Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 07:56 AM EDT

PDB ID	:	1HWJ
Title	:	COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH CERIVASTATIN
Authors	:	Istvan, E.S.; Deisenhofer, J.
Deposited on	:	2001-01-09
Resolution	:	2.26 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 (i) 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 (i)) were used in the production of this report:

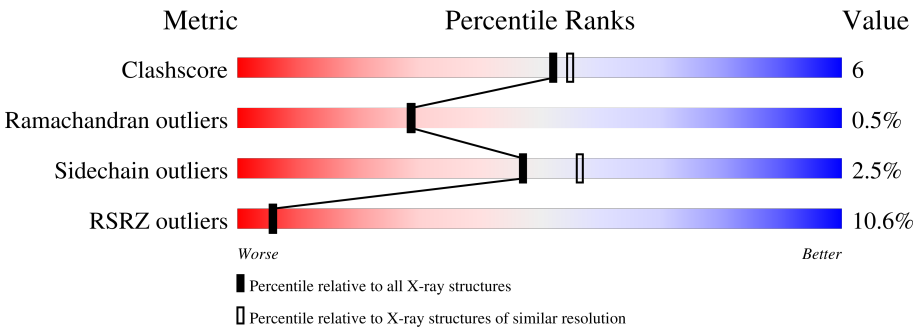
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	11% 75% 11% • 12%
1	B	467	7% 75% 9% • 15%
1	C	467	9% 73% 13% • 13%
1	D	467	9% 74% 9% • 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12418 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.

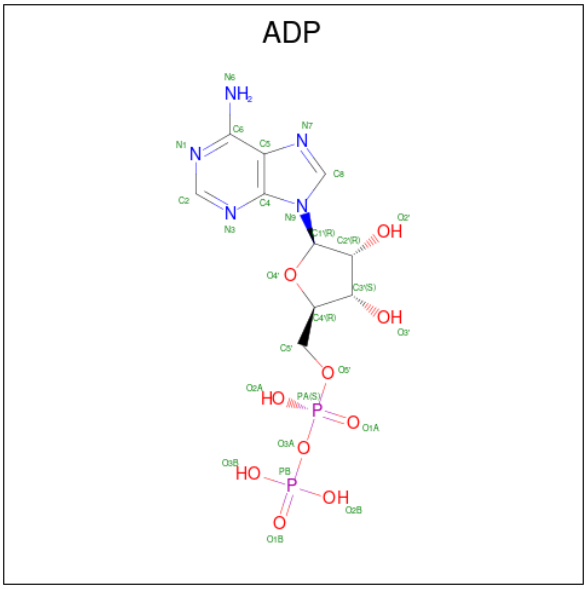
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3052	1900	537	585	30	0	0	0
1	B	398	2952	1838	518	567	29	0	0	0
1	C	408	3034	1888	533	583	30	0	0	0
1	D	392	2900	1803	508	560	29	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

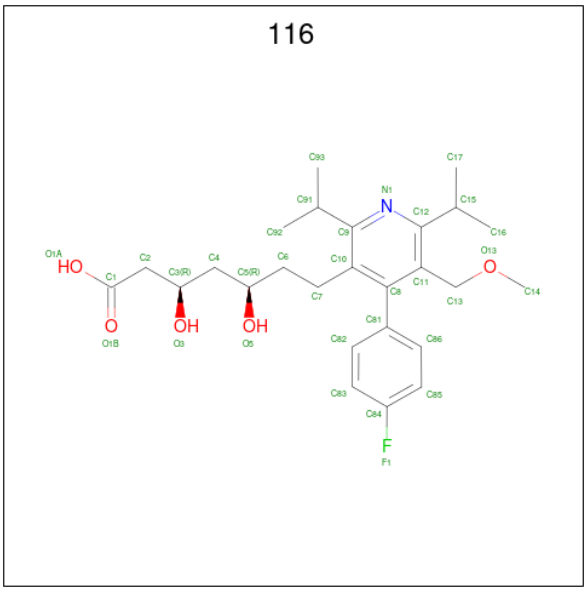
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	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	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	D	1	27	10	5	10	2	0	0

- Molecule 3 is 7-[4-(4-FLUORO-PHENYL)-5-HYDROXYMETHYL-2,6-DIISOPROPYL-PYRIDIN-3-YL]-3,5-DIHYDROXY-HEPTANOIC ACID (three-letter code: 116) (formula: $C_{26}H_{36}FNO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			33	26	1	1	5		
3	B	1	Total	C	F	N	O	0	0
			33	26	1	1	5		
3	C	1	Total	C	F	N	O	0	0
			33	26	1	1	5		
3	D	1	Total	C	F	N	O	0	0
			33	26	1	1	5		

- Molecule 4 is water.

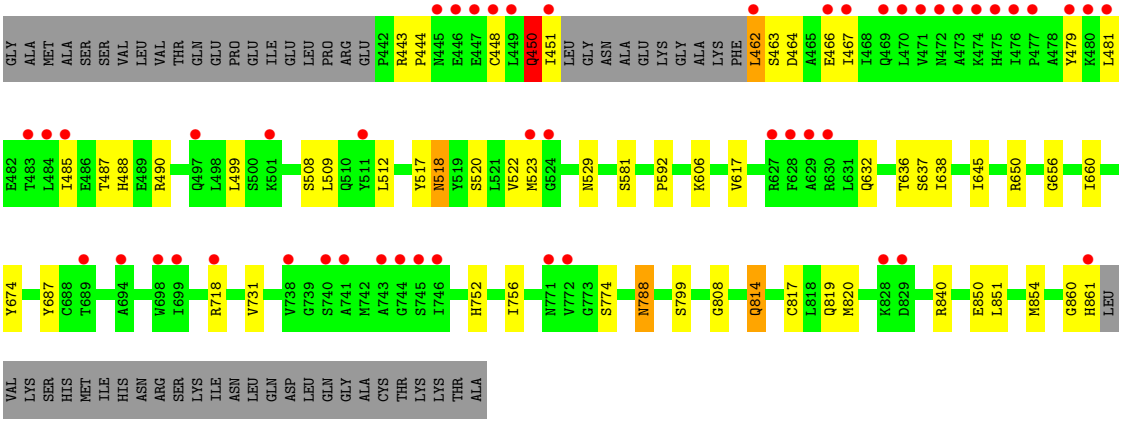
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	52	Total	O	0	0
			52	52		
4	C	33	Total	O	0	0
			33	33		
4	D	49	Total	O	0	0
			49	49		

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.

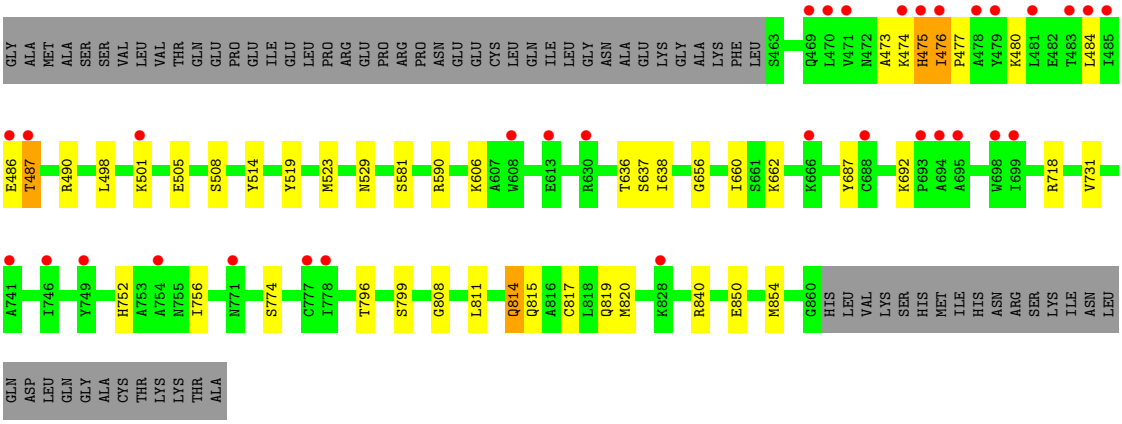
• Molecule 1: HMG-COA REDUCTASE

Chain A:



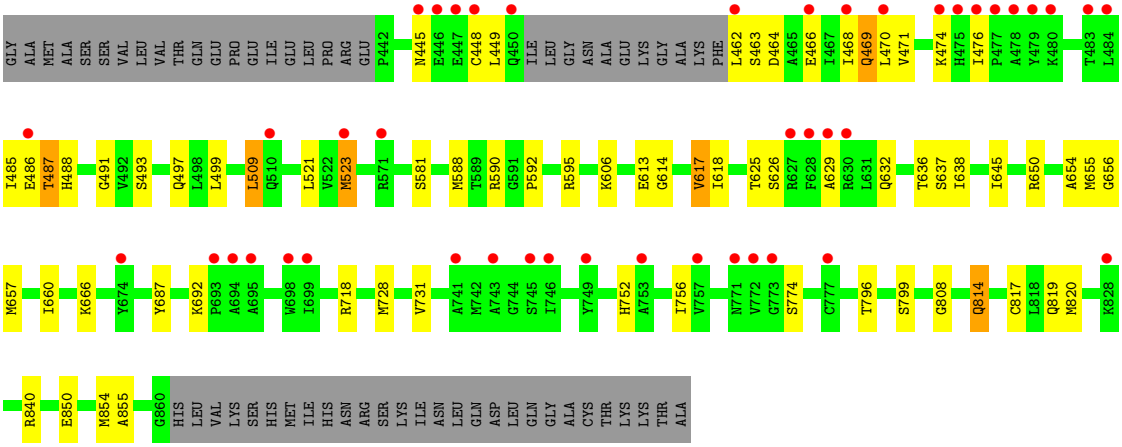
• Molecule 1: HMG-COA REDUCTASE

Chain B:



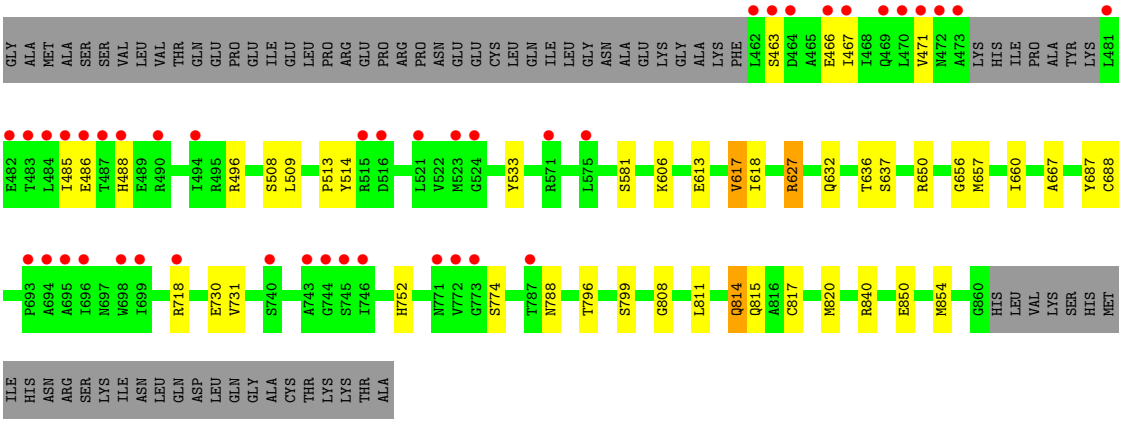
• Molecule 1: HMG-COA REDUCTASE

Chain C:



