



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 01:20 AM EDT

PDB ID : 1HWK
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH ATORVASTATIN
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.22 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.34
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

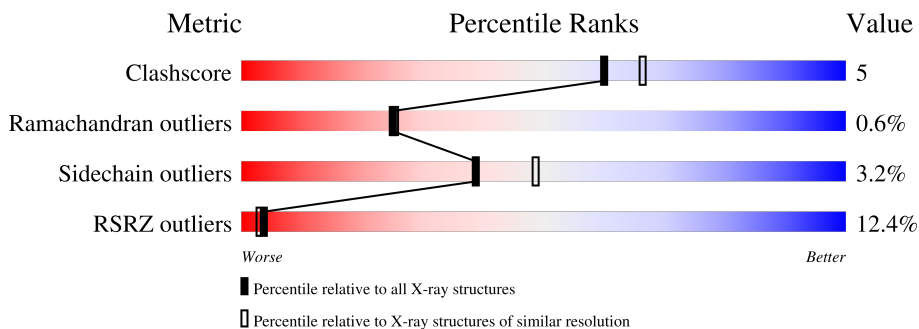
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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))
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	467	
1	B	467	
1	C	467	
1	D	467	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12296 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 HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	Total 3035	C 1889	N 534	O 582	S 30	0	0	0
1	B	393	Total 2913	C 1812	N 510	O 562	S 29	0	0	0
1	C	399	Total 2960	C 1844	N 519	O 568	S 29	0	0	0
1	D	387	Total 2864	C 1779	N 502	O 554	S 29	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

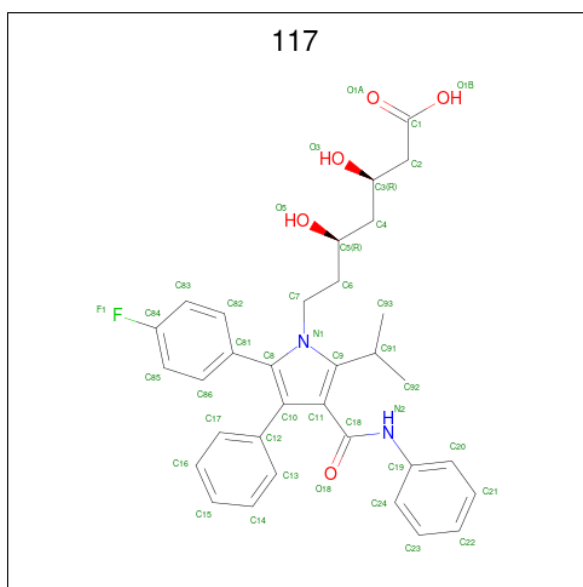
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	insertion	UNP P04035
B	425	ALA	-	insertion	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	422	GLY	-	insertion	UNP P04035
C	423	ALA	-	insertion	UNP P04035
C	424	MET	-	insertion	UNP P04035
C	425	ALA	-	insertion	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035
D	422	GLY	-	insertion	UNP P04035
D	423	ALA	-	insertion	UNP P04035
D	424	MET	-	insertion	UNP P04035
D	425	ALA	-	insertion	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]- 3,5-DIHYDROXY-HEPTANOIC ACID (three-letter code: 117) (formula: $C_{33}H_{35}FN_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	B	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	C	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	D	1	Total	C	F	N	O	0	0
			41	33	1	2	5		

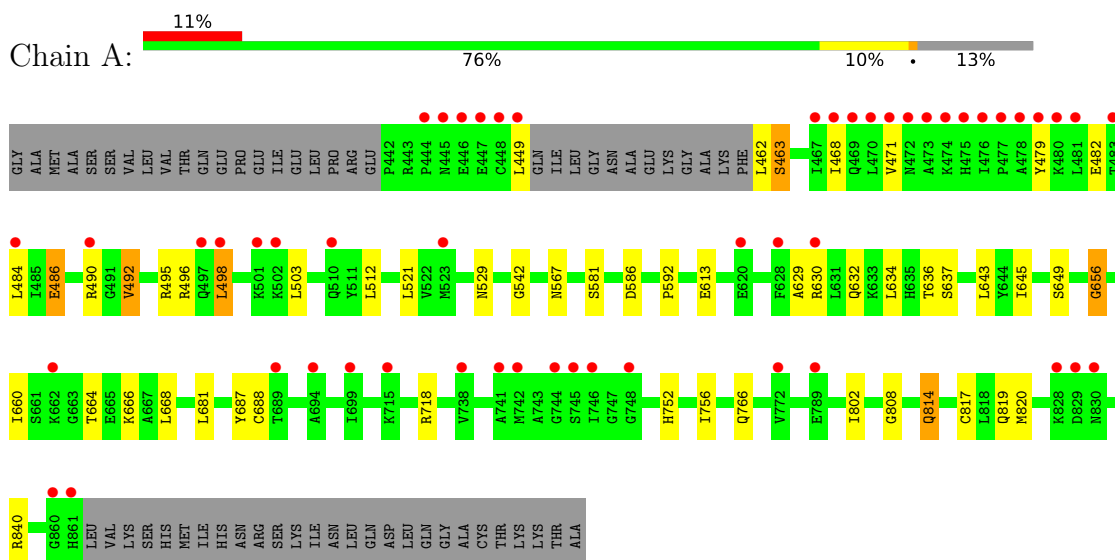
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	48	Total	O	0	0
			48	48		
4	C	57	Total	O	0	0
			57	57		
4	D	61	Total	O	0	0
			61	61		

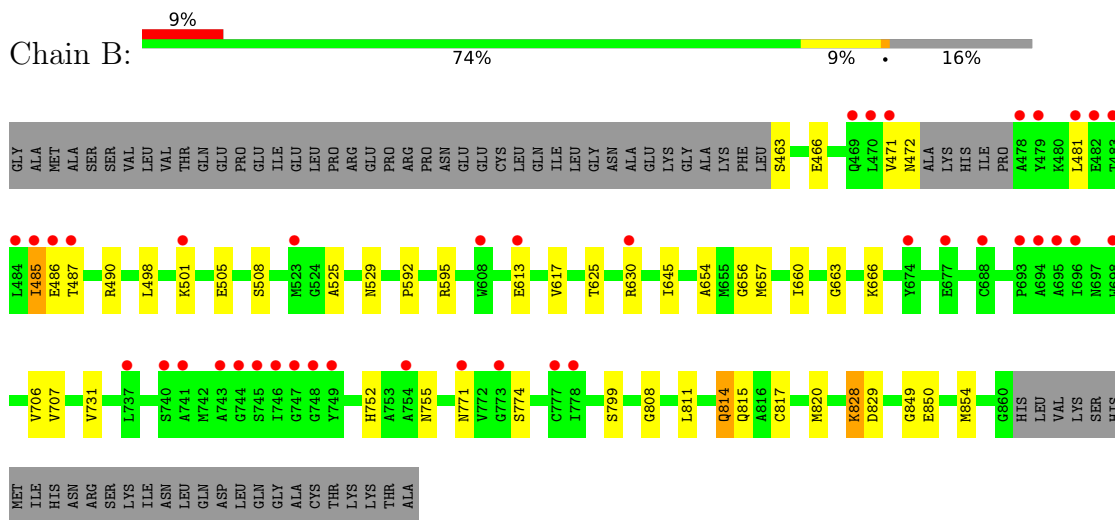
3 Residue-property plots [i](#)

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.

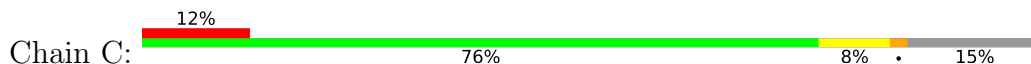
- Molecule 1: HMG-COA REDUCTASE

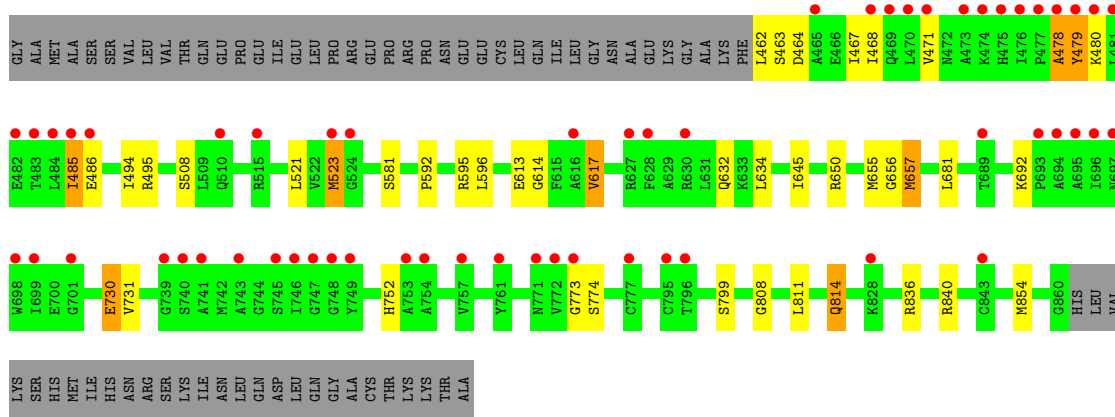


- Molecule 1: HMG-COA REDUCTASE

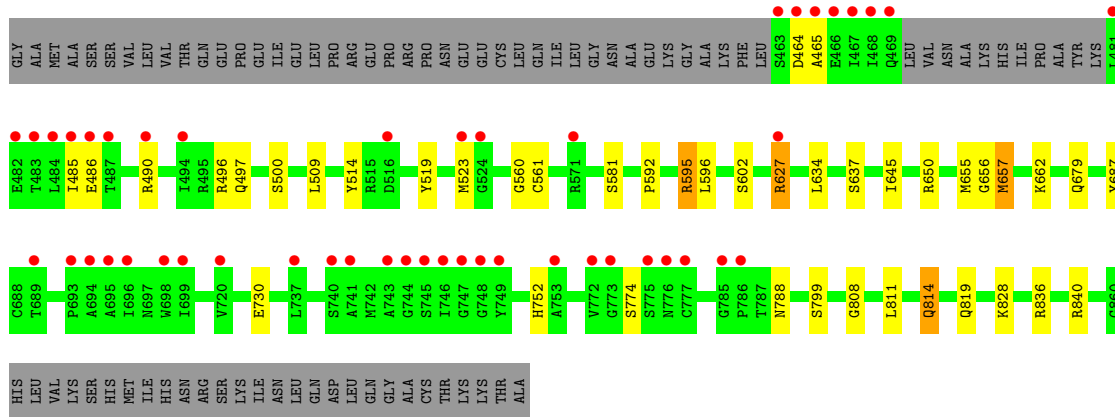
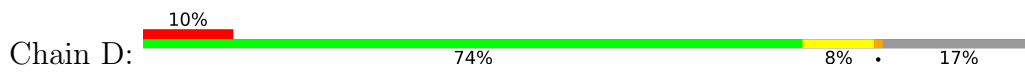


