1.06	2 (7%)
4	17C	D	403	-	20,20,20	1.17	2 (10%)	27,27,27	0.89	1 (3%)
2	PRP	C	401	3	20,22,22	1.81	4 (20%)	32,35,35	2.18	6 (18%)
5	DPO	D	401	-	6,8,8	2.29	3 (50%)	12,13,13	1.63	3 (25%)

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
4	17C	C	404	-	-	4/12/12/12	0/2/2/2
4	17C	A	404	-	-	0/12/12/12	0/2/2/2
4	17C	D	402	-	-	0/12/12/12	0/2/2/2
2	PRP	B	401	3	-	8/16/33/33	0/1/1/1
4	17C	B	404	-	-	4/12/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	17C	C	405	-	-	2/12/12/12	0/2/2/2
2	PRP	A	401	3	-	2/16/33/33	0/1/1/1
4	17C	C	403	-	-	3/12/12/12	0/2/2/2
4	17C	D	403	-	-	6/12/12/12	0/2/2/2
2	PRP	C	401	3	-	5/16/33/33	0/1/1/1
5	DPO	D	401	-	-	0/6/6/6	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PRP	P-O1P	4.07	1.63	1.50
2	B	401	PRP	PB-O1B	4.06	1.63	1.50
2	B	401	PRP	P-O1P	3.99	1.62	1.50
2	A	401	PRP	P-O1P	3.96	1.62	1.50
5	D	401	DPO	P1-O1	3.93	1.62	1.50
2	C	401	PRP	PB-O1B	3.89	1.62	1.50
2	A	401	PRP	PA-O3A	-3.74	1.55	1.59
2	B	401	PRP	PA-O1A	3.25	1.62	1.50
2	C	401	PRP	PA-O1A	3.24	1.62	1.50
2	A	401	PRP	PB-O1B	3.23	1.60	1.50
4	C	405	17C	CAR-CAN	2.96	1.56	1.49
5	D	401	DPO	P2-O6	2.41	1.63	1.54
4	C	405	17C	CAS-CAO	2.36	1.54	1.49
4	D	403	17C	CAS-CAO	2.32	1.54	1.49
4	C	403	17C	CAR-CAN	2.30	1.54	1.49
5	D	401	DPO	P2-O7	2.22	1.63	1.54
2	C	401	PRP	PB-O2B	2.16	1.62	1.54
2	B	401	PRP	P-O5	-2.15	1.53	1.60
2	A	401	PRP	PB-O3B	-2.13	1.46	1.54
4	D	403	17C	OAB-CAO	-2.11	1.24	1.30
4	D	402	17C	CAS-CAO	2.11	1.54	1.49
4	B	404	17C	CAR-CAN	2.07	1.54	1.49
2	B	401	PRP	PB-O3B	-2.06	1.47	1.54
2	A	401	PRP	O5-C5	-2.05	1.36	1.44
2	B	401	PRP	C1-C2	2.03	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PRP	O4-C1-O1	-9.67	90.74	109.16
2	B	401	PRP	O4-C1-O1	-8.39	93.18	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PRP	O4-C1-O1	-8.27	93.39	109.16
2	A	401	PRP	O1-C1-C2	7.30	118.49	106.65
2	A	401	PRP	O4-C4-C3	-6.19	92.86	105.15
2	A	401	PRP	C2-C3-C4	-6.15	90.73	102.61
2	B	401	PRP	C2-C3-C4	-5.81	91.38	102.61
2	B	401	PRP	O4-C4-C3	-5.09	95.04	105.15
2	C	401	PRP	O1-C1-C2	4.86	114.53	106.65
2	B	401	PRP	O1-C1-C2	4.17	113.41	106.65
5	D	401	DPO	O3-P1-O4	3.64	116.86	104.64
2	C	401	PRP	C5-C4-C3	-3.56	102.39	115.21
2	B	401	PRP	O2-C2-C3	-3.40	100.92	111.82
2	B	401	PRP	O3B-PB-O3A	3.36	115.91	104.64
2	A	401	PRP	O3B-PB-O3A	3.27	115.59	104.64
4	C	404	17C	OAD-CAO-CAS	-2.98	114.86	121.97
2	B	401	PRP	O4-C4-C5	2.91	118.67	109.33
4	C	403	17C	CAL-CAS-CAQ	2.86	122.03	118.81
2	C	401	PRP	O3P-P-O5	2.85	114.10	106.67
2	C	401	PRP	O4-C4-C3	-2.85	99.50	105.15
5	D	401	DPO	O6-P2-O4	2.68	113.64	104.64
2	A	401	PRP	O2A-PA-O3A	2.65	114.43	107.27
2	A	401	PRP	O3P-P-O5	2.58	113.40	106.67
2	B	401	PRP	O3P-P-O5	2.54	113.30	106.67
4	A	404	17C	CAK-CAR-CAP	2.54	121.67	118.81
2	A	401	PRP	O2-C2-C3	-2.49	103.84	111.82
2	A	401	PRP	O4-C1-C2	-2.48	101.83	104.98
2	C	401	PRP	O2A-PA-O3A	2.44	113.88	107.27
4	C	405	17C	CAE-CAG-CAK	-2.43	117.24	120.24
2	A	401	PRP	O3A-PB-O1B	-2.31	98.89	111.04
5	D	401	DPO	O2-P1-O1	-2.23	102.13	110.83
4	D	402	17C	OAC-CAN-CAR	-2.14	116.87	121.97
4	C	403	17C	OAC-CAN-CAR	-2.09	116.98	121.97
4	D	403	17C	OAC-CAN-CAR	-2.04	117.10	121.97
4	B	404	17C	OAD-CAO-CAS	-2.01	117.16	121.97

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PRP	C1-O1-PA-O2A
2	A	401	PRP	C1-O1-PA-O3A
2	B	401	PRP	C1-O1-PA-O2A
2	B	401	PRP	C1-O1-PA-O3A