- Molecule 1: HMG-COA REDUCTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.62Å 172.98Å 80.16Å 90.00° 117.35° 90.00°	Depositor
Resolution (Å)	43.50 – 2.26 54.97 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.50-2.26) 93.0 (54.97-2.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.237 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12418	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, 116

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	0/3096	0.66	0/4186
1	B	0.46	0/2994	0.65	0/4049
1	C	0.47	0/3077	0.66	1/4160 (0.0%)
1	D	0.51	0/2938	0.65	0/3972
All	All	0.48	0/12105	0.65	1/16367 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	656	GLY	N-CA-C	5.29	126.34	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	3052	0	3087	33	0
1	B	2952	0	2989	29	0
1	C	3034	0	3069	45	0
1	D	2900	0	2934	27	0
2	A	54	0	24	1	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	54	0	24	1	0
2	D	27	0	12	0	0
3	A	33	0	35	2	0
3	B	33	0	35	2	0
3	C	33	0	35	3	0
3	D	33	0	35	1	0
4	A	52	0	0	1	0
4	B	52	0	0	1	0
4	C	33	0	0	1	0
4	D	49	0	0	2	0
All	All	12418	0	12291	135	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 6.

All (135) 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:485:ILE:HG22	1:C:486:GLU:H	1.37	0.89
1:A:487:THR:HG22	1:A:488:HIS:H	1.43	0.83
1:B:523:MET:HE1	4:B:1019:HOH:O	1.81	0.79
1:B:817:CYS:HA	1:B:820:MET:HE3	1.68	0.76
1:D:817:CYS:HA	1:D:820:MET:HE3	1.70	0.74
1:C:817:CYS:HA	1:C:820:MET:HE3	1.70	0.72
3:B:1:116:H91	3:B:1:116:H61	1.73	0.69
1:A:817:CYS:HA	1:A:820:MET:HE3	1.74	0.69
1:C:448:CYS:HB3	1:C:462:LEU:HD22	1.73	0.68
1:A:523:MET:HE1	4:A:1086:HOH:O	1.95	0.67
1:D:688:CYS:SG	4:D:1163:HOH:O	2.54	0.66
1:C:466:GLU:O	1:C:470:LEU:HG	1.96	0.65
1:D:467:ILE:O	1:D:471:VAL:HG23	1.97	0.64
1:C:655:MET:SD	1:C:657:MET:HG2	2.38	0.63
1:C:590:ARG:NH2	1:C:657:MET:HE3	2.14	0.62
1:C:485:ILE:HG22	1:C:486:GLU:N	2.11	0.62
1:C:632:GLN:HE21	1:C:650:ARG:HG3	1.65	0.60
3:A:2:116:H91	3:A:2:116:H61	1.84	0.60
1:D:656:GLY:O	1:D:660:ILE:HG12	2.03	0.58
1:B:476:ILE:HG21	1:B:484:LEU:HD11	1.86	0.57
1:C:588:MET:HB3	1:C:660:ILE:CD1	2.34	0.57
1:D:808:GLY:O	1:D:814:GLN:HG3	2.04	0.57
1:C:581:SER:OG	1:C:840:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:SER:OG	1:D:840:ARG:HD2	2.04	0.57
1:C:523:MET:HE1	4:C:1102:HOH:O	2.03	0.57
1:B:656:GLY:O	1:B:660:ILE:HG12	2.05	0.57
1:B:477:PRO:HD2	1:B:480:LYS:CG	2.35	0.57
1:A:581:SER:OG	1:A:840:ARG:HD2	2.05	0.56
1:C:808:GLY:O	1:C:814:GLN:HG3	2.07	0.55
1:A:656:GLY:O	1:A:660:ILE:HG12	2.06	0.54
1:B:581:SER:OG	1:B:840:ARG:HD2	2.08	0.54
3:C:4:116:H61	3:C:4:116:H91	1.90	0.53
3:D:3:116:H91	3:D:3:116:H61	1.90	0.53
1:C:463:SER:OG	1:C:466:GLU:HG2	2.08	0.53
1:C:654:ALA:HB1	2:C:104:ADP:O1B	2.09	0.52
1:B:519:TYR:O	1:B:523:MET:HG2	2.08	0.52
1:D:627:ARG:HD3	1:D:627:ARG:H	1.75	0.52
1:B:477:PRO:HD2	1:B:480:LYS:HG3	1.92	0.51
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.93	0.51
1:C:625:THR:HG23	1:C:666:LYS:HD3	1.93	0.51
1:A:487:THR:HG22	1:A:488:HIS:N	2.21	0.50
1:B:808:GLY:O	1:B:814:GLN:HG3	2.11	0.50
1:C:632:GLN:NE2	1:C:650:ARG:HG3	2.26	0.50
1:C:626:SER:HB3	1:C:629:ALA:HB2	1.93	0.50
1:D:485:ILE:HG22	1:D:486:GLU:N	2.27	0.50
1:B:774:SER:HA	1:B:799:SER:O	2.13	0.48
1:A:774:SER:HA	1:A:799:SER:O	2.13	0.48
1:D:774:SER:HA	1:D:799:SER:O	2.14	0.48
1:C:606:LYS:HG3	1:C:636:THR:OG1	2.14	0.48
1:C:637:SER:HB2	1:C:687:TYR:OH	2.13	0.48
1:A:448:CYS:HA	1:A:462:LEU:HD21	1.95	0.47
1:A:632:GLN:HE21	1:A:650:ARG:HG3	1.79	0.47
1:A:479:TYR:HB3	1:A:529:ASN:OD1	2.15	0.47
1:C:464:ASP:O	1:C:468:ILE:HG12	2.15	0.47
1:B:637:SER:HB2	1:B:687:TYR:OH	2.15	0.47
1:C:487:THR:OG1	1:C:488:HIS:N	2.48	0.47
1:A:637:SER:HB2	1:A:687:TYR:OH	2.14	0.47
1:C:523:MET:HA	1:C:523:MET:CE	2.45	0.47
1:D:463:SER:HB2	1:D:466:GLU:HG3	1.97	0.47
1:D:637:SER:HB2	1:D:687:TYR:OH	2.15	0.47
1:B:473:ALA:O	1:B:475:HIS:N	2.49	0.46
1:A:518:ASN:ND2	1:A:520:SER:OG	2.49	0.46
1:C:499:LEU:HD23	1:C:509:LEU:HD21	1.98	0.46
1:A:808:GLY:O	1:A:814:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:MET:HE2	1:A:820:MET:HB2	1.73	0.46
1:C:850:GLU:O	1:C:854:MET:HG2	2.14	0.46
1:C:474:LYS:HB2	1:C:476:ILE:HG13	1.98	0.46
1:C:655:MET:CE	1:C:657:MET:HG2	2.45	0.46
1:A:463:SER:HB3	1:A:466:GLU:CD	2.37	0.45
1:C:613:GLU:O	1:C:617:VAL:HG12	2.17	0.45
1:C:774:SER:HA	1:C:799:SER:O	2.16	0.45
1:C:471:VAL:HG13	1:C:476:ILE:O	2.17	0.45
1:A:467:ILE:HD11	1:A:490:ARG:HH21	1.82	0.45
1:A:606:LYS:HG3	1:A:636:THR:OG1	2.17	0.45
1:C:820:MET:HE2	1:C:820:MET:HB2	1.86	0.44
1:B:850:GLU:O	1:B:854:MET:HG2	2.16	0.44
1:A:499:LEU:HD23	1:A:509:LEU:HD21	2.00	0.44
1:D:820:MET:HE2	1:D:820:MET:HB2	1.85	0.44
1:C:485:ILE:HD12	1:C:491:GLY:HA2	1.98	0.44
1:D:850:GLU:O	1:D:854:MET:HG2	2.17	0.44
1:B:638:ILE:O	1:C:796:THR:HG21	2.18	0.44
1:C:592:PRO:HD2	1:C:645:ILE:O	2.17	0.43
1:D:606:LYS:HG3	1:D:636:THR:OG1	2.18	0.43
1:C:614:GLY:O	1:C:618:ILE:HG12	2.17	0.43
1:C:731:VAL:HG12	1:C:854:MET:CE	2.48	0.43
1:A:850:GLU:O	1:A:854:MET:HG2	2.19	0.43
1:B:796:THR:HG21	1:C:638:ILE:O	2.18	0.43
1:A:450:GLN:HB2	1:A:451:ILE:H	1.60	0.43
1:D:731:VAL:HG12	1:D:854:MET:HE3	2.00	0.43
1:B:606:LYS:HG3	1:B:636:THR:OG1	2.18	0.43
1:A:638:ILE:O	1:D:796:THR:HG21	2.19	0.43
1:B:731:VAL:HG12	1:B:854:MET:CE	2.48	0.43
1:C:595:ARG:HH22	1:D:730:GLU:HG2	1.84	0.43
1:A:617:VAL:HG11	1:A:674:TYR:CE1	2.53	0.43
1:A:508:SER:HB2	1:B:819:GLN:CB	2.48	0.42
1:B:498:LEU:O	1:B:501:LYS:HG2	2.20	0.42
2:A:102:ADP:H2	1:B:529:ASN:HD21	1.66	0.42
1:C:692:LYS:HE2	1:C:692:LYS:HB2	1.91	0.42
1:D:618:ILE:HG23	1:D:667:ALA:HB1	2.02	0.42
1:A:731:VAL:HG12	1:A:854:MET:CE	2.49	0.42
1:B:486:GLU:O	1:B:487:THR:HB	2.20	0.42
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.80	0.42
1:A:632:GLN:NE2	1:A:650:ARG:HG3	2.34	0.42
1:D:731:VAL:HG12	1:D:854:MET:CE	2.50	0.42
1:A:481:LEU:O	1:A:485:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ILE:HD12	1:A:756:ILE:N	2.34	0.42
1:A:819:GLN:CB	1:B:508:SER:HB2	2.50	0.42
1:D:627:ARG:HD3	1:D:627:ARG:N	2.35	0.42
1:D:811:LEU:O	1:D:815:GLN:HG3	2.19	0.42
1:C:756:ILE:HD12	1:C:756:ILE:N	2.35	0.41
1:D:513:PRO:HB2	1:D:533:TYR:CZ	2.55	0.41
1:D:613:GLU:O	1:D:617:VAL:HG13	2.20	0.41
1:B:692:LYS:HE2	1:B:692:LYS:HB2	1.94	0.41
1:C:731:VAL:HG12	1:C:854:MET:HE3	2.01	0.41
1:A:462:LEU:HB2	1:A:463:SER:H	1.52	0.41
1:A:788:ASN:HD22	1:A:788:ASN:HA	1.68	0.41
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.80	0.41
1:A:592:PRO:HD2	1:A:645:ILE:O	2.20	0.41
3:A:2:116:C86	3:A:2:116:H72	2.51	0.41
1:A:517:TYR:HE2	1:A:522:VAL:HG21	1.86	0.41
1:B:662:LYS:HE2	1:B:662:LYS:HB3	1.93	0.41
1:B:476:ILE:HG22	1:B:480:LYS:HB2	2.02	0.41
3:C:4:116:C86	3:C:4:116:H72	2.51	0.41
1:C:493:SER:O	1:C:497:GLN:HG3	2.21	0.41
1:D:496:ARG:NH2	1:D:509:LEU:O	2.53	0.41
1:B:811:LEU:O	1:B:815:GLN:HG3	2.21	0.41
3:B:1:116:H61	3:B:1:116:C91	2.46	0.40
1:C:728:MET:SD	1:C:855:ALA:HA	2.61	0.40
3:C:4:116:H61	3:C:4:116:C91	2.51	0.40
1:A:443:ARG:HA	1:A:444:PRO:HD3	1.86	0.40
1:B:756:ILE:HD12	1:B:756:ILE:N	2.36	0.40
1:C:445:ASN:OD1	1:C:469:GLN:HB3	2.21	0.40
1:C:819:GLN:HB2	1:D:508:SER:HB2	2.02	0.40
1:D:632:GLN:HE21	1:D:650:ARG:HG3	1.85	0.40
1:D:657:MET:HG2	4:D:1186:HOH:O	2.21	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	406/467 (87%)	386 (95%)	18 (4%)	2 (0%)	29	29
1	B	396/467 (85%)	375 (95%)	17 (4%)	4 (1%)	15	13
1	C	404/467 (86%)	379 (94%)	24 (6%)	1 (0%)	47	55
1	D	388/467 (83%)	371 (96%)	16 (4%)	1 (0%)	41	46
All	All	1594/1868 (85%)	1511 (95%)	75 (5%)	8 (0%)	29	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	860	GLY
1	B	474	LYS
1	B	475	HIS
1	B	487	THR
1	C	449	LEU
1	B	514	TYR
1	D	514	TYR