- Molecule 1: HMG-COA REDUCTASE





• Molecule 1: HMG-COA REDUCTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.60Å 172.72Å 80.01Å 90.00° 117.73° 90.00°	Depositor
Resolution (Å)	43.40 – 2.22 54.76 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.40-2.22) 92.9 (54.76-2.21)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.22Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.235 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 117, ADP

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	0.49	0/3079	0.67	1/4163 (0.0%)
1	B	0.48	0/2952	0.66	1/3990 (0.0%)
1	C	0.47	0/3002	0.65	2/4060 (0.0%)
1	D	0.51	0/2902	0.66	1/3922 (0.0%)
All	All	0.49	0/11935	0.66	5/16135 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	LEU	CA-CB-CG	-5.42	102.84	115.30
1	A	656	GLY	N-CA-C	5.28	126.29	113.10
1	D	656	GLY	N-CA-C	5.24	126.21	113.10
1	B	656	GLY	N-CA-C	5.21	126.12	113.10
1	C	656	GLY	N-CA-C	5.04	125.71	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3035	0	3068	31	0
1	B	2913	0	2945	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2960	0	3000	31	0
1	D	2864	0	2892	23	0
2	A	81	0	36	3	0
2	B	27	0	12	1	0
2	D	27	0	12	0	0
3	A	41	0	34	0	0
3	B	41	0	34	0	0
3	C	41	0	34	0	0
3	D	41	0	34	0	0
4	A	59	0	0	0	0
4	B	48	0	0	1	0
4	C	57	0	0	2	0
4	D	61	0	0	0	0
All	All	12296	0	12101	111	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 5.

All (111) 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:B:625:THR:HG22	1:B:666:LYS:HD2	1.44	1.00
1:B:485:ILE:HG22	1:B:486:GLU:H	1.31	0.96
1:C:485:ILE:HG22	1:C:486:GLU:H	1.30	0.95
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.58	0.85
1:C:479:TYR:HA	1:C:495:ARG:HH11	1.47	0.80
1:A:542:GLY:H	1:A:567:ASN:ND2	1.78	0.79
1:B:752:HIS:HD2	1:B:755:ASN:HD22	1.30	0.79
1:C:632:GLN:HE21	1:C:650:ARG:HG3	1.52	0.74
1:C:479:TYR:HA	1:C:495:ARG:NH1	2.04	0.73
1:D:485:ILE:HG22	1:D:486:GLU:H	1.55	0.71
1:B:654:ALA:HB1	2:B:104:ADP:O1B	1.93	0.69
1:D:485:ILE:HG22	1:D:486:GLU:N	2.11	0.65
1:D:581:SER:OG	1:D:840:ARG:HD2	1.96	0.65
1:C:581:SER:OG	1:C:840:ARG:HD2	1.96	0.63
1:C:485:ILE:HG22	1:C:486:GLU:N	2.11	0.62
1:C:485:ILE:HD11	1:C:494:ILE:HD12	1.80	0.62
1:B:485:ILE:HG22	1:B:486:GLU:N	2.10	0.61
1:C:523:MET:HE1	4:C:1227:HOH:O	2.01	0.60
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.84	0.60
1:B:817:CYS:HA	1:B:820:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASN:HD21	2:A:101:ADP:H2	1.52	0.58
1:C:613:GLU:O	1:C:617:VAL:HG12	2.04	0.58
1:A:462:LEU:O	1:A:463:SER:HB3	2.04	0.58
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.34	0.57
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.87	0.56
1:C:467:ILE:O	1:C:471:VAL:HG23	2.05	0.56
1:C:730:GLU:HG2	1:D:595:ARG:HH12	1.71	0.56
1:A:629:ALA:O	1:A:630:ARG:HD2	2.06	0.56
1:A:656:GLY:O	1:A:660:ILE:HG12	2.06	0.56
1:B:752:HIS:CD2	1:B:755:ASN:HD22	2.18	0.55
1:A:479:TYR:HB3	1:A:529:ASN:OD1	2.07	0.55
1:D:519:TYR:O	1:D:523:MET:HG2	2.07	0.55
1:C:808:GLY:O	1:C:814:GLN:HG3	2.08	0.54
1:D:808:GLY:O	1:D:814:GLN:HG3	2.07	0.54
1:C:464:ASP:O	1:C:468:ILE:HG12	2.07	0.54
1:C:463:SER:O	1:C:467:ILE:HG12	2.08	0.54
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.08	0.53
1:A:542:GLY:H	1:A:567:ASN:HD21	1.55	0.53
1:A:581:SER:OG	1:A:840:ARG:HD2	2.08	0.53
1:A:819:GLN:HB3	1:B:508:SER:CB	2.38	0.53
1:D:595:ARG:HD2	1:D:679:GLN:OE1	2.08	0.53
1:A:718:ARG:HH11	1:A:718:ARG:HG3	1.75	0.52
1:D:596:LEU:HD13	1:D:602:SER:HA	1.92	0.51
1:B:498:LEU:O	1:B:501:LYS:HG2	2.10	0.51
1:A:613:GLU:H	1:A:613:GLU:CD	2.14	0.51
1:B:752:HIS:HE1	1:B:849:GLY:O	1.94	0.50
1:A:819:GLN:HB3	1:B:508:SER:HB2	1.92	0.50
1:A:542:GLY:H	1:A:567:ASN:HD22	1.58	0.49
1:A:808:GLY:O	1:A:814:GLN:HG3	2.12	0.48
1:D:655:MET:SD	1:D:657:MET:HG2	2.52	0.48
1:A:492:VAL:O	1:A:496:ARG:HG2	2.14	0.48
1:B:811:LEU:O	1:B:815:GLN:HG3	2.14	0.47
1:B:481:LEU:HD22	1:B:481:LEU:H	1.78	0.47
1:B:808:GLY:O	1:B:814:GLN:HG3	2.15	0.47
1:A:649:SER:HB3	1:A:660:ILE:HD12	1.96	0.47
1:C:655:MET:SD	1:C:657:MET:HG2	2.55	0.46
1:B:828:LYS:HD2	1:B:829:ASP:H	1.81	0.46
1:D:485:ILE:CG2	1:D:486:GLU:H	2.25	0.46
1:B:471:VAL:O	1:B:472:ASN:HB2	2.16	0.45
1:D:485:ILE:CG2	1:D:486:GLU:N	2.80	0.45
1:D:662:LYS:HE2	1:D:662:LYS:HB3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:VAL:HG12	1:B:854:MET:CE	2.46	0.45
1:B:706:VAL:HG12	1:B:707:VAL:N	2.32	0.45
1:B:811:LEU:HB2	1:B:814:GLN:HG2	1.99	0.45
1:A:817:CYS:HA	1:A:820:MET:HE3	2.00	0.44
1:A:586:ASP:O	1:A:632:GLN:NE2	2.45	0.44
1:C:478:ALA:O	1:C:480:LYS:N	2.47	0.44
1:C:692:LYS:HE2	1:C:692:LYS:HB2	1.86	0.44
1:C:523:MET:HA	1:C:523:MET:CE	2.48	0.44
1:A:637:SER:HB2	1:A:687:TYR:OH	2.17	0.43
1:B:595:ARG:HD3	4:B:1036:HOH:O	2.18	0.43
1:B:850:GLU:O	1:B:854:MET:HG2	2.18	0.43
1:C:462:LEU:HD12	1:C:462:LEU:N	2.33	0.43
1:A:484:LEU:HD23	1:A:484:LEU:O	2.19	0.43
1:C:508:SER:HB2	1:D:819:GLN:HB3	2.01	0.43
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:A:756:ILE:HD12	1:A:756:ILE:N	2.33	0.43
1:B:463:SER:OG	1:B:466:GLU:HG2	2.17	0.43
1:C:614:GLY:O	1:C:617:VAL:HG13	2.18	0.43
1:D:650:ARG:NH1	1:D:836:ARG:HH21	2.17	0.43
1:D:485:ILE:HG21	1:D:490:ARG:HD3	1.99	0.43
1:D:627:ARG:N	1:D:627:ARG:HD3	2.34	0.43
2:A:102:ADP:H2	1:B:529:ASN:HD21	1.66	0.42
1:C:773:GLY:HA3	4:C:1171:HOH:O	2.19	0.42
1:A:664:THR:O	1:A:668:LEU:HG	2.20	0.42
1:B:613:GLU:O	1:B:617:VAL:HG23	2.20	0.42
1:C:592:PRO:HD2	1:C:645:ILE:O	2.19	0.42
1:C:595:ARG:HD2	1:C:681:LEU:HD22	2.00	0.42
1:B:625:THR:HG21	1:B:663:GLY:HA2	2.00	0.42
1:A:529:ASN:ND2	2:A:101:ADP:H2	2.17	0.42
1:B:774:SER:HA	1:B:799:SER:O	2.20	0.42
1:C:478:ALA:C	1:C:480:LYS:H	2.22	0.41
1:B:592:PRO:HD2	1:B:645:ILE:O	2.19	0.41
1:A:479:TYR:HA	1:A:495:ARG:HH21	1.85	0.41
1:C:811:LEU:HB2	1:C:814:GLN:HG2	2.02	0.41
1:D:637:SER:HB2	1:D:687:TYR:OH	2.20	0.41
1:C:650:ARG:NH1	1:C:836:ARG:HH21	2.18	0.41
1:A:819:GLN:HB3	1:B:508:SER:HB3	2.01	0.41
1:C:731:VAL:HG12	1:C:854:MET:CE	2.51	0.41
1:C:774:SER:HA	1:C:799:SER:O	2.20	0.41
1:D:496:ARG:NH2	1:D:509:LEU:O	2.54	0.41
1:D:592:PRO:HD2	1:D:645:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:THR:HG23	1:B:490:ARG:CB	2.50	0.41
1:A:468:ILE:HG23	1:A:498:LEU:CD1	2.51	0.40
1:C:657:MET:HA	1:C:657:MET:CE	2.51	0.40
1:D:497:GLN:O	1:D:500:SER:HB3	2.21	0.40
1:A:592:PRO:HD2	1:A:645:ILE:O	2.21	0.40
1:B:731:VAL:HG12	1:B:854:MET:HE3	2.04	0.40
1:C:467:ILE:HG21	1:C:494:ILE:HD13	2.02	0.40
1:D:811:LEU:HB2	1:D:814:GLN:HG2	2.04	0.40
1:D:560:GLY:O	1:D:561:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	404/467 (86%)	385 (95%)	17 (4%)	2 (0%)	29	30
1	B	389/467 (83%)	372 (96%)	15 (4%)	2 (0%)	29	30
1	C	397/467 (85%)	382 (96%)	12 (3%)	3 (1%)	19	18
1	D	383/467 (82%)	366 (96%)	15 (4%)	2 (0%)	29	30
All	All	1573/1868 (84%)	1505 (96%)	59 (4%)	9 (1%)	25	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	C	478	ALA
1	C	479	TYR
1	D	465	ALA
1	B	525	ALA
1	D	514	TYR