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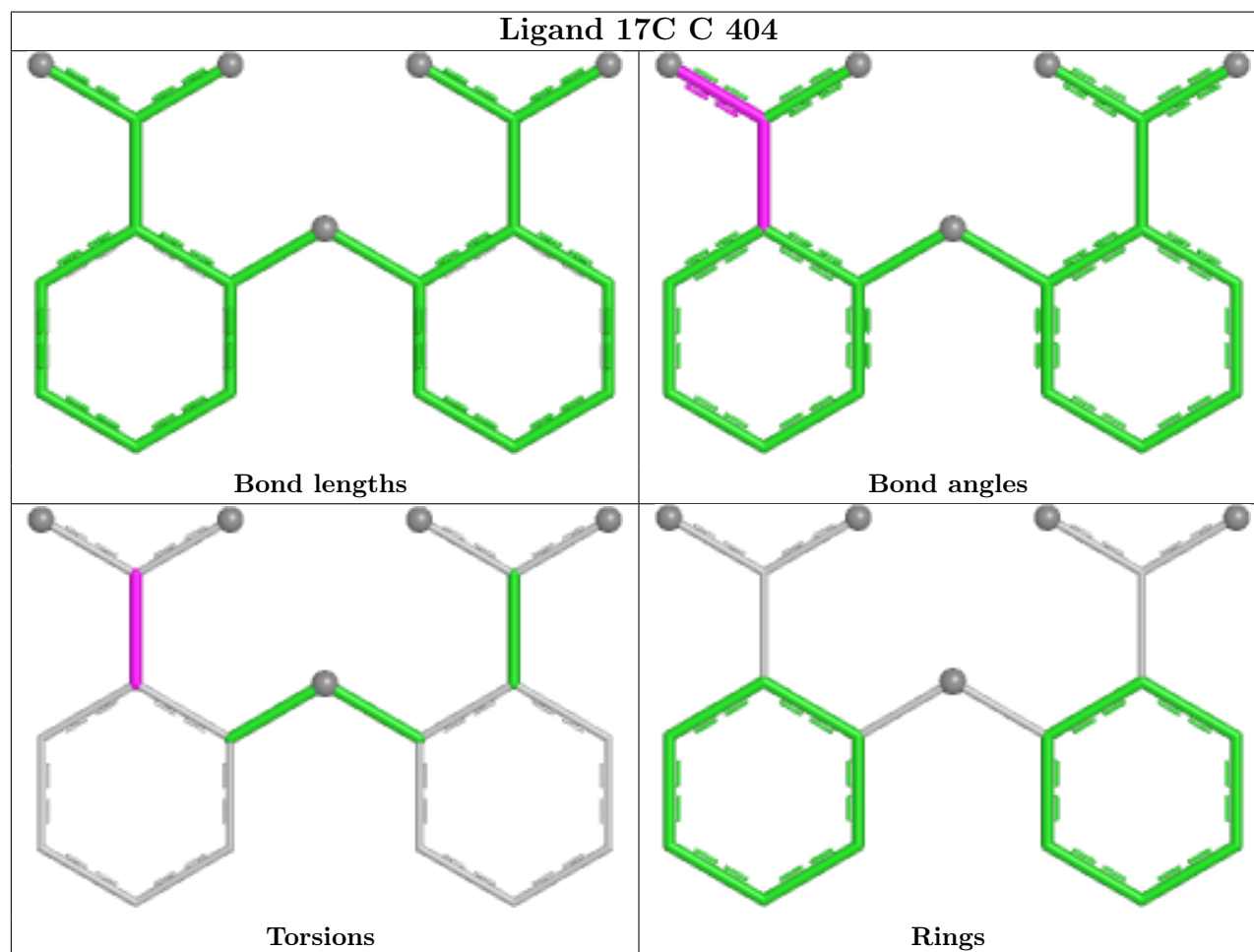
Mol	Chain	Res	Type	Atoms
2	B	401	PRP	C5-O5-P-O1P
2	B	401	PRP	C5-O5-P-O2P
2	B	401	PRP	C5-O5-P-O3P
2	C	401	PRP	C5-O5-P-O1P
2	C	401	PRP	C5-O5-P-O2P
2	C	401	PRP	C5-O5-P-O3P
2	B	401	PRP	C3-C4-C5-O5
2	C	401	PRP	C3-C4-C5-O5
4	D	403	17C	OAD-CAO-CAS-CAQ
4	D	403	17C	OAB-CAO-CAS-CAQ
2	C	401	PRP	O4-C4-C5-O5
2	B	401	PRP	O4-C4-C5-O5
4	C	404	17C	OAD-CAO-CAS-CAL
4	C	404	17C	OAB-CAO-CAS-CAL
4	C	404	17C	OAB-CAO-CAS-CAQ
4	B	404	17C	OAD-CAO-CAS-CAQ
4	C	404	17C	OAD-CAO-CAS-CAQ
4	B	404	17C	OAB-CAO-CAS-CAQ
4	D	403	17C	OAD-CAO-CAS-CAL
4	D	403	17C	OAB-CAO-CAS-CAL
4	C	403	17C	OAC-CAN-CAR-CAP
4	B	404	17C	OAD-CAO-CAS-CAL
4	C	405	17C	OAB-CAO-CAS-CAQ
4	C	403	17C	OAA-CAN-CAR-CAP
4	B	404	17C	OAB-CAO-CAS-CAL
2	B	401	PRP	PA-O3A-PB-O2B
4	C	405	17C	OAD-CAO-CAS-CAQ
4	D	403	17C	OAA-CAN-CAR-CAP
4	D	403	17C	OAC-CAN-CAR-CAP
4	C	403	17C	OAC-CAN-CAR-CAK

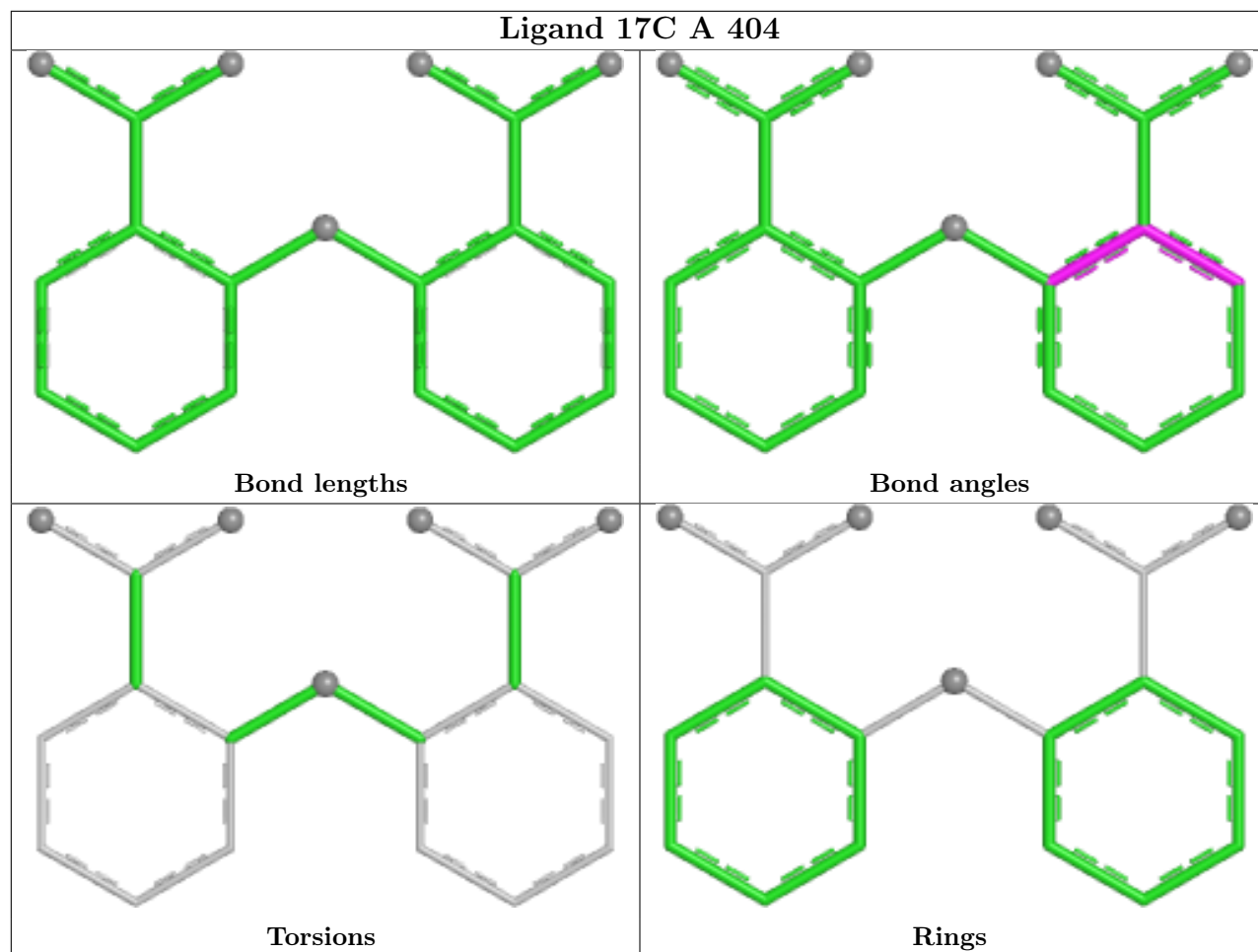
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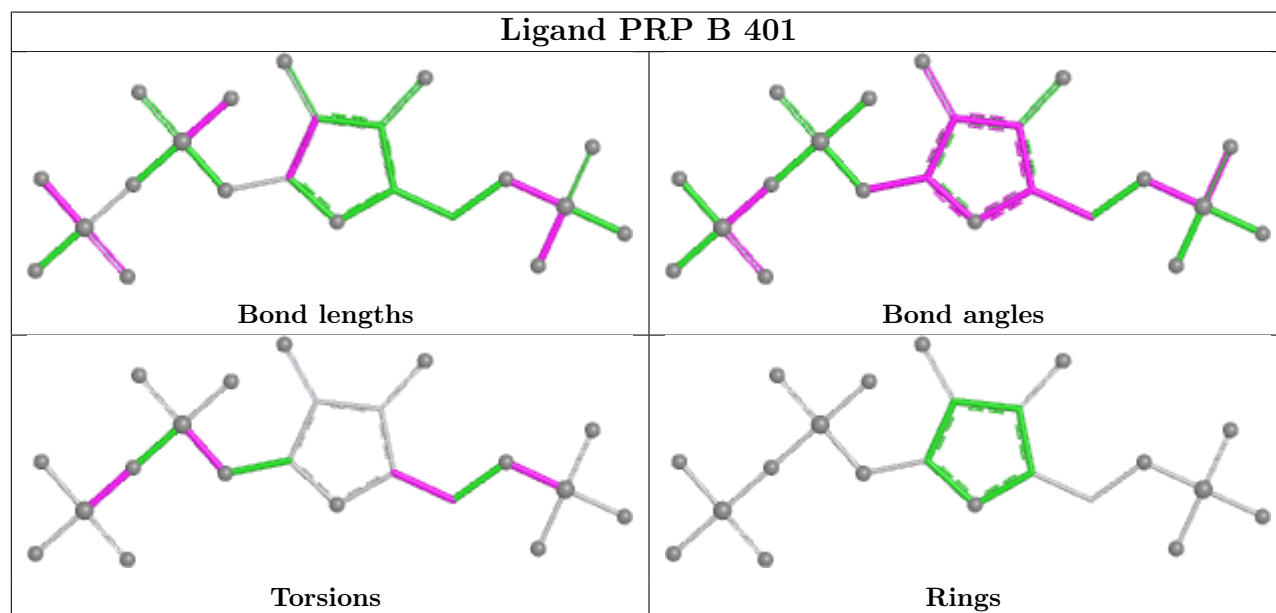
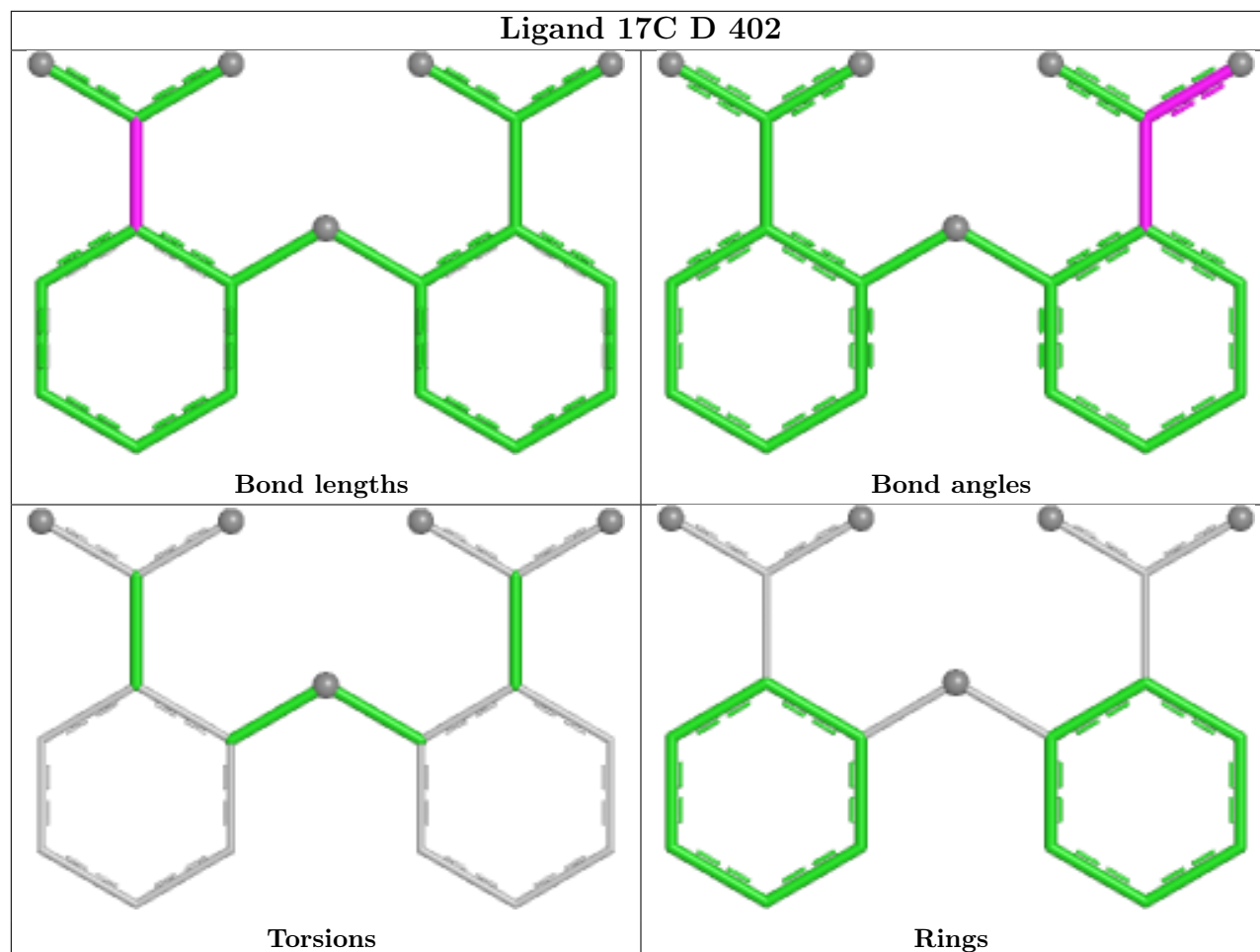
7 monomers are involved in 25 short contacts:

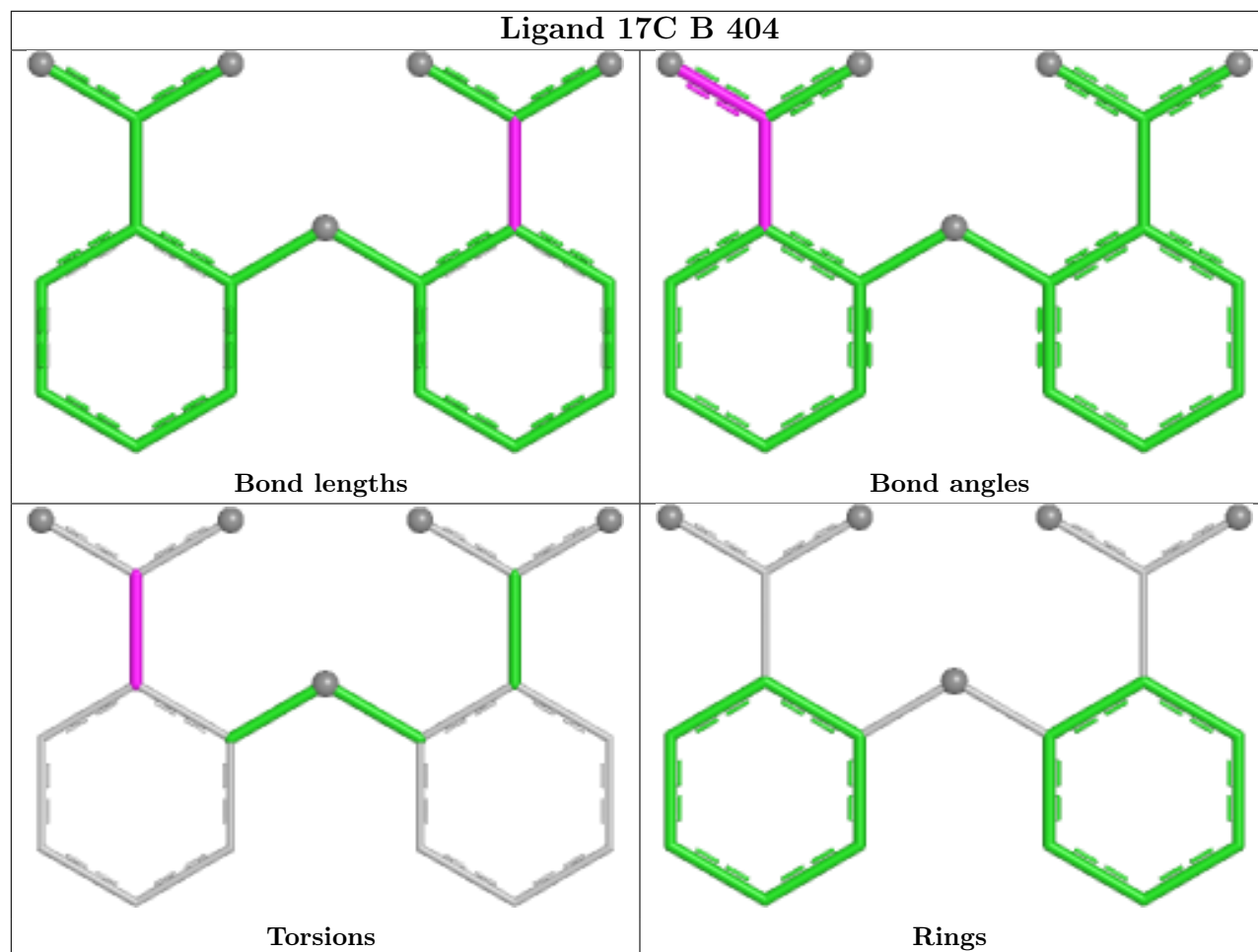
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	17C	1	0
4	A	404	17C	4	0
4	D	402	17C	5	0
4	B	404	17C	2	0
4	C	405	17C	4	0
4	D	403	17C	5	0
2	C	401	PRP	4	0