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	328/375 (88%)	317 (97%)	11 (3%)	37	45
1	B	316/375 (84%)	311 (98%)	5 (2%)	62	73
1	C	326/375 (87%)	317 (97%)	9 (3%)	43	52
1	D	311/375 (83%)	304 (98%)	7 (2%)	50	59
All	All	1281/1500 (85%)	1249 (98%)	32 (2%)	47	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	462	LEU
1	A	464	ASP
1	A	512	LEU
1	A	518	ASN
1	A	718	ARG
1	A	752	HIS
1	A	788	ASN
1	A	814	GLN
1	A	851	LEU
1	A	861	HIS
1	B	476	ILE
1	B	505	GLU
1	B	718	ARG
1	B	752	HIS
1	B	814	GLN
1	C	469	GLN
1	C	487	THR
1	C	509	LEU
1	C	521	LEU
1	C	523	MET
1	C	617	VAL
1	C	718	ARG
1	C	752	HIS
1	C	814	GLN
1	D	488	HIS
1	D	617	VAL
1	D	627	ARG
1	D	718	ARG
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	635	HIS
1	A	788	ASN
1	A	819	GLN
1	B	469	GLN
1	B	488	HIS
1	B	635	HIS

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Mol	Chain	Res	Type
1	B	819	GLN
1	C	450	GLN
1	C	469	GLN
1	C	510	GLN
1	C	632	GLN
1	C	635	HIS
1	C	819	GLN
1	D	469	GLN
1	D	635	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)

10 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	C	103	-	24,29,29	1.27	2 (8%)	29,45,45	0.99	1 (3%)
2	ADP	A	101	-	24,29,29	1.21	1 (4%)	29,45,45	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	116	D	3	-	33,34,34	1.85	5 (15%)	35,47,47	1.52	5 (14%)
2	ADP	A	102	-	24,29,29	1.29	2 (8%)	29,45,45	0.78	1 (3%)
2	ADP	C	104	-	24,29,29	1.37	3 (12%)	29,45,45	0.72	1 (3%)
2	ADP	D	106	-	24,29,29	1.46	4 (16%)	29,45,45	0.74	1 (3%)
3	116	A	2	-	33,34,34	1.72	7 (21%)	35,47,47	1.56	4 (11%)
3	116	C	4	-	33,34,34	1.78	7 (21%)	35,47,47	1.64	5 (14%)
3	116	B	1	-	33,34,34	1.84	5 (15%)	35,47,47	1.62	8 (22%)
2	ADP	B	105	-	24,29,29	1.59	5 (20%)	29,45,45	0.77	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	C	103	-	-	2/12/32/32	0/3/3/3
2	ADP	A	101	-	-	2/12/32/32	0/3/3/3
3	116	D	3	-	-	3/24/28/28	0/2/2/2
2	ADP	A	102	-	-	2/12/32/32	0/3/3/3
2	ADP	C	104	-	-	6/12/32/32	0/3/3/3
2	ADP	D	106	-	-	6/12/32/32	0/3/3/3
3	116	A	2	-	-	3/24/28/28	0/2/2/2
3	116	C	4	-	-	3/24/28/28	0/2/2/2
3	116	B	1	-	-	6/24/28/28	0/2/2/2
2	ADP	B	105	-	-	1/12/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	116	C12-C15	6.07	1.59	1.51
3	A	2	116	C12-C15	5.08	1.58	1.51
3	C	4	116	C12-C15	5.06	1.58	1.51
3	B	1	116	C12-C15	4.86	1.58	1.51
3	B	1	116	C13-C11	4.64	1.57	1.51
3	D	3	116	C6-C7	-4.37	1.33	1.52
3	C	4	116	C9-C91	4.22	1.57	1.51
3	B	1	116	C9-C91	4.19	1.57	1.51
3	A	2	116	C6-C7	-4.16	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	116	C6-C7	-4.14	1.34	1.52
3	D	3	116	C9-C91	4.07	1.56	1.51
3	B	1	116	C6-C7	-3.82	1.35	1.52
2	C	103	ADP	C8-N7	-3.81	1.27	1.34
3	A	2	116	C9-C91	3.66	1.56	1.51
2	B	105	ADP	O4'-C1'	3.53	1.46	1.41
2	D	106	ADP	C8-N7	-3.49	1.28	1.34
2	A	101	ADP	C8-N7	-3.41	1.28	1.34
2	A	102	ADP	C8-N7	-3.38	1.28	1.34
2	B	105	ADP	C8-N7	-3.31	1.28	1.34
2	C	104	ADP	C8-N7	-3.26	1.28	1.34
3	D	3	116	C13-C11	3.09	1.55	1.51
2	B	105	ADP	O4'-C4'	3.02	1.51	1.45
3	A	2	116	C13-C11	2.96	1.54	1.51
3	C	4	116	C7-C10	2.74	1.57	1.52
2	C	104	ADP	O4'-C4'	2.73	1.51	1.45
2	D	106	ADP	O4'-C4'	2.70	1.51	1.45
3	C	4	116	C13-C11	2.61	1.54	1.51
2	D	106	ADP	O4'-C1'	2.54	1.44	1.41
2	B	105	ADP	C2'-C3'	2.45	1.60	1.53
2	C	104	ADP	O4'-C1'	2.40	1.44	1.41
2	A	102	ADP	O4'-C4'	2.25	1.50	1.45
3	B	1	116	C7-C10	2.23	1.56	1.52
3	C	4	116	C82-C83	2.20	1.41	1.36
3	A	2	116	C7-C10	2.17	1.56	1.52
2	D	106	ADP	C2'-C3'	2.16	1.59	1.53
3	C	4	116	C83-C84	2.14	1.41	1.37
2	B	105	ADP	O2'-C2'	2.11	1.47	1.43
3	A	2	116	C4-C5	2.07	1.57	1.52
2	C	103	ADP	C2'-C3'	2.06	1.59	1.53
3	D	3	116	C9-N1	-2.03	1.31	1.34
3	A	2	116	C86-C85	2.02	1.40	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	116	C7-C6-C5	6.04	126.68	115.05
3	D	3	116	C7-C6-C5	5.40	125.44	115.05
3	B	1	116	C7-C6-C5	5.25	125.14	115.05
3	A	2	116	C7-C6-C5	5.20	125.06	115.05
3	C	4	116	C10-C9-N1	-3.86	119.40	122.67
3	D	3	116	C11-C12-N1	-3.57	119.65	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	116	C10-C9-N1	-3.42	119.78	122.67
3	B	1	116	C10-C9-N1	-3.38	119.82	122.67
3	D	3	116	C10-C9-N1	-3.24	119.93	122.67
3	A	2	116	C11-C12-N1	-3.21	119.96	122.67
3	B	1	116	C11-C12-N1	-3.11	120.04	122.67
3	C	4	116	C11-C12-N1	-2.99	120.14	122.67
3	A	2	116	C13-C11-C12	-2.95	118.58	121.79
3	D	3	116	C13-C11-C12	-2.89	118.64	121.79
3	B	1	116	C13-C11-C12	-2.79	118.75	121.79
3	C	4	116	C13-C11-C12	-2.68	118.88	121.79
3	C	4	116	C92-C91-C9	2.39	114.99	110.96
3	B	1	116	C13-C11-C8	2.37	123.07	120.41
3	B	1	116	O13-C13-C11	2.26	112.58	108.72
2	C	104	ADP	C5-C6-N6	2.24	123.75	120.35
2	B	105	ADP	C5-C6-N6	2.18	123.67	120.35
2	C	103	ADP	C3'-C2'-C1'	2.14	104.21	100.98
2	D	106	ADP	C5-C6-N6	2.13	123.59	120.35
2	A	101	ADP	C5-C6-N6	2.09	123.53	120.35
3	B	1	116	C85-C84-C83	-2.08	120.06	122.83
3	B	1	116	C92-C91-C9	2.07	114.45	110.96
2	A	102	ADP	C5-C6-N6	2.02	123.42	120.35
3	D	3	116	C13-C11-C8	2.01	122.66	120.41