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Mol	Chain	Res	Type
1	A	463	SER
1	C	485	ILE
1	B	485	ILE

5.3.2 Protein sidechains [i](#)

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	326/375 (87%)	311 (95%)	15 (5%)	27	32
1	B	312/375 (83%)	305 (98%)	7 (2%)	52	64
1	C	317/375 (84%)	309 (98%)	8 (2%)	47	58
1	D	307/375 (82%)	297 (97%)	10 (3%)	38	47
All	All	1262/1500 (84%)	1222 (97%)	40 (3%)	39	49

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	LEU
1	A	482	GLU
1	A	486	GLU
1	A	490	ARG
1	A	492	VAL
1	A	498	LEU
1	A	503	LEU
1	A	512	LEU
1	A	521	LEU
1	A	634	LEU
1	A	666	LYS
1	A	681	LEU
1	A	688	CYS
1	A	752	HIS
1	A	814	GLN
1	B	505	GLU
1	B	630	ARG
1	B	657	MET

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Mol	Chain	Res	Type
1	B	660	ILE
1	B	771	ASN
1	B	814	GLN
1	B	828	LYS
1	C	521	LEU
1	C	523	MET
1	C	617	VAL
1	C	634	LEU
1	C	657	MET
1	C	730	GLU
1	C	752	HIS
1	C	814	GLN
1	D	464	ASP
1	D	595	ARG
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	730	GLU
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN
1	D	828	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	469	GLN
1	A	567	ASN
1	A	814	GLN
1	B	632	GLN
1	B	635	HIS
1	B	752	HIS
1	C	469	GLN
1	C	819	GLN
1	D	488	HIS
1	D	788	ASN
1	D	819	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	102	-	24,29,29	1.32	3 (12%)	29,45,45	0.91	2 (6%)
2	ADP	A	103	-	24,29,29	1.56	4 (16%)	29,45,45	0.93	2 (6%)
2	ADP	D	105	-	24,29,29	1.39	4 (16%)	29,45,45	0.76	1 (3%)
3	117	C	4	-	38,44,44	1.76	9 (23%)	44,61,61	1.19	4 (9%)
3	117	A	2	-	38,44,44	1.83	7 (18%)	44,61,61	1.25	5 (11%)
2	ADP	A	101	-	24,29,29	1.32	2 (8%)	29,45,45	0.74	0
3	117	B	1	-	38,44,44	1.80	8 (21%)	44,61,61	1.20	4 (9%)
3	117	D	3	-	38,44,44	1.67	6 (15%)	44,61,61	1.29	4 (9%)
2	ADP	B	104	-	24,29,29	1.68	4 (16%)	29,45,45	0.79	1 (3%)

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	ADP	A	102	-	-	2/12/32/32	0/3/3/3
2	ADP	A	103	-	-	6/12/32/32	0/3/3/3
2	ADP	D	105	-	-	3/12/32/32	0/3/3/3
3	117	C	4	-	-	1/21/33/33	0/4/4/4
3	117	A	2	-	-	2/21/33/33	0/4/4/4
2	ADP	A	101	-	-	2/12/32/32	0/3/3/3
3	117	B	1	-	-	3/21/33/33	0/4/4/4
3	117	D	3	-	-	2/21/33/33	0/4/4/4
2	ADP	B	104	-	-	1/12/32/32	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	117	C19-N2	-6.95	1.27	1.41
3	B	1	117	C19-N2	-6.48	1.28	1.41
3	C	4	117	C19-N2	-6.27	1.28	1.41
3	D	3	117	C19-N2	-5.21	1.31	1.41
2	B	104	ADP	O4'-C1'	3.88	1.46	1.41
3	D	3	117	O1A-C1	3.78	1.34	1.22
3	B	1	117	O1A-C1	3.72	1.34	1.22
3	A	2	117	C9-C91	3.54	1.58	1.51
2	A	103	ADP	C8-N7	-3.47	1.28	1.34
2	D	105	ADP	C8-N7	-3.46	1.28	1.34
2	A	101	ADP	C8-N7	-3.44	1.28	1.34
3	C	4	117	O1A-C1	3.44	1.33	1.22
2	B	104	ADP	C8-N7	-3.42	1.28	1.34
3	A	2	117	O1A-C1	3.33	1.33	1.22
2	A	103	ADP	O4'-C4'	3.30	1.52	1.45
3	B	1	117	C18-N2	3.30	1.44	1.35
2	A	102	ADP	C8-N7	-3.25	1.28	1.34
3	D	3	117	C18-N2	3.20	1.44	1.35
3	D	3	117	C11-C18	3.19	1.55	1.51
3	D	3	117	C9-C91	3.18	1.57	1.51
2	B	104	ADP	O4'-C4'	3.14	1.52	1.45
3	C	4	117	C18-N2	3.11	1.44	1.35
3	C	4	117	C9-C91	3.08	1.57	1.51
3	B	1	117	C82-C83	2.86	1.42	1.36
2	A	103	ADP	O4'-C1'	2.83	1.45	1.41
3	A	2	117	C18-N2	2.63	1.42	1.35
3	B	1	117	C9-C91	2.63	1.56	1.51
3	A	2	117	O1B-C1	-2.62	1.21	1.30
2	D	105	ADP	O4'-C4'	2.60	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	117	C83-C84	2.59	1.42	1.37
2	B	104	ADP	C2'-C3'	2.55	1.60	1.53
3	C	4	117	C83-C84	2.53	1.42	1.37
2	A	101	ADP	O4'-C4'	2.48	1.50	1.45
2	D	105	ADP	O4'-C1'	2.44	1.44	1.41
3	B	1	117	O1B-C1	-2.43	1.22	1.30
2	A	103	ADP	C2'-C3'	2.43	1.60	1.53
3	B	1	117	C11-C18	2.34	1.54	1.51
3	C	4	117	O1B-C1	-2.33	1.22	1.30
3	C	4	117	C24-C19	2.32	1.43	1.39
3	A	2	117	C14-C13	2.25	1.41	1.36
2	A	102	ADP	O4'-C4'	2.24	1.50	1.45
2	A	102	ADP	C2'-C3'	2.21	1.59	1.53
3	A	2	117	C82-C83	2.17	1.41	1.36
3	C	4	117	C14-C13	2.15	1.41	1.36
3	C	4	117	C82-C83	2.10	1.41	1.36
2	D	105	ADP	C2'-C3'	2.07	1.59	1.53
3	D	3	117	C24-C19	2.03	1.42	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	117	C11-C18-N2	5.03	121.63	114.81
3	A	2	117	C11-C18-N2	4.88	121.42	114.81
3	C	4	117	C11-C18-N2	4.27	120.60	114.81
3	B	1	117	C11-C18-N2	3.60	119.69	114.81
3	B	1	117	O1A-C1-C2	-3.32	112.15	122.80
3	C	4	117	O1A-C1-C2	-3.30	112.22	122.80
3	D	3	117	O1A-C1-C2	-3.29	112.26	122.80
3	B	1	117	O1B-C1-C2	3.27	124.55	114.07
3	C	4	117	O1B-C1-C2	3.06	123.89	114.07
3	A	2	117	O1A-C1-C2	-3.00	113.16	122.80
3	D	3	117	O1B-C1-C2	2.98	123.62	114.07
3	A	2	117	O1B-C1-C2	2.80	123.05	114.07
3	B	1	117	C5-C4-C3	-2.65	110.15	114.18
3	A	2	117	O18-C18-C11	-2.56	116.71	122.63
2	A	103	ADP	C5-C6-N6	2.43	124.05	120.35
2	A	102	ADP	C3'-C2'-C1'	2.31	104.46	100.98
3	D	3	117	O18-C18-C11	-2.25	117.42	122.63
3	C	4	117	O18-C18-C11	-2.19	117.57	122.63
2	A	102	ADP	C5-C6-N6	2.11	123.56	120.35
2	B	104	ADP	C5-C6-N6	2.07	123.49	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	103	ADP	C3'-C2'-C1'	2.05	104.07	100.98
2	D	105	ADP	C5-C6-N6	2.03	123.44	120.35
3	A	2	117	C3-C2-C1	-2.02	108.91	112.97