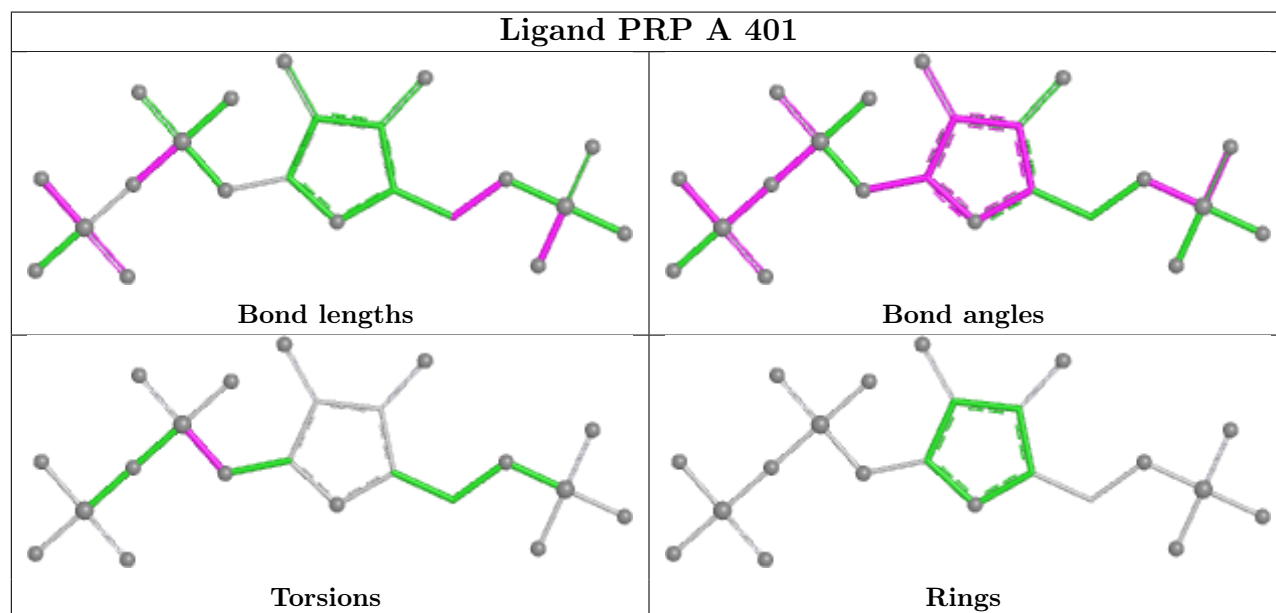
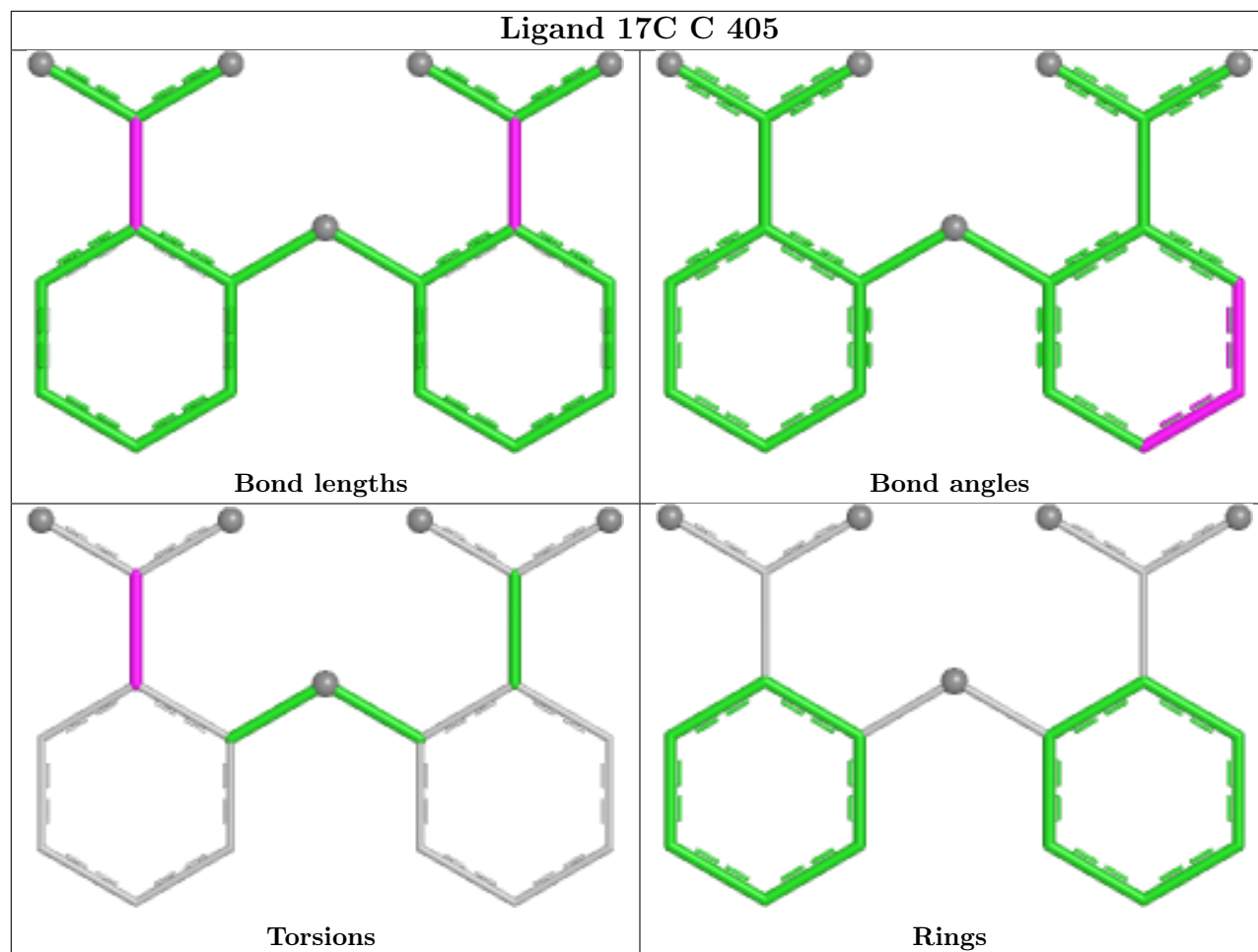
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