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	104	ADP	PA-O3A-PB-O3B
2	C	104	ADP	C3'-C4'-C5'-O5'
2	D	106	ADP	PA-O3A-PB-O3B
3	A	2	116	C9-C10-C7-C6
3	A	2	116	C4-C5-C6-C7
3	B	1	116	C9-C10-C7-C6
3	B	1	116	C4-C5-C6-C7
3	C	4	116	C9-C10-C7-C6
3	C	4	116	C4-C5-C6-C7
3	D	3	116	C9-C10-C7-C6
3	D	3	116	C4-C5-C6-C7
3	D	3	116	O5-C5-C6-C7
2	D	106	ADP	C3'-C4'-C5'-O5'
2	C	103	ADP	C3'-C4'-C5'-O5'
3	A	2	116	O5-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	B	1	116	O5-C5-C6-C7
3	C	4	116	O5-C5-C6-C7
2	C	103	ADP	O4'-C4'-C5'-O5'
2	C	104	ADP	O4'-C4'-C5'-O5'
2	A	102	ADP	O4'-C4'-C5'-O5'
2	D	106	ADP	O4'-C4'-C5'-O5'
2	A	102	ADP	C3'-C4'-C5'-O5'
2	C	104	ADP	C4'-C5'-O5'-PA
2	A	101	ADP	C3'-C4'-C5'-O5'
2	B	105	ADP	C4'-C5'-O5'-PA
2	D	106	ADP	C4'-C5'-O5'-PA
2	A	101	ADP	O4'-C4'-C5'-O5'
3	B	1	116	O1A-C1-C2-C3
3	B	1	116	O1B-C1-C2-C3
2	C	104	ADP	PA-O3A-PB-O1B
3	B	1	116	C8-C10-C7-C6
2	D	106	ADP	PA-O3A-PB-O1B
2	C	104	ADP	PA-O3A-PB-O2B
2	D	106	ADP	PA-O3A-PB-O2B

There are no ring outliers.

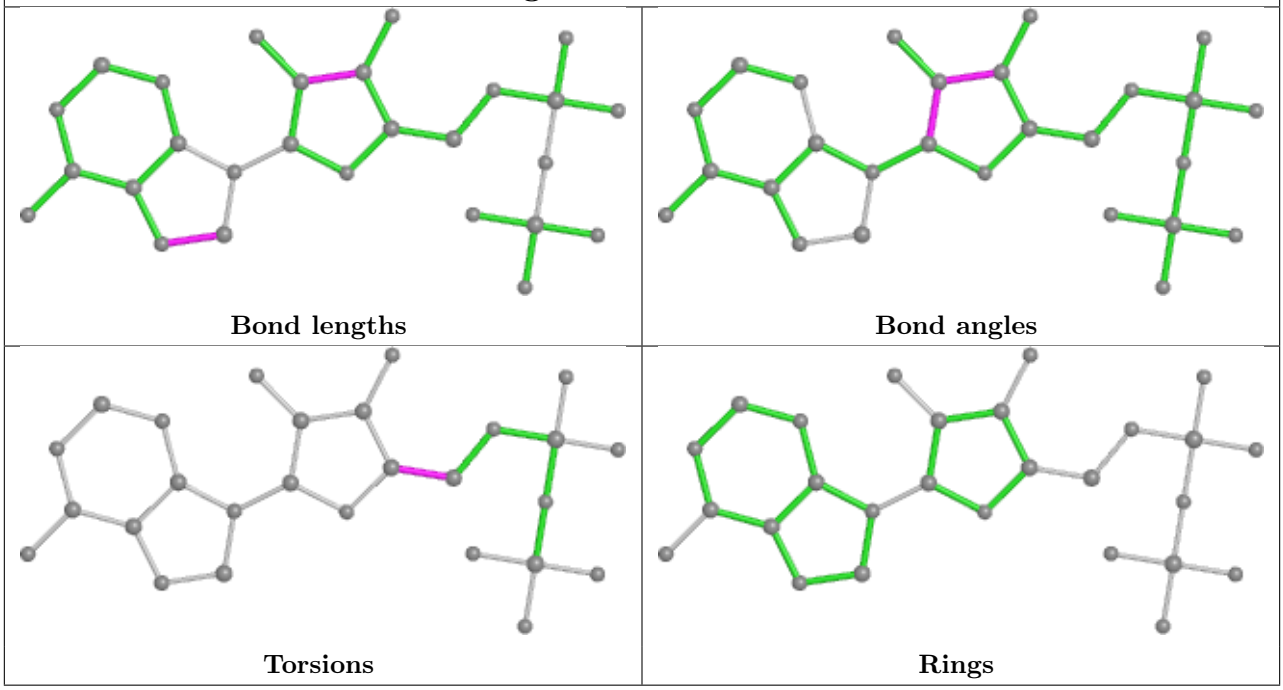
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	116	1	0
2	A	102	ADP	1	0
2	C	104	ADP	1	0
3	A	2	116	2	0
3	C	4	116	3	0
3	B	1	116	2	0

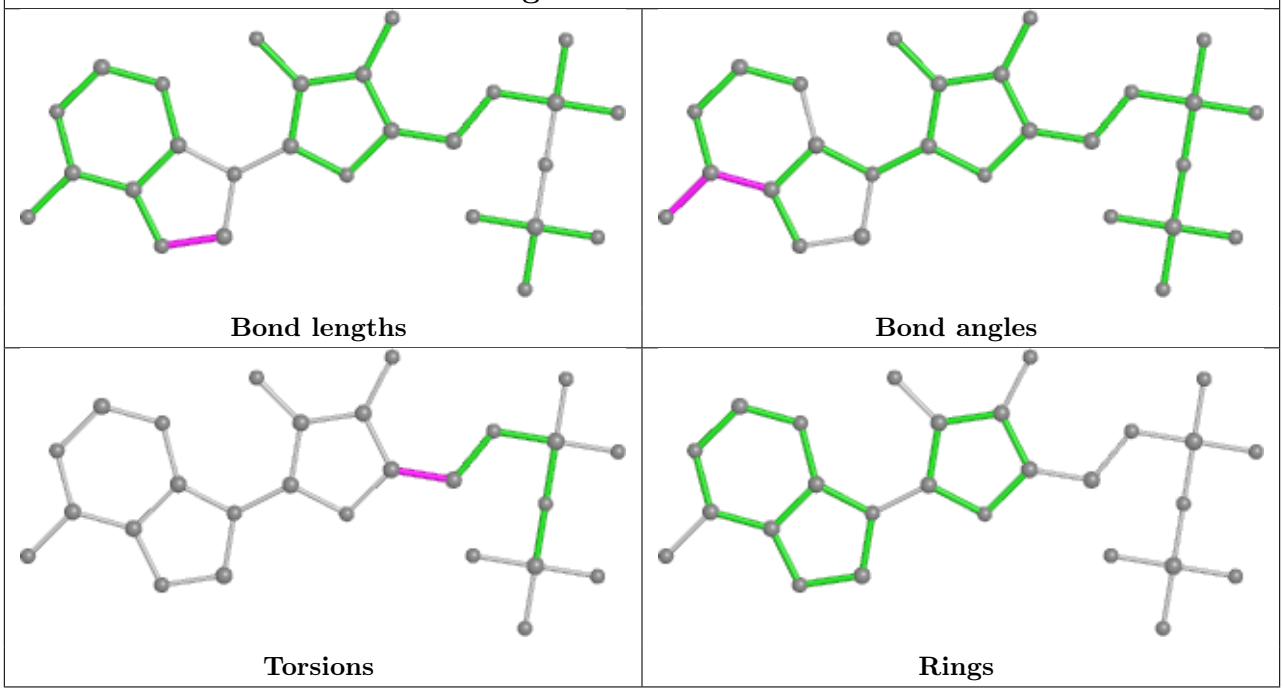
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