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	ADP	O4'-C4'-C5'-O5'
2	A	101	ADP	C3'-C4'-C5'-O5'
2	A	103	ADP	PA-O3A-PB-O2B
2	A	103	ADP	C3'-C4'-C5'-O5'
2	D	105	ADP	PA-O3A-PB-O3B
3	A	2	117	O5-C5-C6-C7
3	B	1	117	O5-C5-C6-C7
3	D	3	117	O5-C5-C6-C7
2	A	103	ADP	O4'-C4'-C5'-O5'
2	A	102	ADP	C3'-C4'-C5'-O5'
2	A	102	ADP	O4'-C4'-C5'-O5'
2	A	103	ADP	C4'-C5'-O5'-PA
3	B	1	117	C4-C5-C6-C7
3	D	3	117	C4-C5-C6-C7
2	B	104	ADP	C4'-C5'-O5'-PA
2	A	103	ADP	PA-O3A-PB-O3B
3	A	2	117	C4-C5-C6-C7
2	D	105	ADP	C4'-C5'-O5'-PA
2	A	103	ADP	PA-O3A-PB-O1B
3	C	4	117	O5-C5-C6-C7
3	B	1	117	O1B-C1-C2-C3
2	D	105	ADP	PA-O3A-PB-O1B

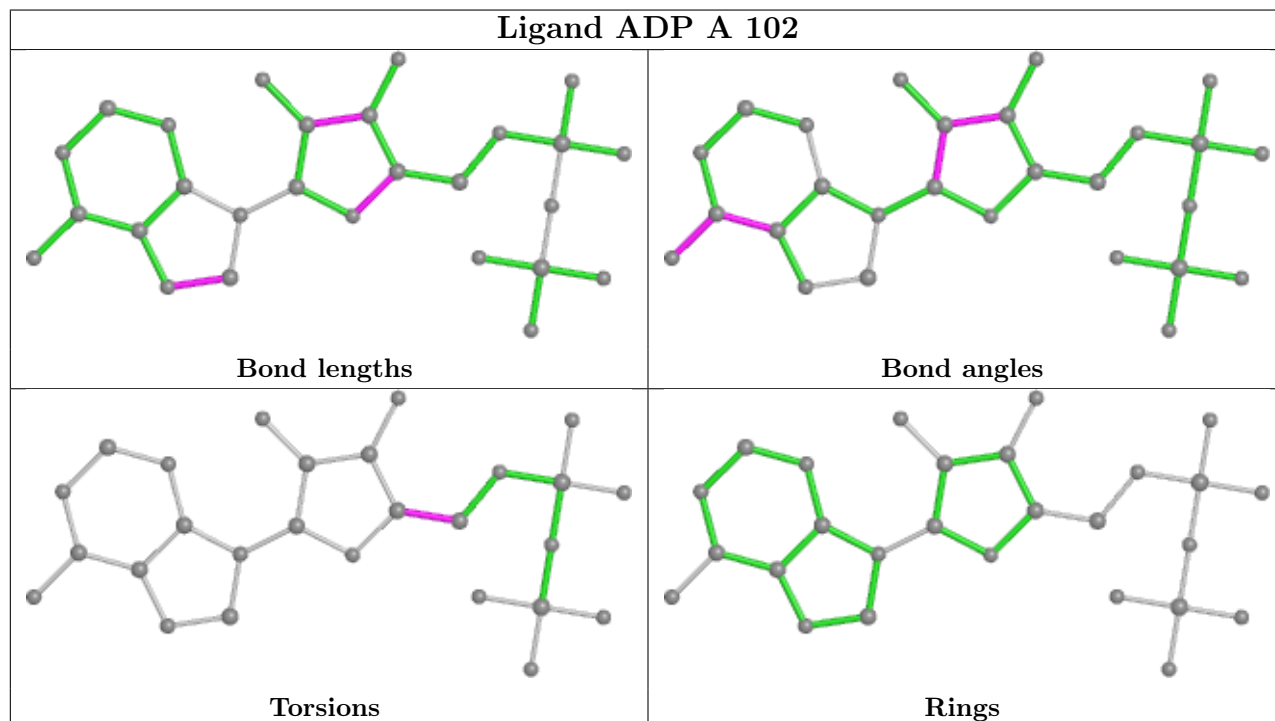
There are no ring outliers.

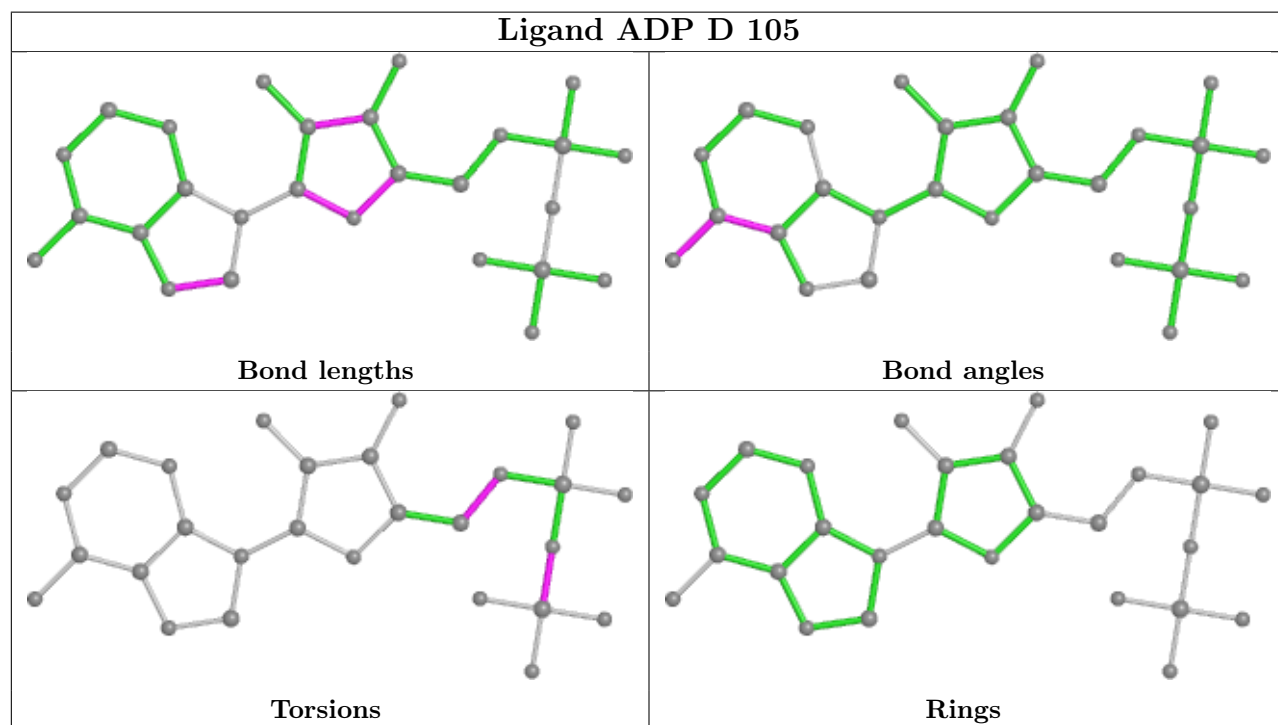
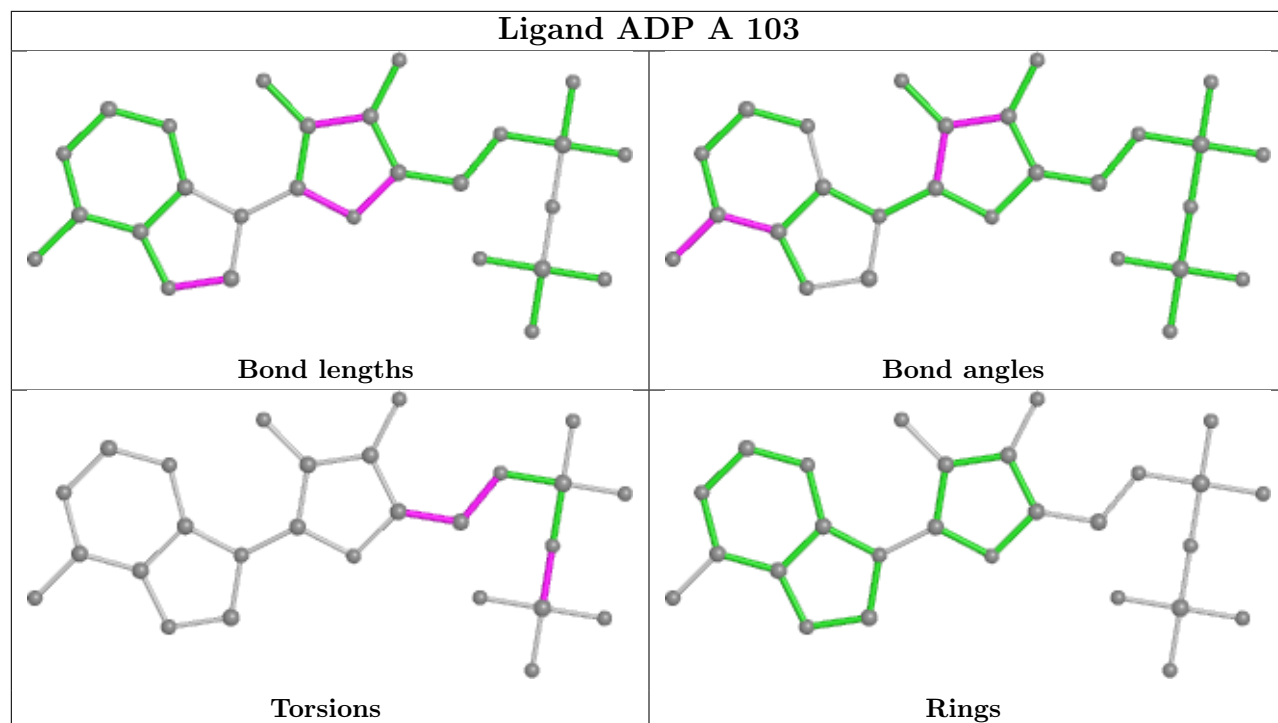
3 monomers are involved in 4 short contacts:

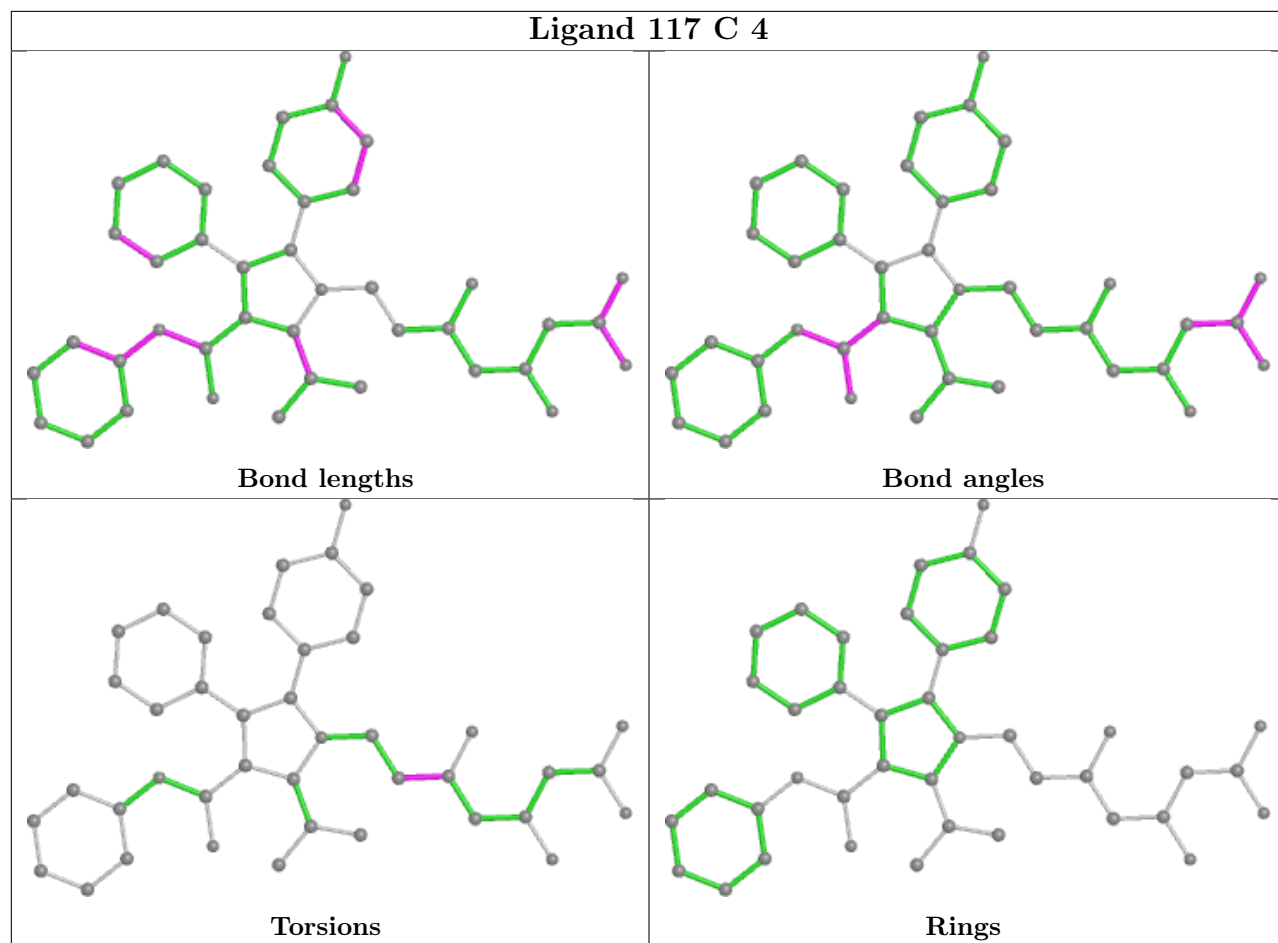
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	ADP	1	0
2	A	101	ADP	2	0
2	B	104	ADP	1	0

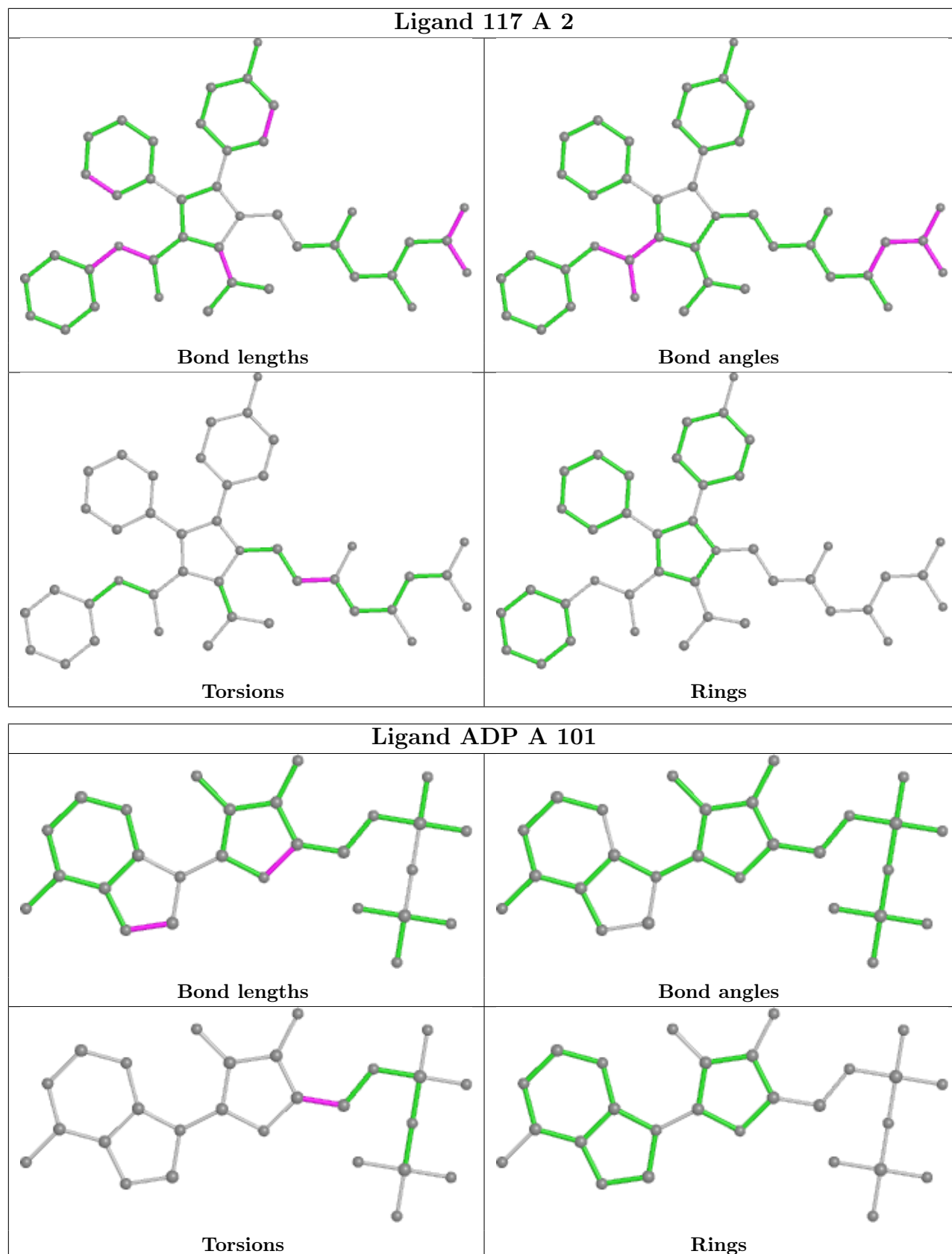
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

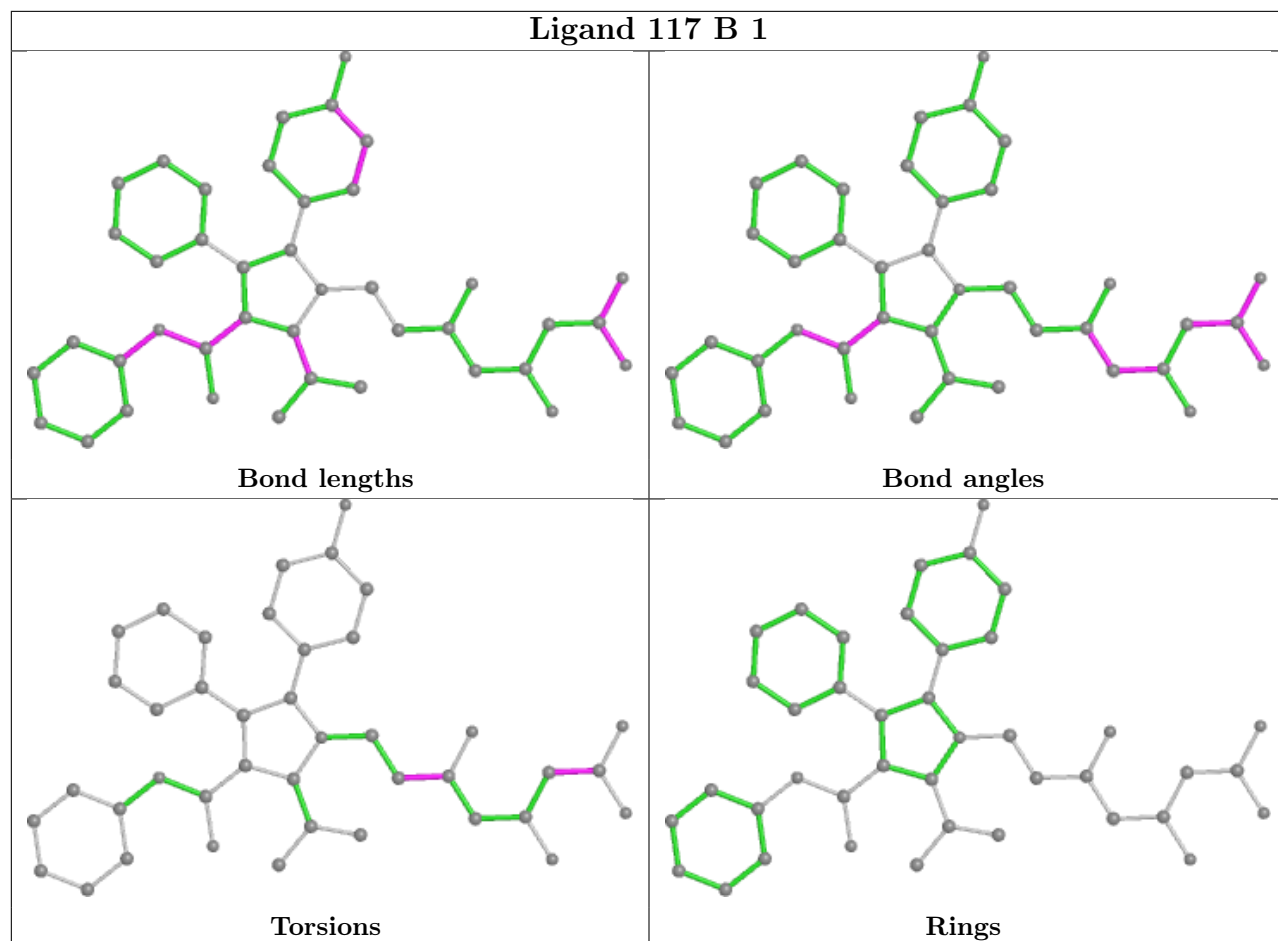
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