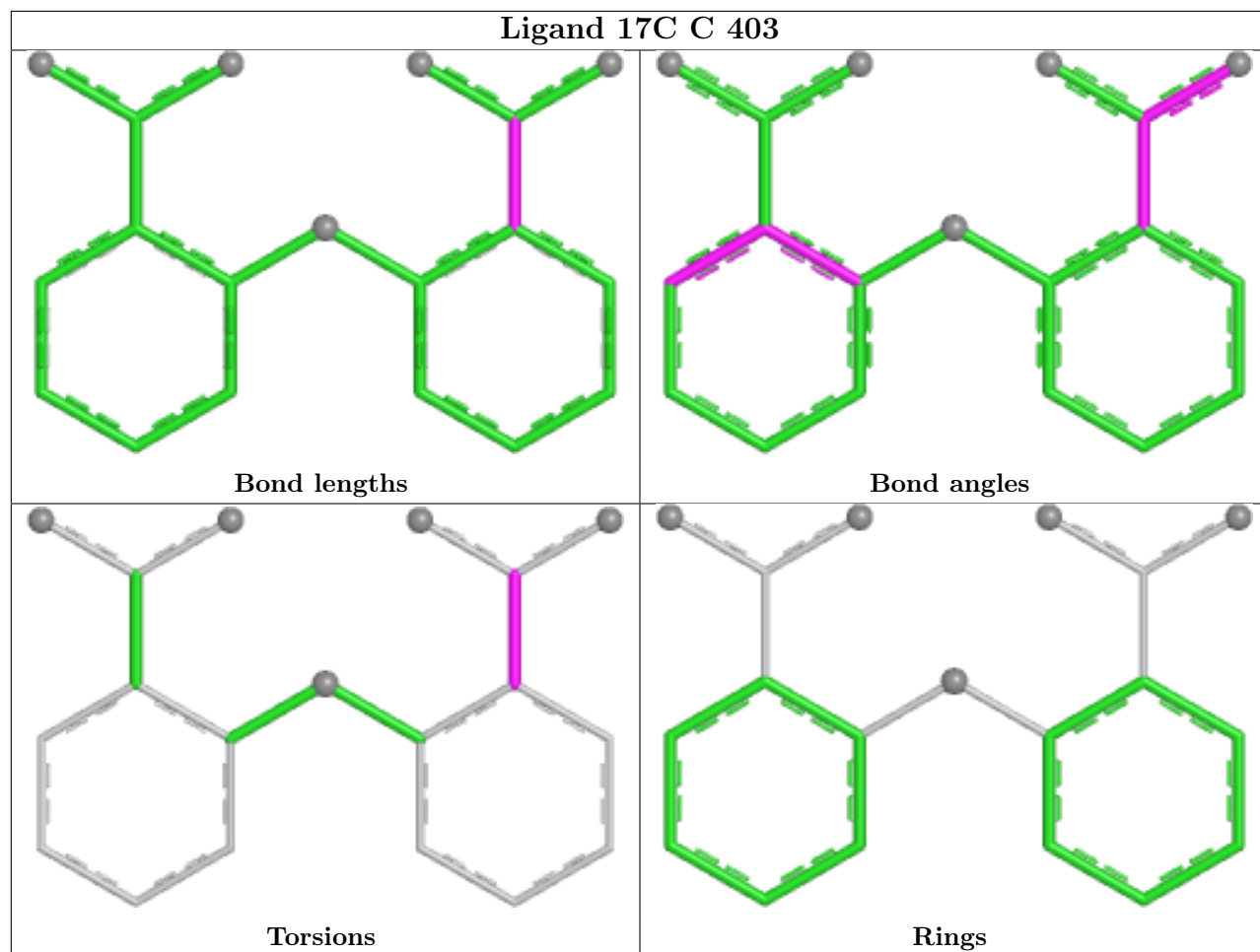


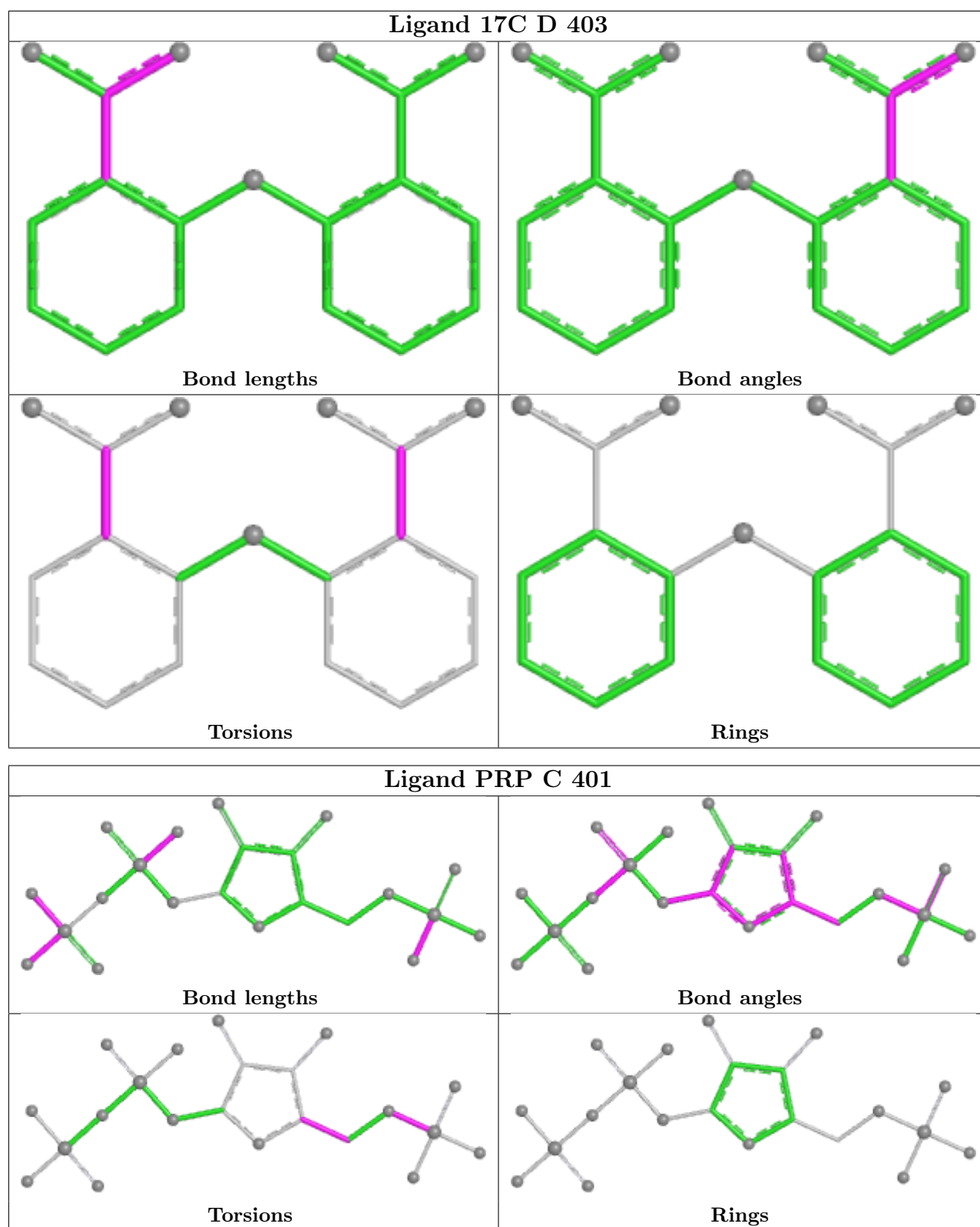












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	346/377 (91%)	-0.06	10 (2%) 53 63	11, 19, 33, 49	0
1	B	346/377 (91%)	-0.04	9 (2%) 57 67	10, 20, 34, 47	0
1	C	343/377 (90%)	0.91	61 (17%) 4 4	15, 28, 56, 65	0
1	D	330/377 (87%)	0.77	46 (13%) 6 9	16, 27, 47, 66	0
All	All	1365/1508 (90%)	0.39	126 (9%) 14 20	10, 23, 46, 66	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	289	LEU	7.0
1	D	286	LEU	6.8
1	C	286	LEU	5.7
1	D	110	GLY	5.4
1	C	223	PHE	5.3
1	A	370	ILE	5.3
1	D	267	GLY	5.3
1	D	223	PHE	5.2
1	C	141	ALA	5.1
1	A	142	SER	4.9
1	C	113	VAL	4.8
1	C	289	LEU	4.8
1	C	142	SER	4.7
1	C	296	ALA	4.5
1	C	144	LEU	4.3
1	C	114	ASN	4.1
1	A	141	ALA	4.1
1	D	284	ALA	4.1
1	C	292	GLY	4.1
1	D	292	GLY	4.1
1	C	116	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	4.0
1	D	294	ALA	4.0
1	C	266	ALA	3.9
1	C	290	ALA	3.9
1	C	291	GLY	3.9
1	C	294	ALA	3.9
1	B	370	ILE	3.8
1	B	141	ALA	3.7
1	C	284	ALA	3.7
1	D	250	LEU	3.6
1	A	144	LEU	3.5
1	D	138	ASN	3.5
1	D	331	SER	3.4
1	D	269	VAL	3.4
1	C	112	GLY	3.3
1	C	115	THR	3.3
1	D	25	PRO	3.2
1	C	153	ALA	3.2
1	D	224	ALA	3.1
1	D	282	ALA	3.1
1	C	298	ALA	3.1
1	C	109	GLY	3.1
1	D	222	ALA	3.1
1	C	293	ASP	3.0
1	D	264	VAL	3.0
1	D	140	ALA	3.0
1	D	117	ASN	3.0
1	C	299	ALA	3.0
1	C	111	ASP	2.9
1	A	337	LEU	2.9
1	C	146	GLY	2.9
1	C	272	LEU	2.8
1	D	272	LEU	2.8
1	B	144	LEU	2.8
1	C	256	THR	2.8
1	D	277	ALA	2.7
1	D	333	ARG	2.7
1	C	312	VAL	2.7
1	B	140	ALA	2.7
1	A	25	PRO	2.7
1	C	260	THR	2.7
1	D	238	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	297	ASN	2.6
1	D	334	ALA	2.6
1	D	149	ASP	2.6
1	C	269	VAL	2.6
1	C	276	PRO	2.6
1	D	281	PHE	2.6
1	C	250	LEU	2.6
1	C	117	ASN	2.5
1	C	333	ARG	2.5
1	C	110	GLY	2.4
1	D	268	SER	2.4
1	C	262	TRP	2.4
1	C	118	LEU	2.4
1	C	222	ALA	2.4
1	B	113	VAL	2.4
1	A	334	ALA	2.4
1	C	170	ALA	2.4
1	C	367	GLY	2.4
1	D	296	ALA	2.3
1	C	301	VAL	2.3