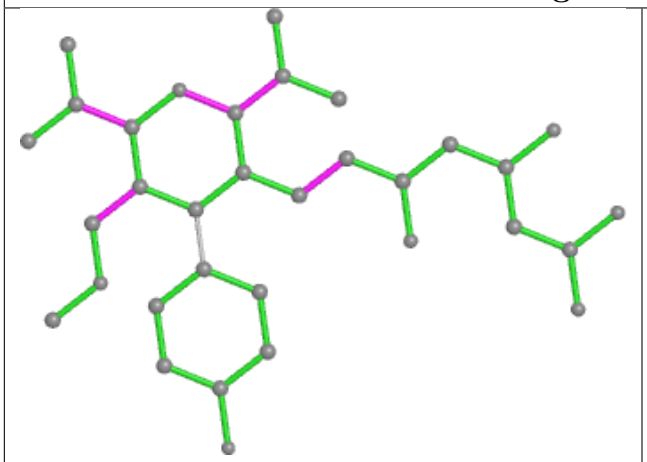
Ligand ADP C 103



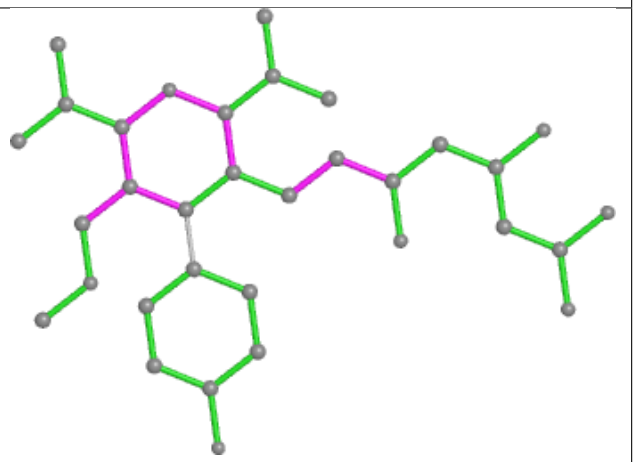
Ligand ADP A 101



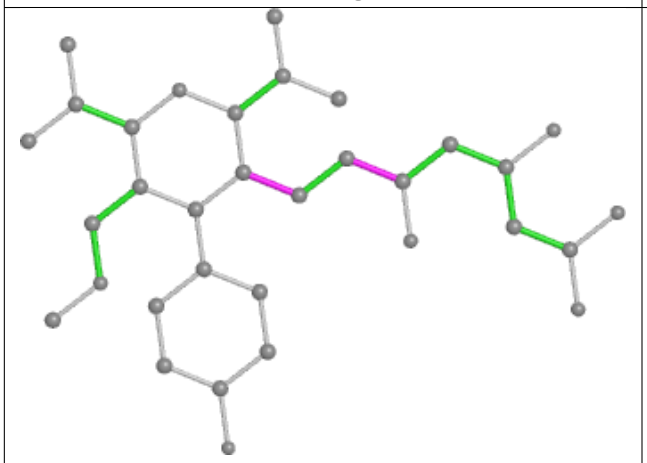
Ligand 116 D 3



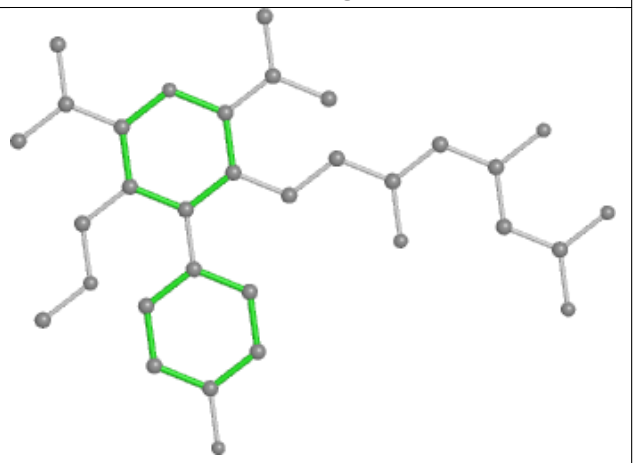
Bond lengths



Bond angles

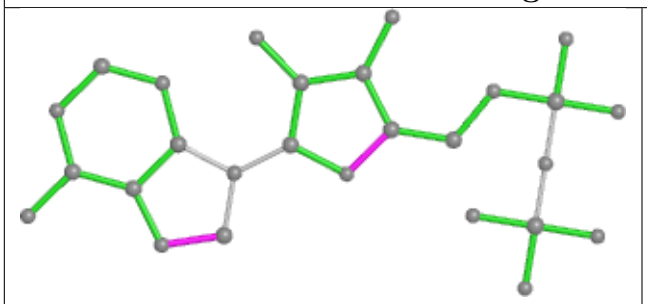


Torsions



Rings

Ligand ADP A 102



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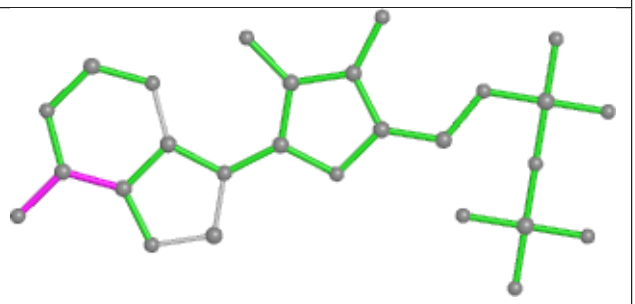
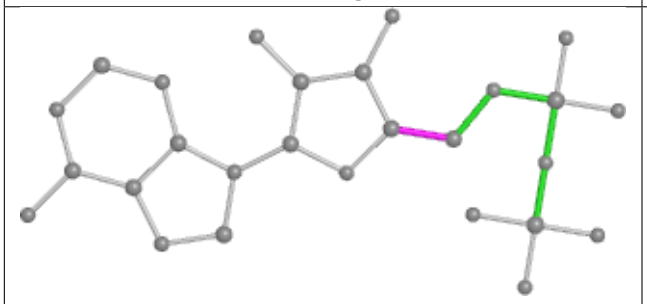
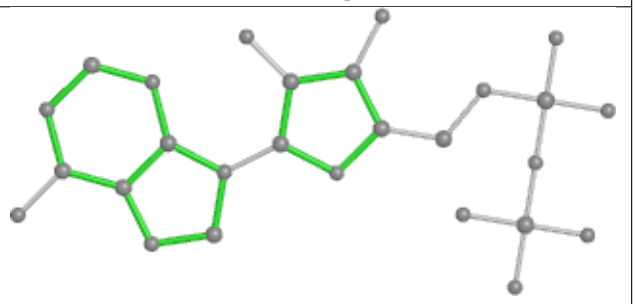