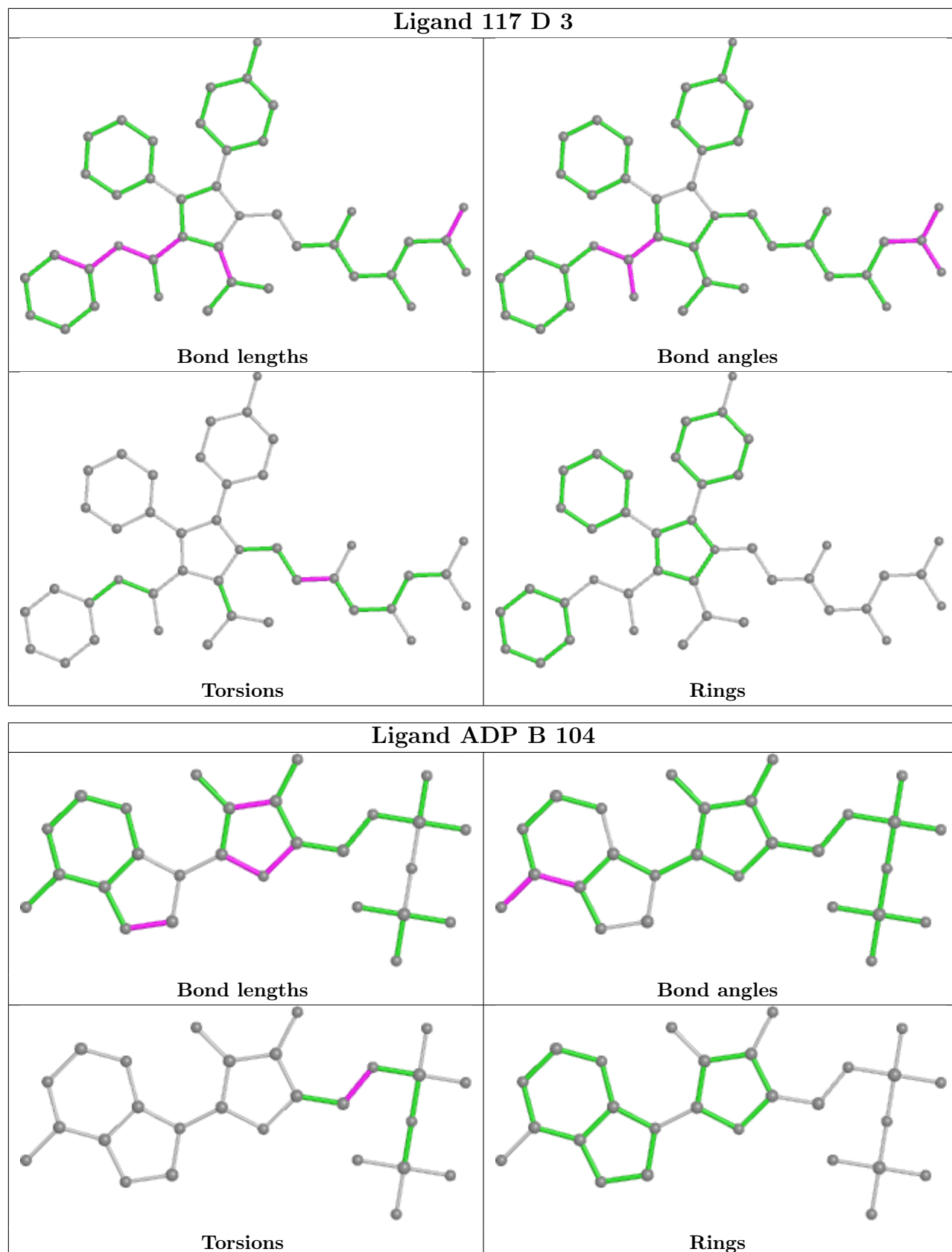












5.7 Other polymers [i](#)

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	408/467 (87%)	0.60	52 (12%) 3 3	30, 48, 93, 100	0
1	B	393/467 (84%)	0.48	40 (10%) 6 5	30, 48, 77, 100	0
1	C	399/467 (85%)	0.78	57 (14%) 2 2	32, 50, 94, 100	0
1	D	387/467 (82%)	0.48	47 (12%) 4 3	30, 45, 75, 100	0
All	All	1587/1868 (84%)	0.58	196 (12%) 4 3	30, 48, 91, 100	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	11.1
1	D	483	THR	9.0
1	C	475	HIS	9.0
1	D	467	ILE	8.5
1	A	484	LEU	8.3
1	C	476	ILE	7.6
1	A	475	HIS	7.5
1	C	477	PRO	7.4
1	A	473	ALA	7.4
1	D	484	LEU	7.1
1	C	483	THR	6.9
1	D	485	ILE	6.9
1	C	627	ARG	6.5
1	B	479	TYR	6.3
1	C	478	ALA	5.9
1	C	484	LEU	5.8
1	C	479	TYR	5.8
1	C	486	GLU	5.7
1	B	486	GLU	5.7
1	A	470	LEU	5.7
1	D	466	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	485	ILE	5.4
1	B	478	ALA	5.3
1	A	479	TYR	5.3
1	D	486	GLU	5.3
1	D	494	ILE	5.3
1	A	448	CYS	5.2
1	A	471	VAL	5.0
1	C	628	PHE	4.9
1	A	449	LEU	4.9
1	C	480	LYS	4.9
1	C	473	ALA	4.8
1	D	463	SER	4.8
1	B	483	THR	4.7
1	D	490	ARG	4.6
1	D	481	LEU	4.6
1	A	480	LYS	4.4
1	A	861	HIS	4.4
1	A	483	THR	4.4
1	D	487	THR	4.4
1	B	487	THR	4.2
1	B	746	ILE	4.2
1	D	464	ASP	4.2
1	A	477	PRO	4.1
1	B	523	MET	4.0
1	D	694	ALA	4.0
1	C	470	LEU	4.0
1	A	497	GLN	4.0
1	B	613	GLU	3.9
1	C	465	ALA	3.8
1	D	524	GLY	3.8
1	A	746	ILE	3.8
1	C	828	LYS	3.8
1	D	693	PRO	3.8
1	A	446	GLU	3.8
1	B	470	LEU	3.7
1	B	630	ARG	3.7
1	A	860	GLY	3.7
1	B	694	ALA	3.7
1	C	694	ALA	3.6
1	A	447	GLU	3.6
1	C	740	SER	3.6
1	A	445	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	485	ILE	3.6
1	C	699	ILE	3.6
1	D	523	MET	3.5
1	D	482	GLU	3.5
1	B	469	GLN	3.4
1	D	786	PRO	3.4
1	C	524	GLY	3.4
1	D	743	ALA	3.3
1	D	772	VAL	3.3
1	B	481	LEU	3.3
1	C	748	GLY	3.3
1	D	695	ALA	3.3
1	C	746	ILE	3.3
1	B	747	GLY	3.2
1	C	698	TRP	3.2
1	C	471	VAL	3.2
1	C	482	GLU	3.2
1	B	695	ALA	3.2
1	D	745	SER	3.2
1	C	757	VAL	3.1
1	A	829	ASP	3.1
1	A	498	LEU	3.1
1	C	772	VAL	3.1
1	C	469	GLN	3.1
1	A	472	ASN	3.1
1	A	772	VAL	3.0
1	B	698	TRP	3.0
1	C	630	ARG	3.0
1	D	746	ILE	3.0
1	B	471	VAL	3.0
1	A	501	LYS	3.0
1	B	741	ALA	2.9
1	A	481	LEU	2.9
1	C	689	THR	2.9
1	A	748	GLY	2.9
1	D	465	ALA	2.9
1	C	773	GLY	2.8
1	B	482	GLU	2.8
1	C	741	ALA	2.8
1	C	749	TYR	2.8
1	C	747	GLY	2.8
1	B	484	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	748	GLY	2.8
1	A	468	ILE	2.8
1	C	693	PRO	2.8
1	C	696	ILE	2.8
1	C	695	ALA	2.7
1	A	630	ARG	2.7
1	A	741	ALA	2.7
1	B	743	ALA	2.7
1	C	510	GLN	2.7
1	A	699	ILE	2.7
1	D	516	ASP	2.7
1	D	740	SER	2.7
1	D	696	ILE	2.7
1	D	747	GLY	2.7
1	C	474	LYS	2.6
1	A	478	ALA	2.6
1	D	469	GLN	2.6
1	C	523	MET	2.6
1	D	741	ALA	2.6
1	A	694	ALA	2.6
1	B	696	ILE	2.6
1	D	698	TRP	2.6
1	B	688	CYS	2.6
1	B	693	PRO	2.5
1	B	677	GLU	2.5
1	B	748	GLY	2.5
1	D	773	GLY	2.5
1	A	467	ILE	2.5
1	B	501	LYS	2.5
1	C	515	ARG	2.5
1	B	749	TYR	2.5
1	A	469	GLN	2.5
1	C	468	ILE	2.5
1	C	754	ALA	2.5
1	B	740	SER	2.4
1	A	523	MET	2.4
1	A	444	PRO	2.4
1	D	699	ILE	2.4
1	A	744	GLY	2.4
1	B	773	GLY	2.4
1	D	744	GLY	2.4
1	C	843	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	628	PHE	2.4
1	A	745	SER	2.4
1	A	828	LYS	2.4
1	C	701	GLY	2.4
1	D	775	SER	2.3
1	D	777	CYS	2.3
1	B	737	LEU	2.3
1	C	481	LEU	2.3
1	D	737	LEU	2.3
1	A	689	THR	2.3
1	C	771	ASN	2.3
1	D	689	THR	2.3
1	C	745	SER	2.3
1	C	743	ALA	2.3
1	C	761	TYR	2.3
1	D	627	ARG	2.3
1	A	620	GLU	2.3
1	B	608	TRP	2.3
1	B	777	CYS	2.3
1	C	616	ALA	2.3
1	C	753	ALA	2.3
1	C	777	CYS	2.3
1	A	474	LYS	2.3
1	A	830	ASN	2.3
1	D	749	TYR	2.3
1	A	789	GLU	2.2
1	A	502	LYS	2.2
1	B	745	SER	2.2
1	D	468	ILE	2.2
1	A	738	VAL	2.2
1	B	754	ALA	2.2
1	B	778	ILE	2.2
1	D	776	ASN	2.1
1	A	742	MET	2.1
1	B	744	GLY	2.1
1	B	771	ASN	2.1
1	A	715	LYS	2.1
1	C	697	ASN	2.1
1	D	720	VAL	2.1
1	C	796	THR	2.1
1	C	739	GLY	2.1
1	A	510	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	753	ALA	2.0
1	A	490	ARG	2.0
1	B	674	TYR	2.0
1	C	795	CYS	2.0
1	D	785	GLY	2.0
1	A	662	LYS	2.0
1	D	571	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