1	D	252	GLU	2.3
1	C	337	LEU	2.3
1	B	196	ILE	2.3
1	B	197	GLY	2.3
1	D	147	GLY	2.3
1	C	332	SER	2.3
1	C	166	ALA	2.3
1	C	261	ILE	2.3
1	D	109	GLY	2.3
1	A	332	SER	2.3
1	C	277	ALA	2.2
1	C	253	LEU	2.2
1	C	285	GLN	2.2
1	D	288	GLN	2.2
1	B	143	SER	2.2
1	D	287	ASP	2.2
1	A	140	ALA	2.2
1	D	148	ALA	2.2
1	D	246	GLY	2.2
1	D	276	PRO	2.2
1	C	328	ALA	2.2
1	D	273	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	157	ARG	2.1
1	D	265	ALA	2.1
1	D	266	ALA	2.1
1	D	299	ALA	2.1
1	A	331	SER	2.1
1	C	145	SER	2.1
1	D	274	PHE	2.1
1	D	279	PHE	2.1
1	C	257	THR	2.1
1	C	273	THR	2.1
1	C	311	PRO	2.1
1	C	287	ASP	2.1
1	C	279	PHE	2.0
1	C	281	PHE	2.0
1	C	268	SER	2.0
1	B	114	ASN	2.0
1	C	336	TRP	2.0
1	D	336	TRP	2.0
1	D	298	ALA	2.0
1	D	293	ASP	2.0
1	D	139	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	DPO	D	401	9/9	0.80	0.20	18,21,24,24	9
4	17C	D	403	19/19	0.81	0.15	20,23,25,25	19

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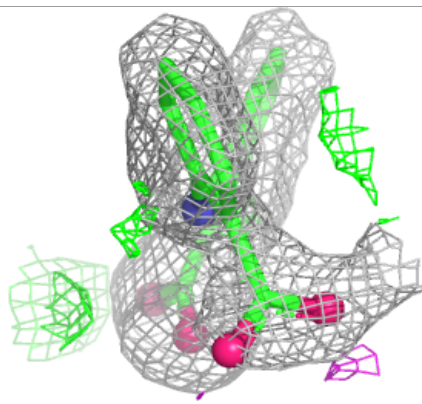
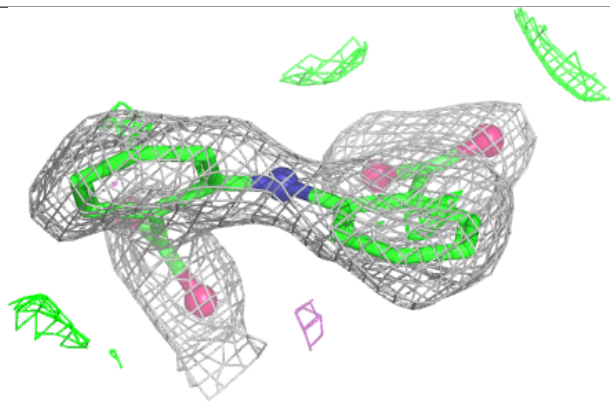
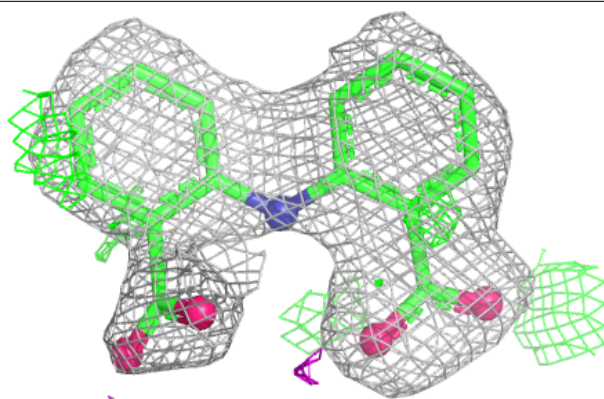
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	17C	D	402	19/19	0.82	0.14	19,23,25,25	19
4	17C	C	404	19/19	0.83	0.14	22,23,27,28	19
2	PRP	C	401	22/22	0.88	0.16	31,34,36,37	22
4	17C	C	405	19/19	0.90	0.08	25,28,32,32	0
4	17C	C	403	19/19	0.90	0.09	23,28,34,37	0
4	17C	B	404	19/19	0.94	0.06	21,23,27,28	0
3	MG	C	402	1/1	0.96	0.04	17,17,17,17	1
4	17C	A	404	19/19	0.96	0.06	17,19,26,27	0
2	PRP	A	401	22/22	0.96	0.09	15,20,21,24	13
2	PRP	B	401	22/22	0.97	0.10	15,20,22,22	13
3	MG	A	403	1/1	0.97	0.03	27,27,27,27	0
3	MG	B	403	1/1	0.97	0.05	22,22,22,22	0
3	MG	A	402	1/1	0.99	0.02	19,19,19,19	0
3	MG	B	402	1/1	0.99	0.03	15,15,15,15	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.

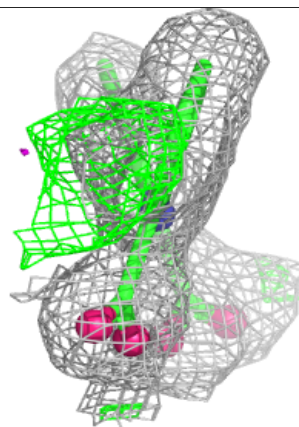
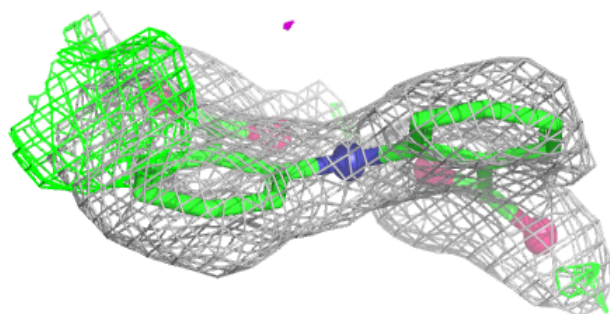
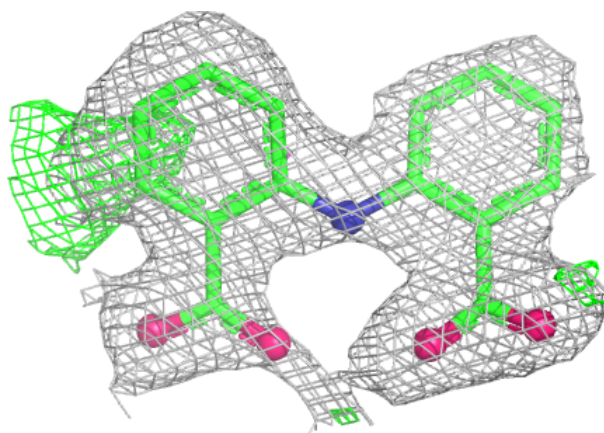
Electron density around 17C D 403:

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



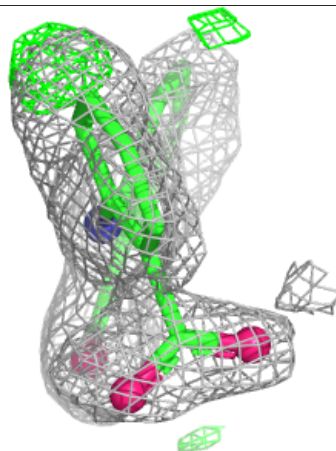
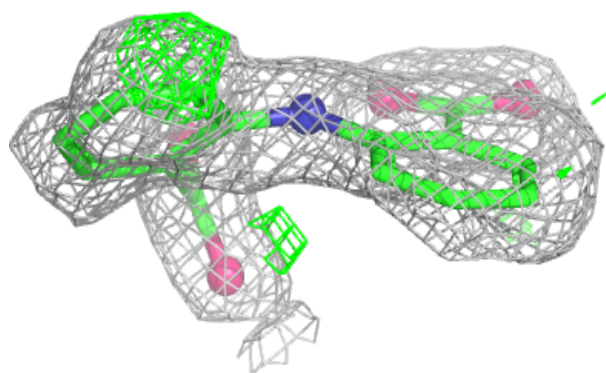
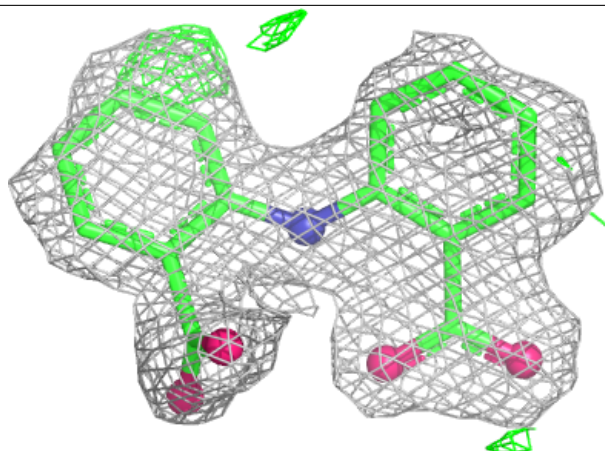
Electron density around 17C D 402:

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

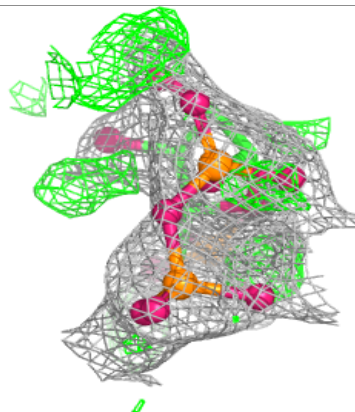
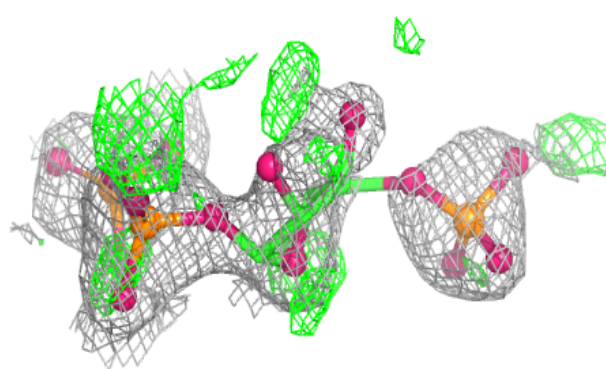
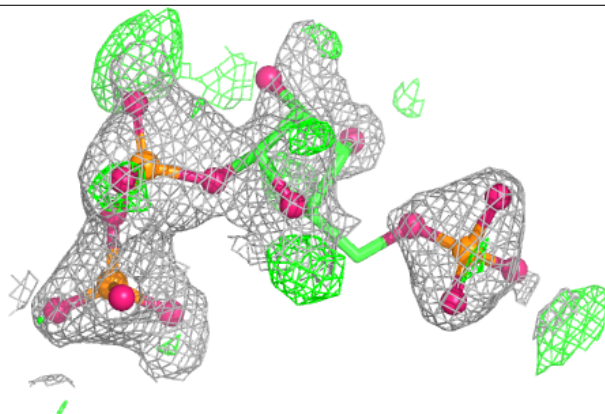


Electron density around 17C C 404:

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

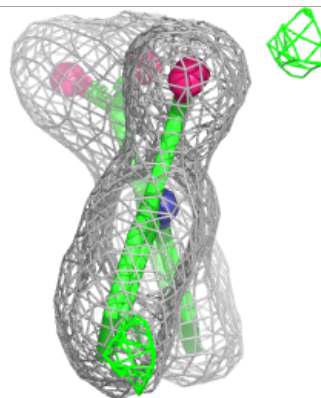
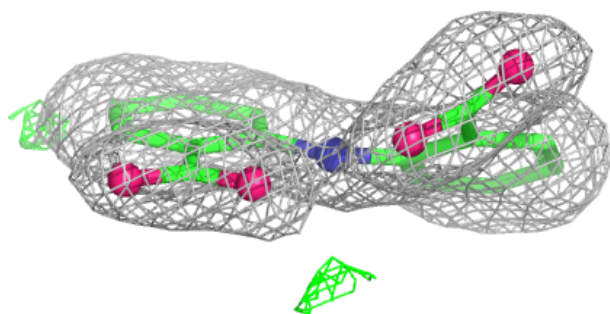
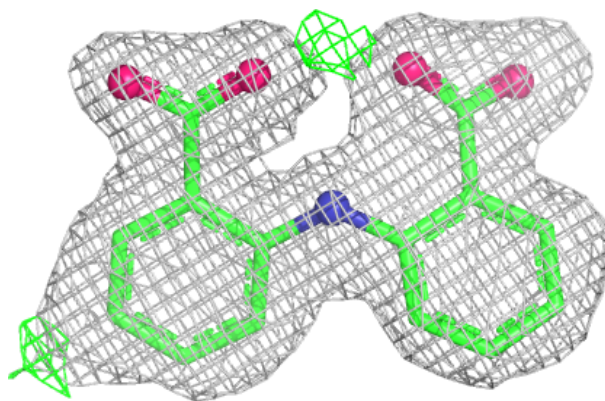
**Electron density around PRP C 401:**

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

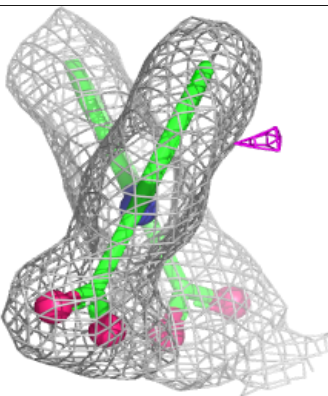
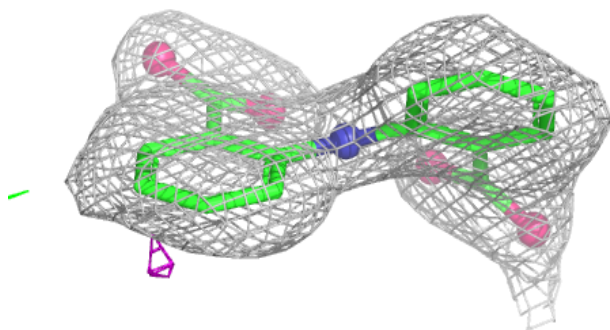
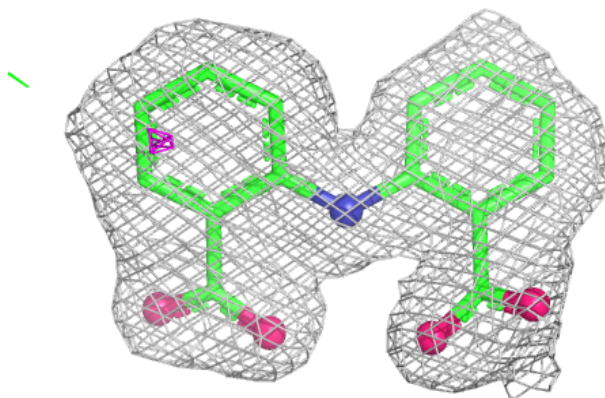


Electron density around 17C C 405:

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

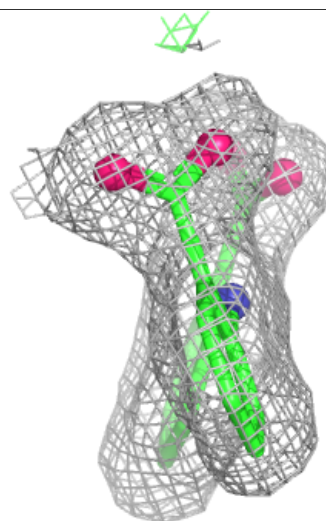
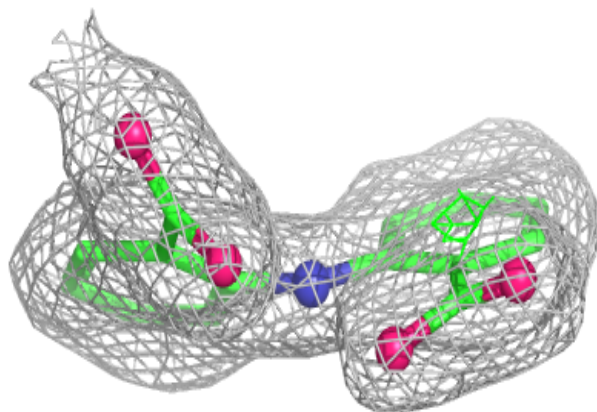
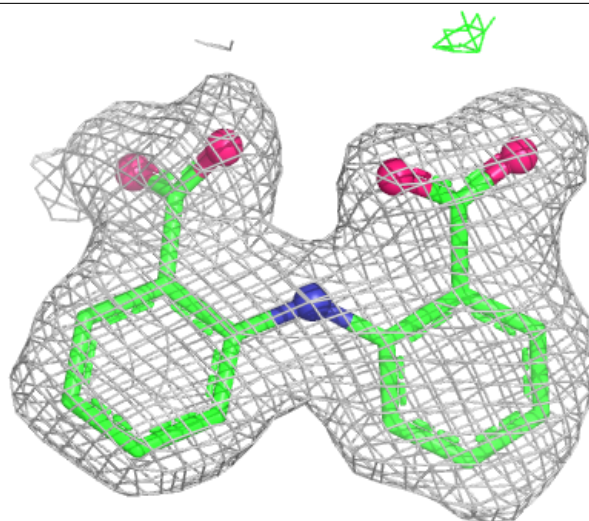
**Electron density around 17C C 403:**

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



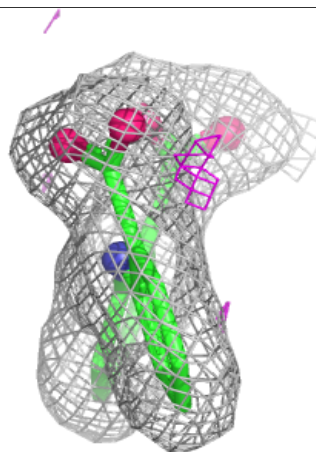
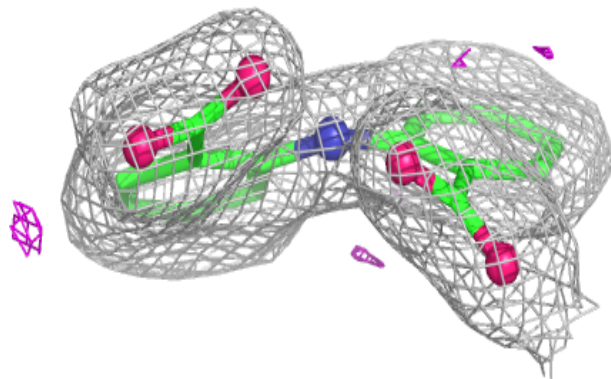
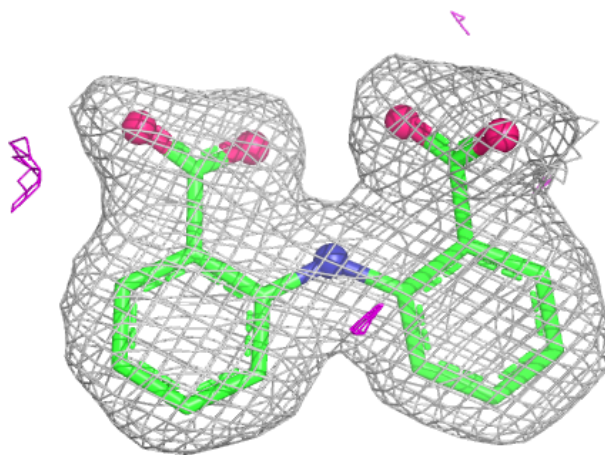
Electron density around 17C B 404:

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



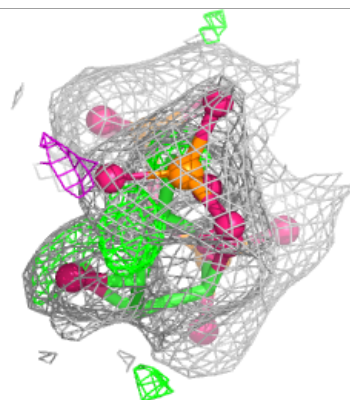
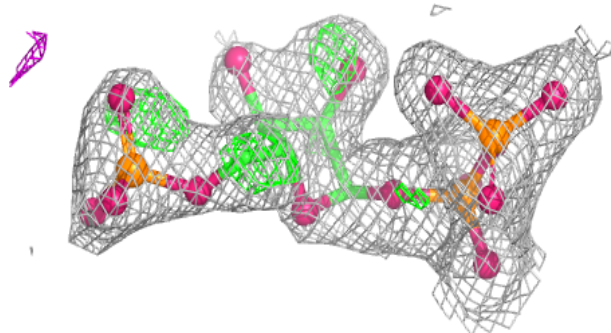
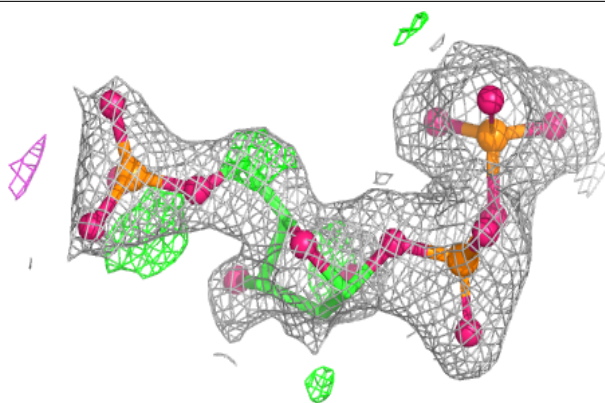
Electron density around 17C A 404:

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

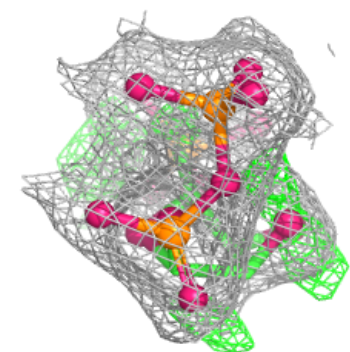
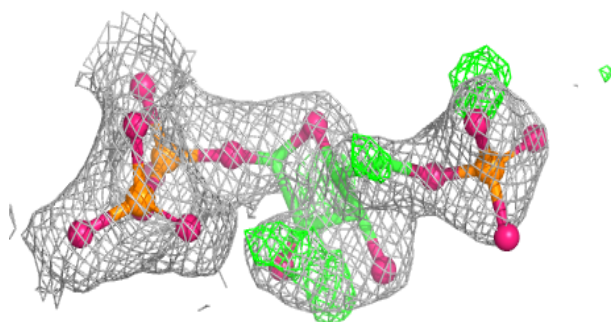
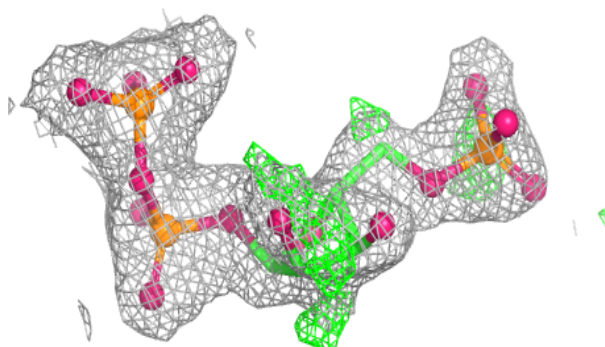


Electron density around PRP A 401:

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

**Electron density around PRP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.