Bond angles

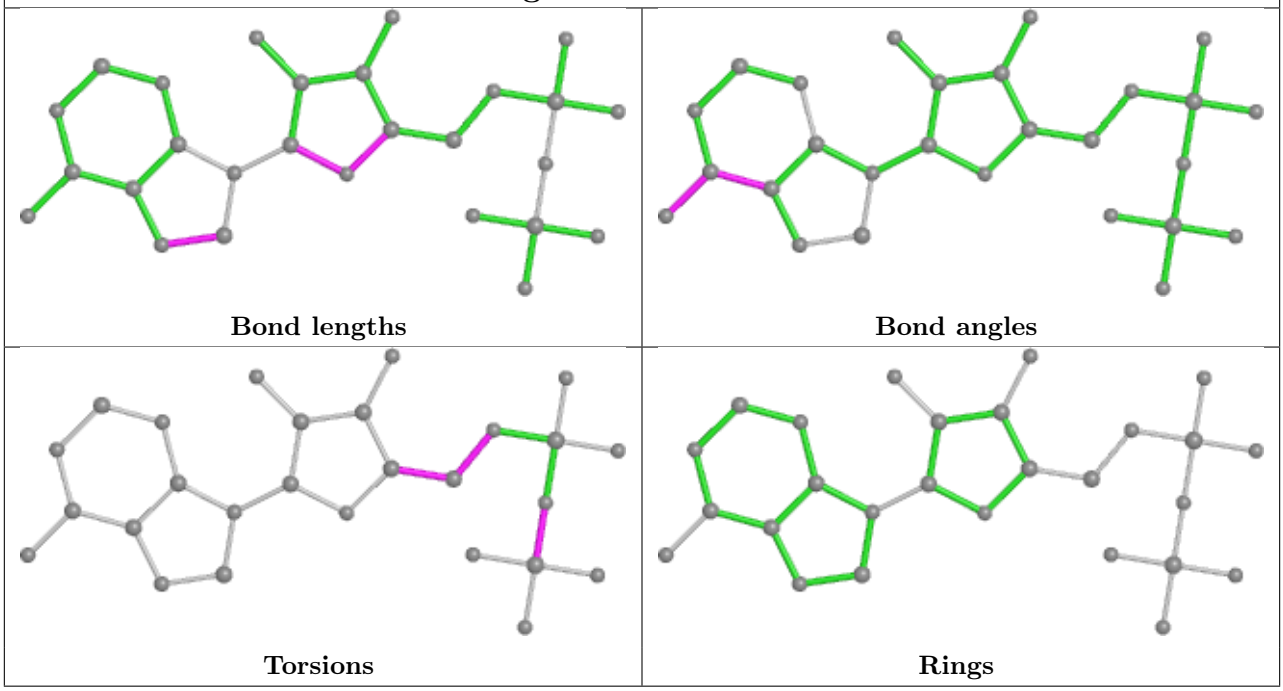


Torsions

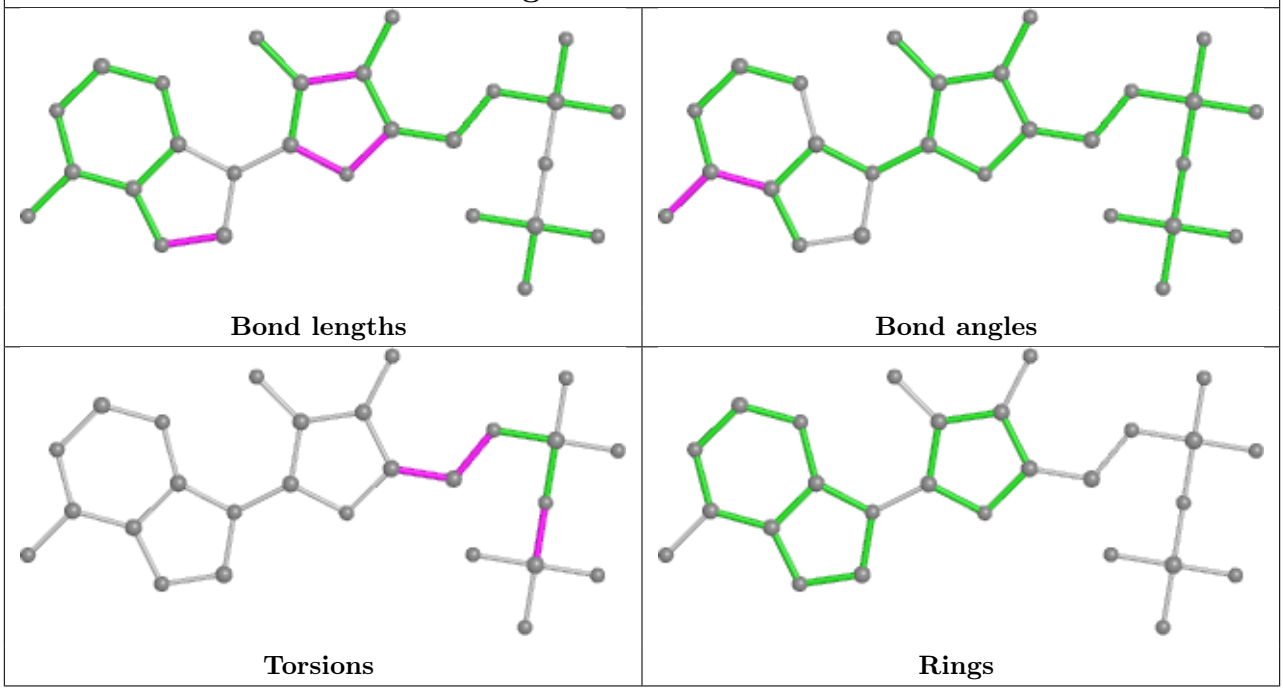


Rings

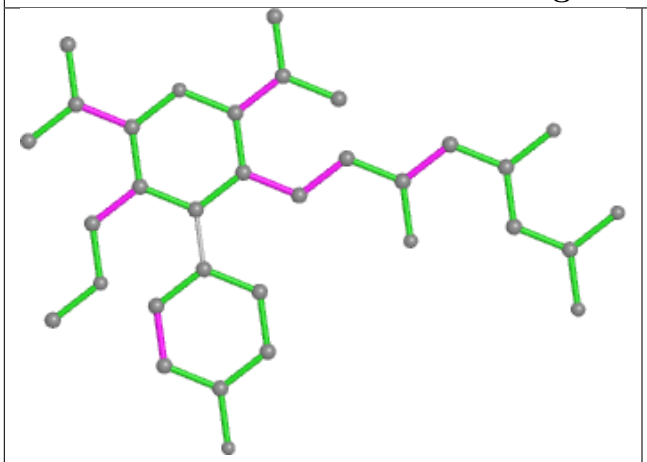
Ligand ADP C 104



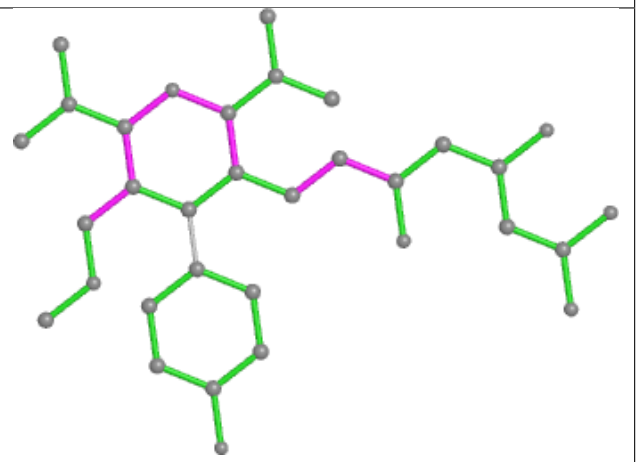
Ligand ADP D 106



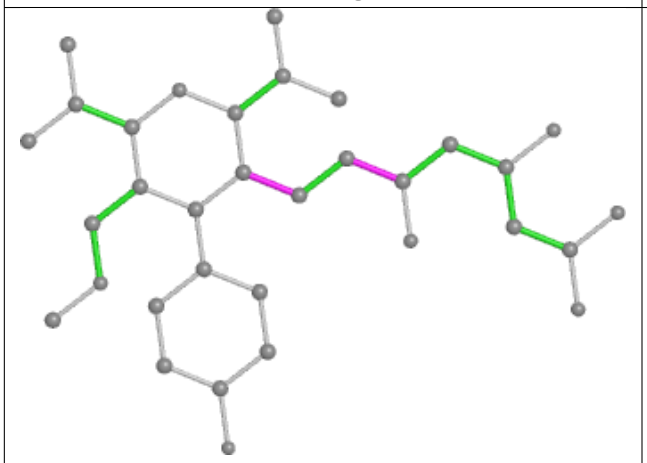
Ligand 116 A 2



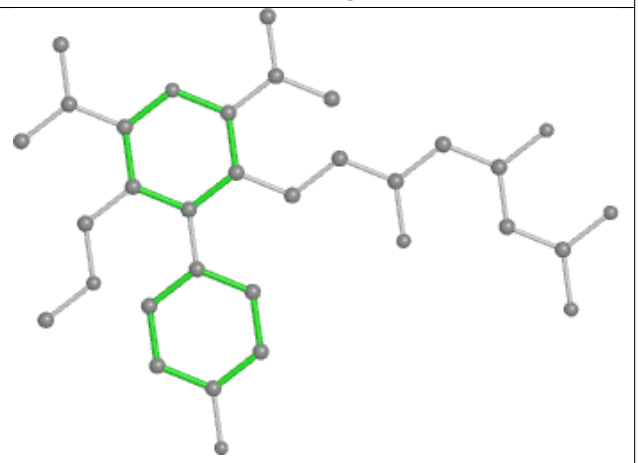
Bond lengths



Bond angles

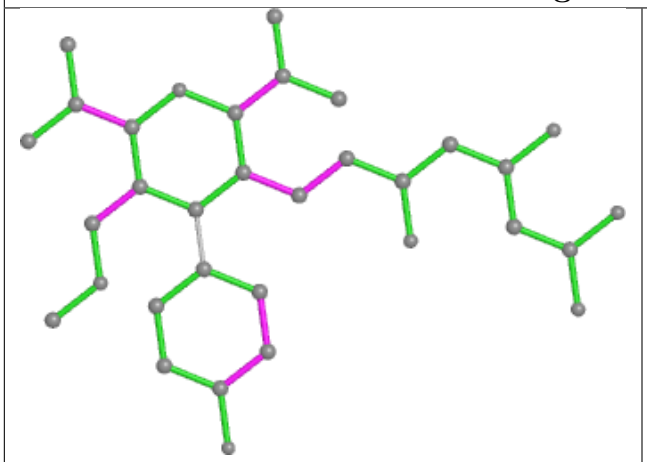


Torsions

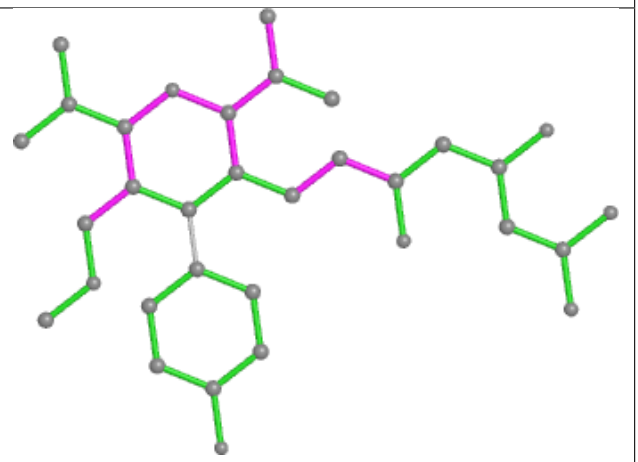


Rings

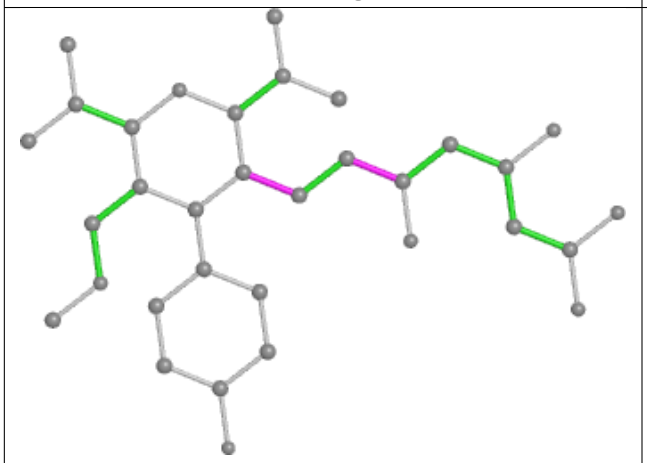
Ligand 116 C 4



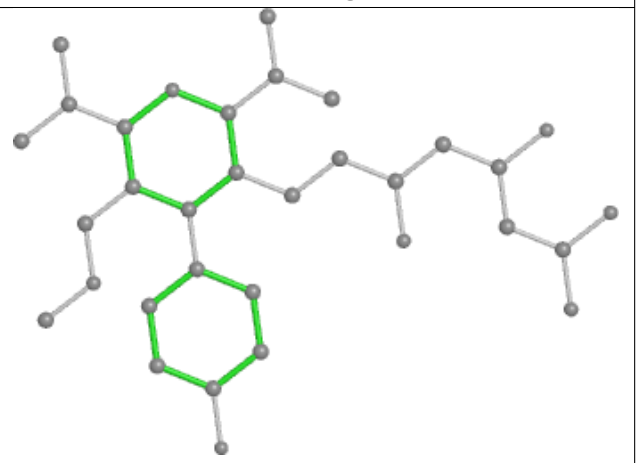
Bond lengths



Bond angles

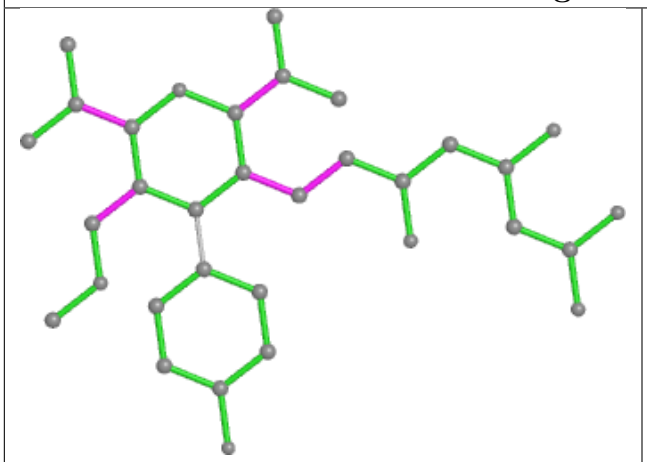


Torsions

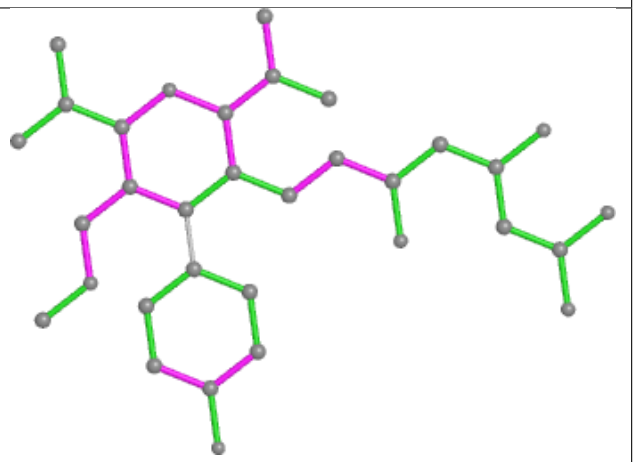


Rings

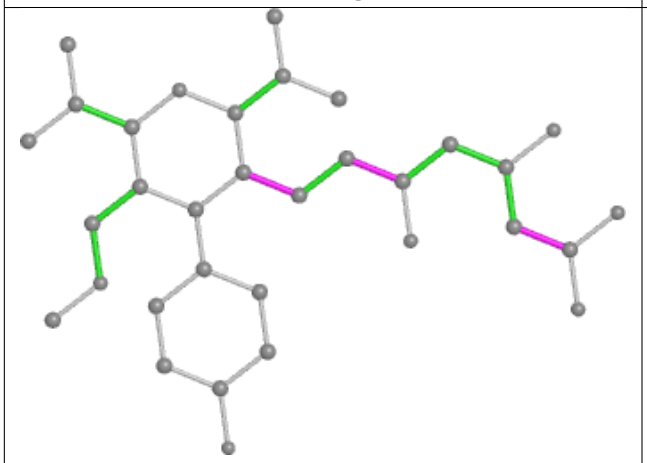
Ligand 116 B 1



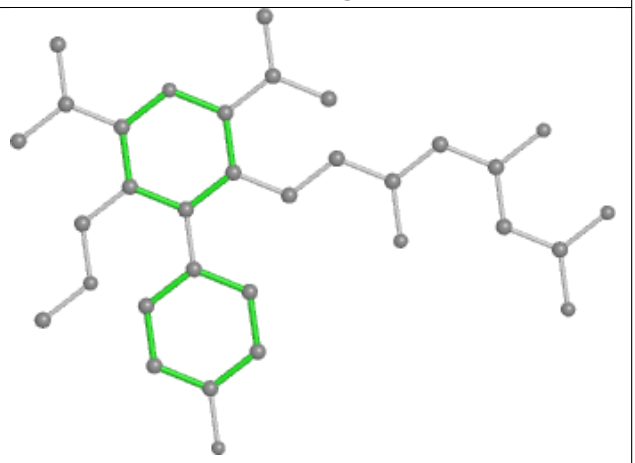
Bond lengths



Bond angles

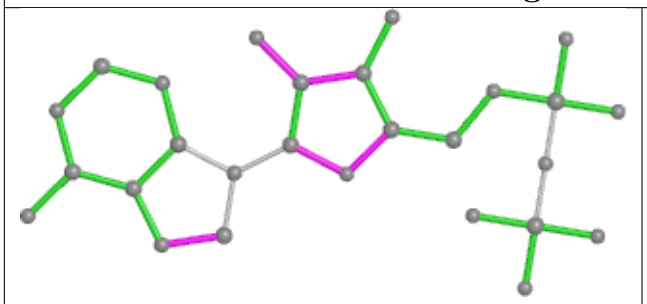


Torsions

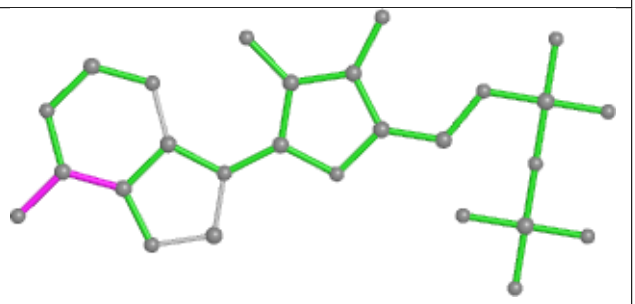


Rings

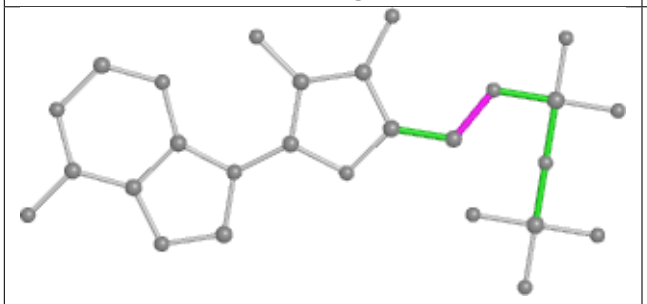
Ligand ADP B 105



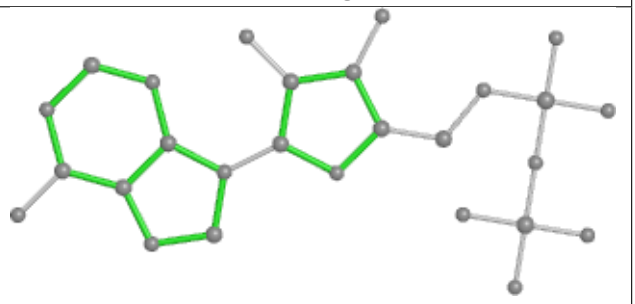
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	410/467 (87%)	0.50	50 (12%)	4	3	27, 51, 99, 101	0
1	B	398/467 (85%)	0.49	33 (8%)	11	12	30, 50, 86, 101	0
1	C	408/467 (87%)	0.63	44 (10%)	5	5	30, 53, 100, 101	0
1	D	392/467 (83%)	0.47	43 (10%)	5	5	29, 48, 93, 101	0
All	All	1608/1868 (86%)	0.52	170 (10%)	6	6	27, 50, 99, 101	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	475	HIS	8.1
1	D	483	THR	7.8
1	D	462	LEU	7.4
1	B	471	VAL	7.2
1	A	861	HIS	7.0
1	A	484	LEU	6.9
1	A	473	ALA	6.7
1	D	484	LEU	6.4
1	C	483	THR	6.3
1	B	475	HIS	6.2
1	D	486	GLU	6.2
1	D	471	VAL	6.0
1	D	523	MET	6.0
1	D	469	GLN	5.8
1	A	449	LEU	5.5
1	A	475	HIS	5.4
1	A	448	CYS	5.4
1	C	484	LEU	5.2
1	B	476	ILE	5.2
1	D	470	LEU	5.2
1	D	524	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	5.0
1	C	486	GLU	5.0
1	C	477	PRO	4.7
1	A	451	ILE	4.6
1	B	470	LEU	4.6
1	D	485	ILE	4.5
1	A	471	VAL	4.5
1	B	485	ILE	4.5
1	B	613	GLU	4.2
1	B	486	GLU	4.1
1	A	479	TYR	4.1
1	A	470	LEU	4.0
1	D	467	ILE	4.0
1	D	694	ALA	4.0
1	A	446	GLU	3.9
1	D	481	LEU	3.9
1	D	487	THR	3.9
1	A	828	LYS	3.7
1	B	487	THR	3.7
1	D	473	ALA	3.6
1	C	627	ARG	3.6
1	C	447	GLU	3.6
1	C	628	PHE	3.5
1	C	448	CYS	3.5
1	A	467	ILE	3.4
1	D	482	GLU	3.4
1	D	466	GLU	3.4
1	B	479	TYR	3.4
1	C	476	ILE	3.3
1	D	494	ILE	3.3
1	D	693	PRO	3.3
1	A	630	ARG	3.3
1	B	746	ILE	3.3
1	D	463	SER	3.2
1	D	743	ALA	3.2
1	A	718	ARG	3.2
1	C	450	GLN	3.2
1	D	472	ASN	3.2
1	B	698	TRP	3.2
1	C	445	ASN	3.2
1	B	630	ARG	3.2
1	A	477	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	695	ALA	3.1