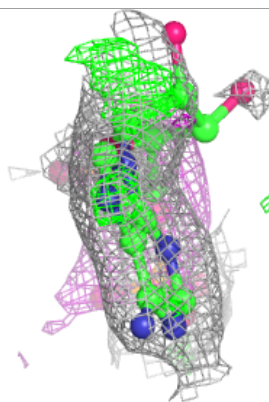
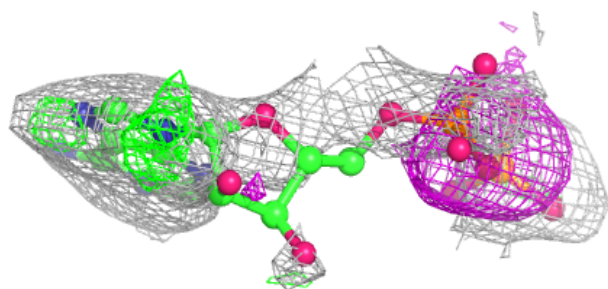
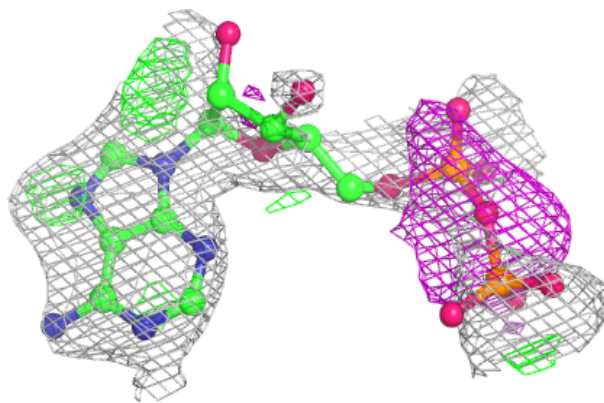
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADP	B	104	27/27	0.52	0.37	99,101,101,101	0
2	ADP	A	103	27/27	0.71	0.32	93,98,100,100	0
2	ADP	A	102	27/27	0.75	0.32	94,98,100,100	0
2	ADP	A	101	27/27	0.76	0.32	93,96,100,100	0
2	ADP	D	105	27/27	0.81	0.23	86,94,100,100	0
3	117	C	4	41/41	0.91	0.15	37,46,52,53	0
3	117	D	3	41/41	0.93	0.15	34,44,49,49	0
3	117	B	1	41/41	0.94	0.12	40,47,50,51	0
3	117	A	2	41/41	0.95	0.14	34,41,45,47	0

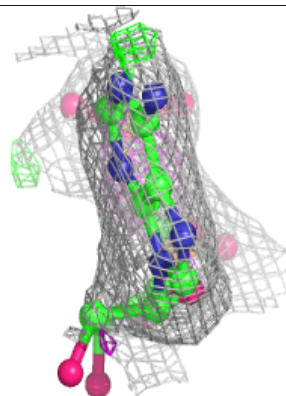
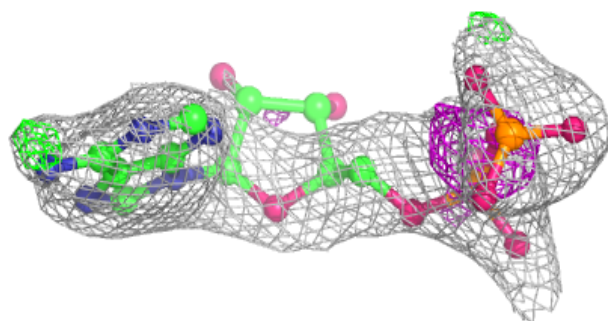
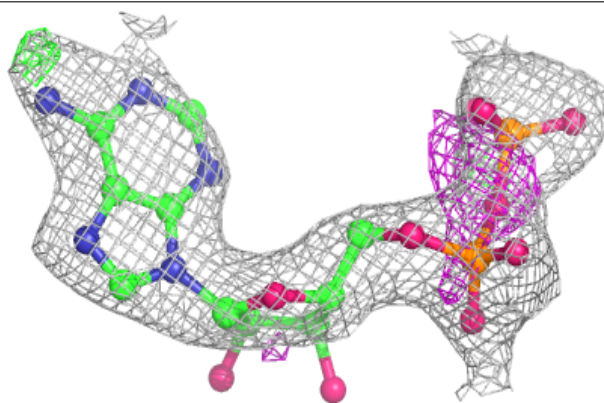
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 104:

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

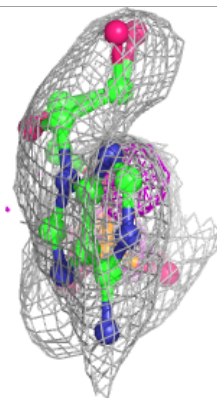
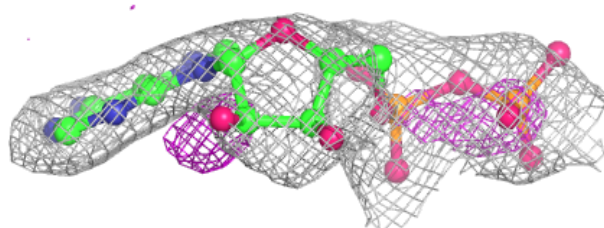
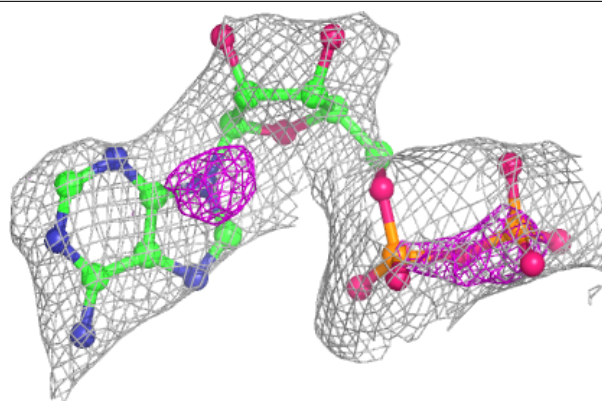
**Electron density around ADP A 103:**

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

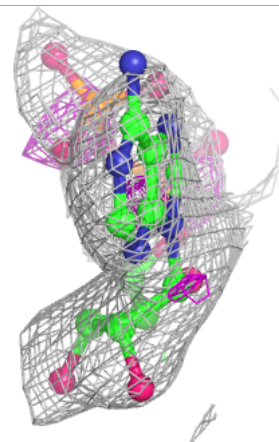
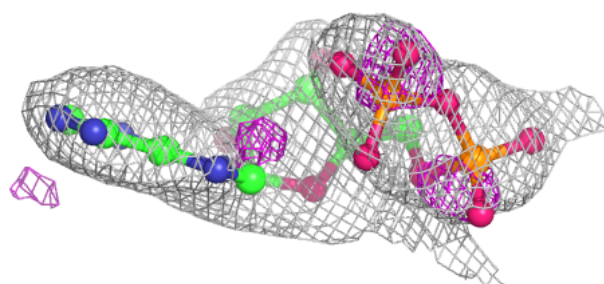
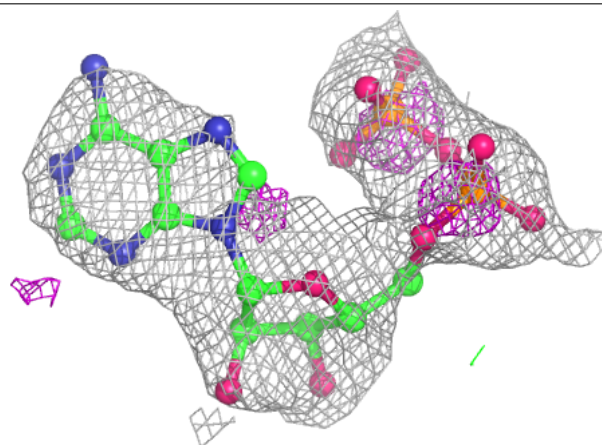


Electron density around ADP A 102:

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

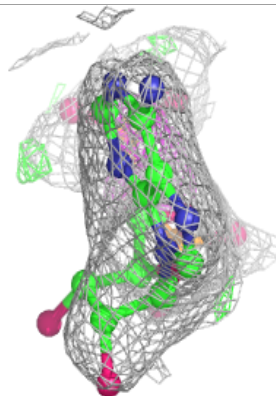
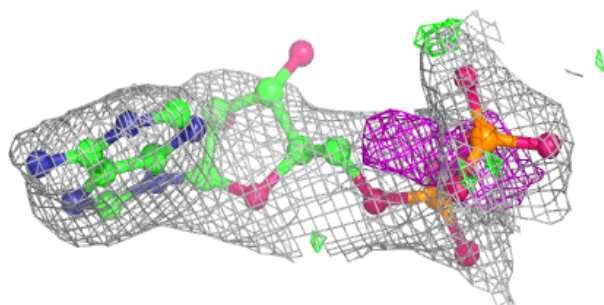
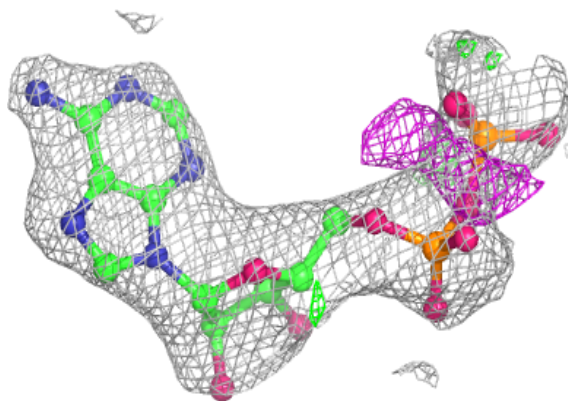
**Electron density around ADP A 101:**

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

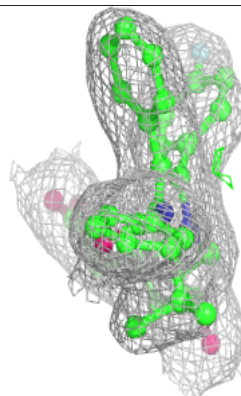
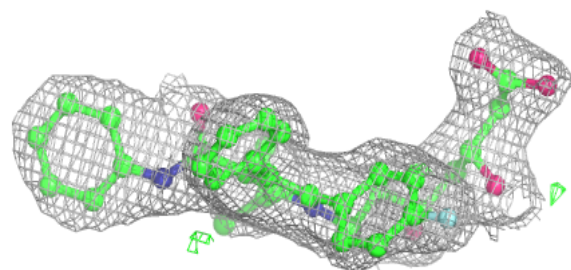
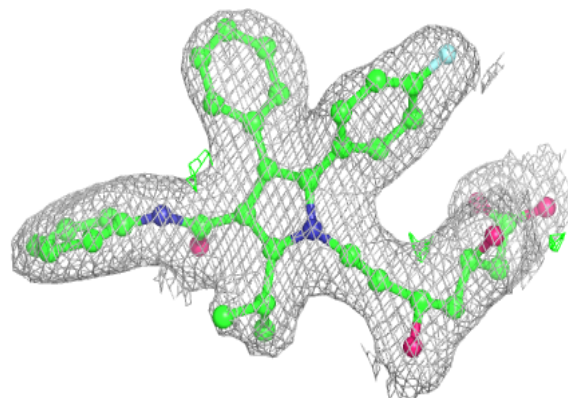


Electron density around ADP D 105:

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

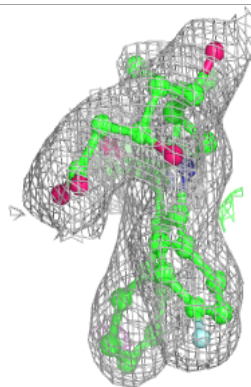
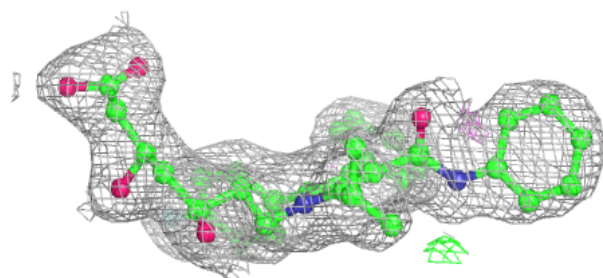
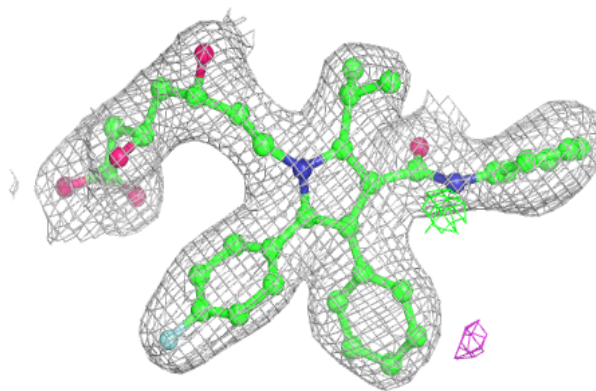
**Electron density around 117 C 4:**

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

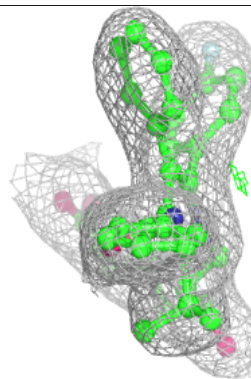
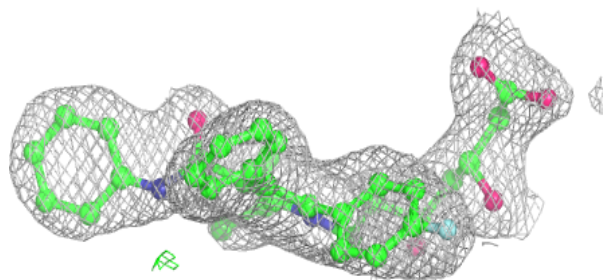
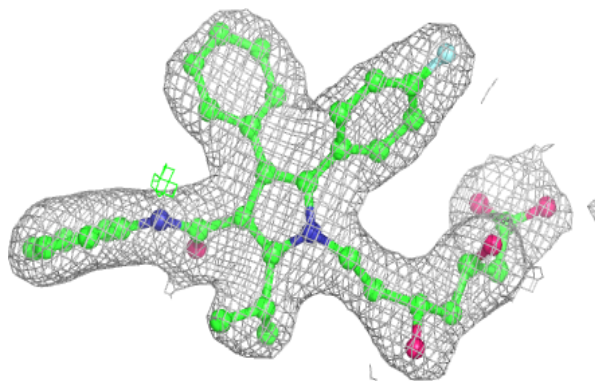


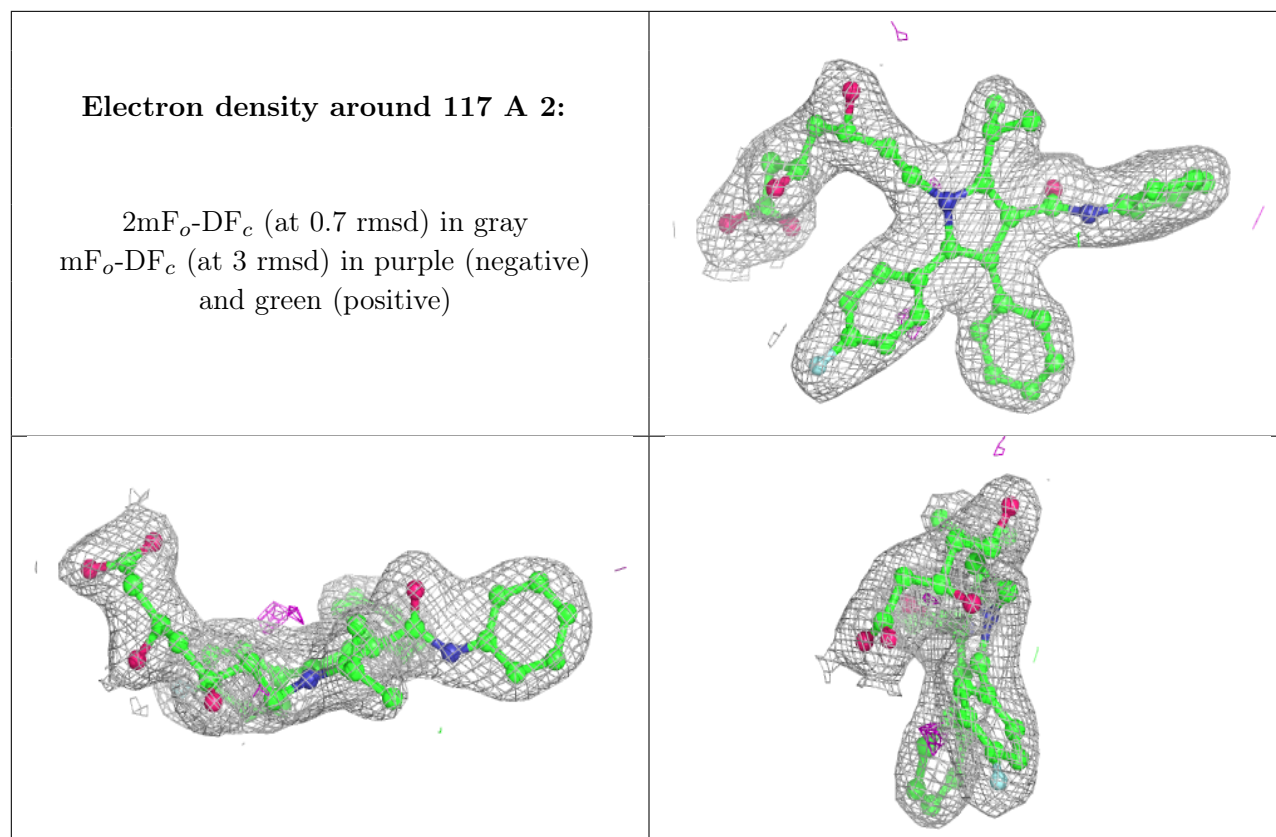
Electron density around 117 D 3:

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

**Electron density around 117 B 1:**

$2mF_o-DF_c$ (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.