1	A	469	GLN	3.1
1	A	472	ASN	3.1
1	A	741	ALA	3.1
1	D	718	ARG	3.0
1	C	630	ARG	3.0
1	C	695	ALA	3.0
1	B	608	TRP	3.0
1	C	446	GLU	3.0
1	B	694	ALA	3.0
1	C	694	ALA	3.0
1	C	479	TYR	2.9
1	C	699	ILE	2.9
1	B	474	LYS	2.9
1	C	480	LYS	2.9
1	A	699	ILE	2.9
1	C	746	ILE	2.9
1	A	447	GLU	2.9
1	B	484	LEU	2.9
1	C	749	TYR	2.9
1	C	828	LYS	2.9
1	C	693	PRO	2.9
1	A	698	TRP	2.9
1	A	481	LEU	2.8
1	A	627	ARG	2.8
1	C	698	TRP	2.8
1	A	497	GLN	2.8
1	D	746	ILE	2.8
1	B	688	CYS	2.7
1	A	466	GLU	2.7
1	A	462	LEU	2.7
1	B	666	LYS	2.7
1	C	523	MET	2.7
1	D	490	ARG	2.7
1	D	772	VAL	2.6
1	D	698	TRP	2.6
1	D	699	ILE	2.6
1	D	516	ASP	2.6
1	D	488	HIS	2.6
1	A	474	LYS	2.5
1	B	478	ALA	2.5
1	C	745	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	699	ILE	2.5
1	C	757	VAL	2.5
1	B	741	ALA	2.5
1	C	771	ASN	2.5
1	D	773	GLY	2.5
1	D	575	LEU	2.5
1	A	445	ASN	2.5
1	B	695	ALA	2.4
1	C	468	ILE	2.4
1	C	741	ALA	2.4
1	B	483	THR	2.4
1	B	828	LYS	2.4
1	C	674	TYR	2.4
1	C	466	GLU	2.4
1	C	773	GLY	2.4
1	B	693	PRO	2.4
1	D	521	LEU	2.3
1	A	772	VAL	2.3
1	A	744	GLY	2.3
1	C	753	ALA	2.3
1	A	689	THR	2.3
1	B	754	ALA	2.3
1	B	501	LYS	2.3
1	A	485	ILE	2.3
1	C	629	ALA	2.3
1	A	483	THR	2.3
1	A	771	ASN	2.3
1	A	829	ASP	2.2
1	C	772	VAL	2.2
1	B	469	GLN	2.2
1	D	745	SER	2.2
1	C	743	ALA	2.2
1	D	696	ILE	2.2
1	A	501	LYS	2.2
1	A	746	ILE	2.2
1	A	743	ALA	2.2
1	B	771	ASN	2.2
1	C	777	CYS	2.2
1	A	524	GLY	2.2
1	D	464	ASP	2.2
1	A	628	PHE	2.2
1	C	571	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	515	ARG	2.2
1	D	740	SER	2.2
1	A	738	VAL	2.1
1	A	629	ALA	2.1
1	D	744	GLY	2.1
1	B	749	TYR	2.1
1	C	474	LYS	2.1
1	A	745	SER	2.1
1	B	778	ILE	2.1
1	C	462	LEU	2.1
1	B	777	CYS	2.1
1	A	740	SER	2.1
1	D	571	ARG	2.1
1	C	470	LEU	2.1
1	A	523	MET	2.1
1	B	481	LEU	2.0
1	D	771	ASN	2.0
1	D	787	THR	2.0
1	C	510	GLN	2.0
1	A	511	TYR	2.0
1	C	478	ALA	2.0
1	A	480	LYS	2.0
1	A	694	ALA	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.

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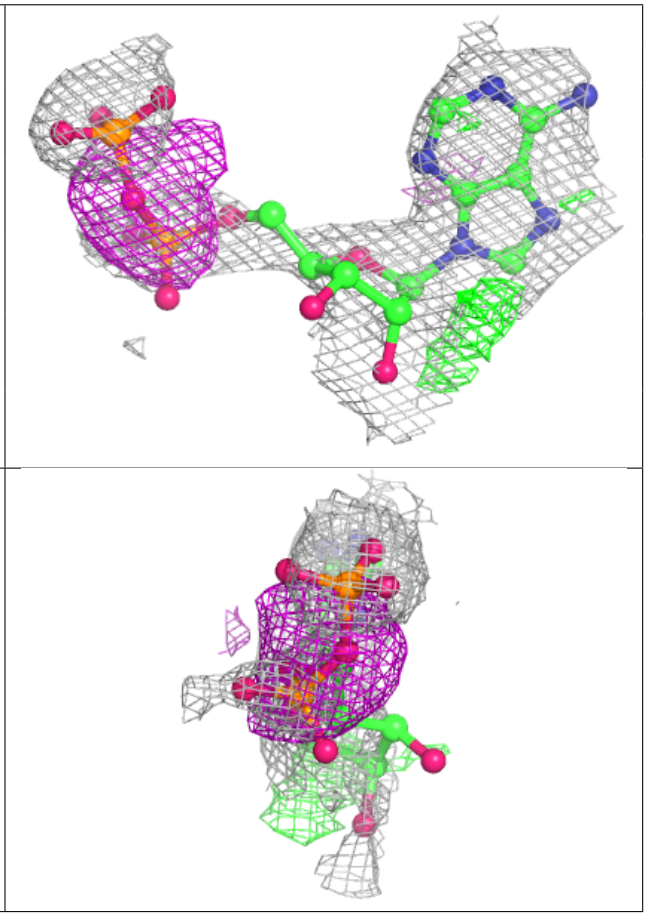
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	105	27/27	0.52	0.33	99,100,100,100	0
2	ADP	C	103	27/27	0.69	0.33	91,95,100,100	0
2	ADP	D	106	27/27	0.72	0.30	99,100,100,100	0
2	ADP	C	104	27/27	0.81	0.25	98,100,100,100	0
2	ADP	A	102	27/27	0.81	0.24	86,91,100,100	0
2	ADP	A	101	27/27	0.82	0.22	88,92,100,100	0
3	116	B	1	33/33	0.93	0.16	42,49,54,55	0
3	116	C	4	33/33	0.93	0.16	39,45,48,50	0
3	116	A	2	33/33	0.96	0.15	35,40,44,46	0
3	116	D	3	33/33	0.96	0.15	39,46,49,49	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.

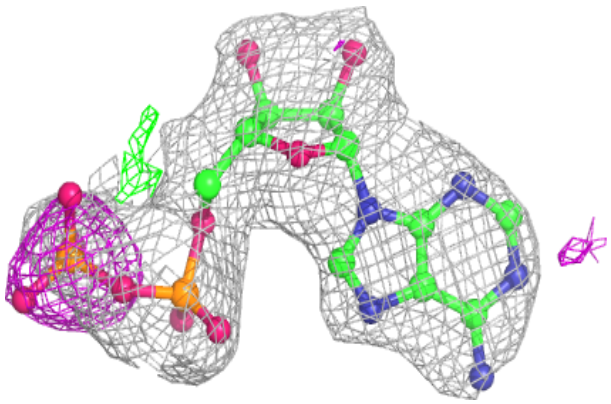
Electron density around ADP B 105:

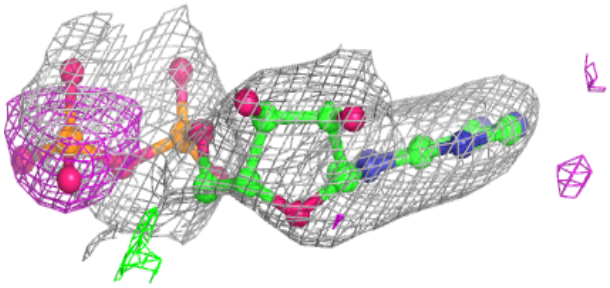
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

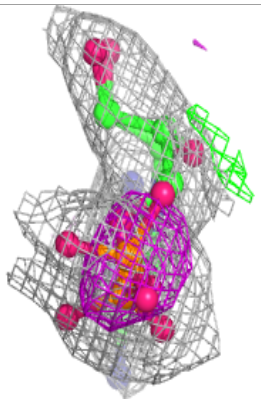


Electron density around ADP C 103:

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

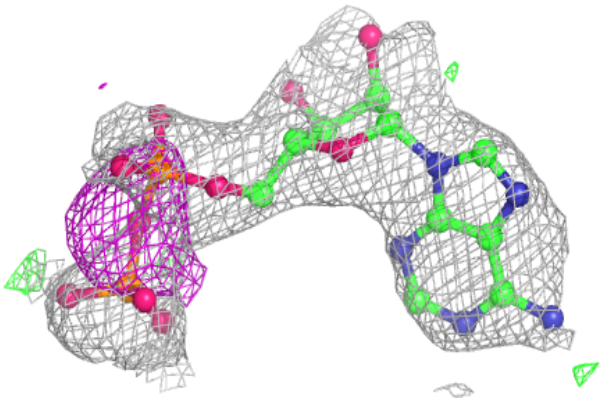


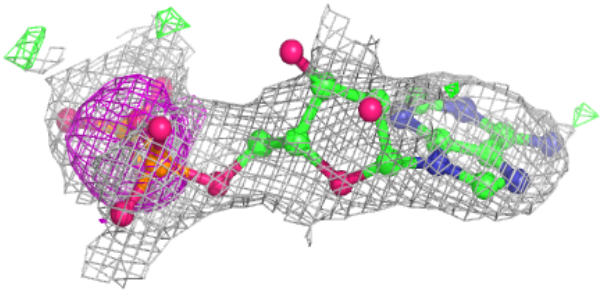


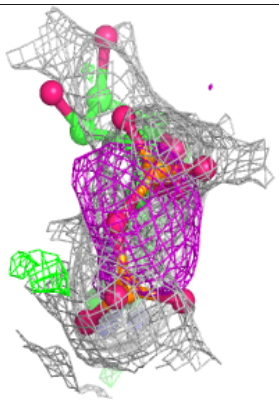


Electron density around ADP D 106:

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

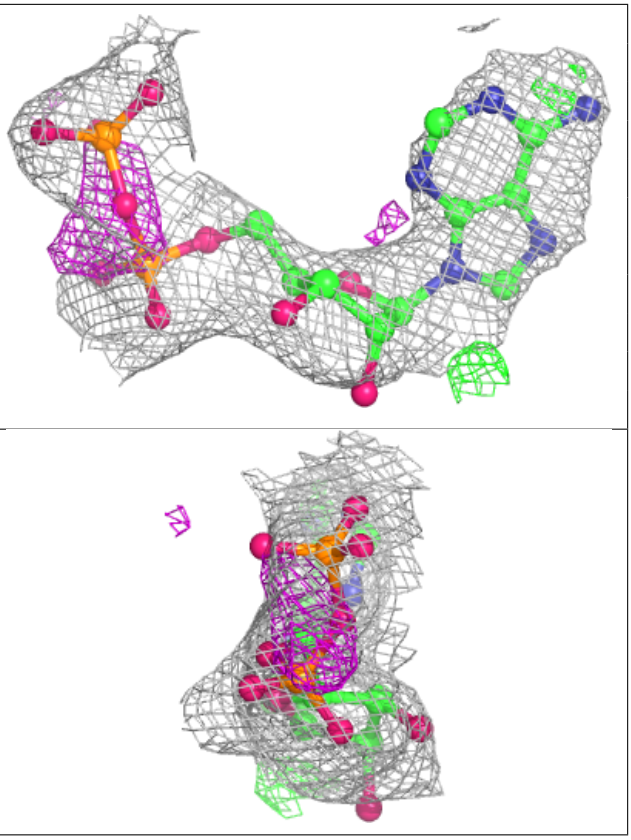


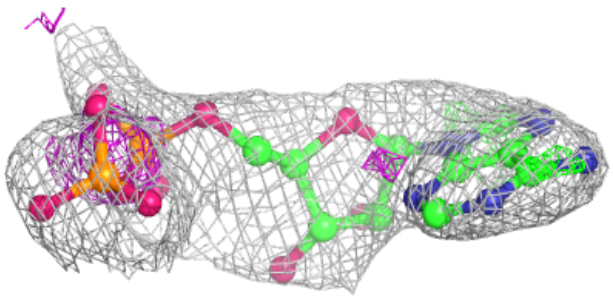




Electron density around ADP C 104:

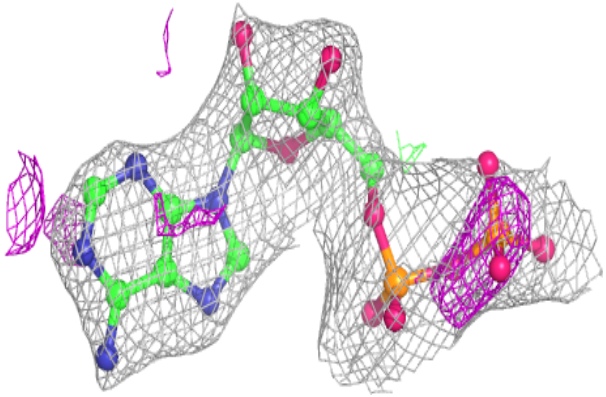
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

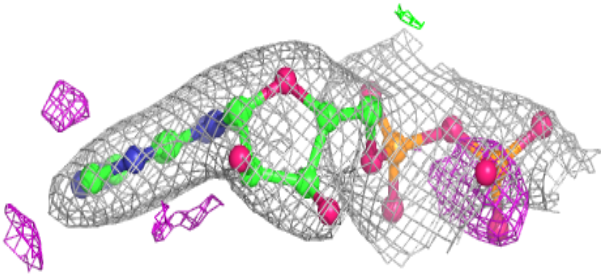


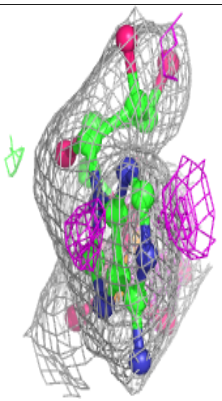


Electron density around ADP A 102:

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

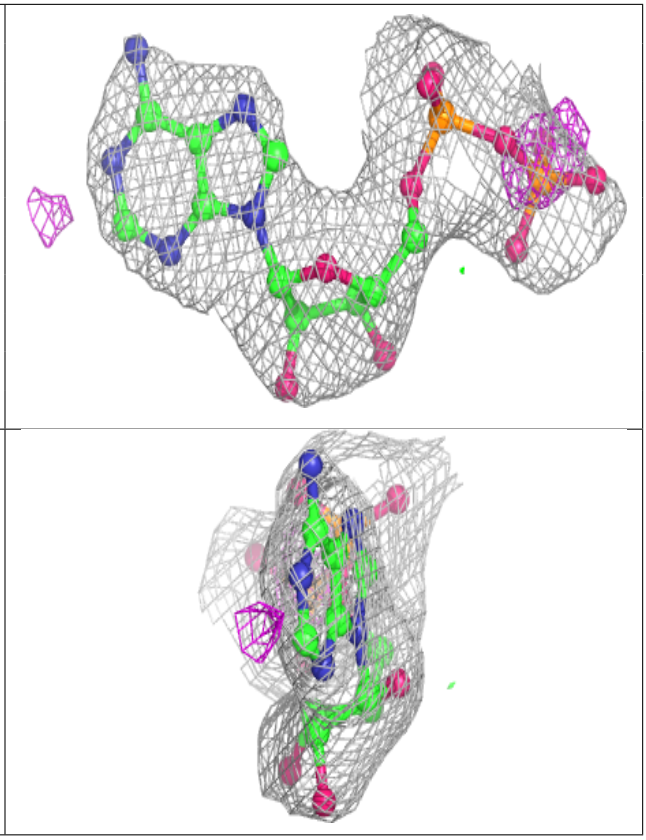






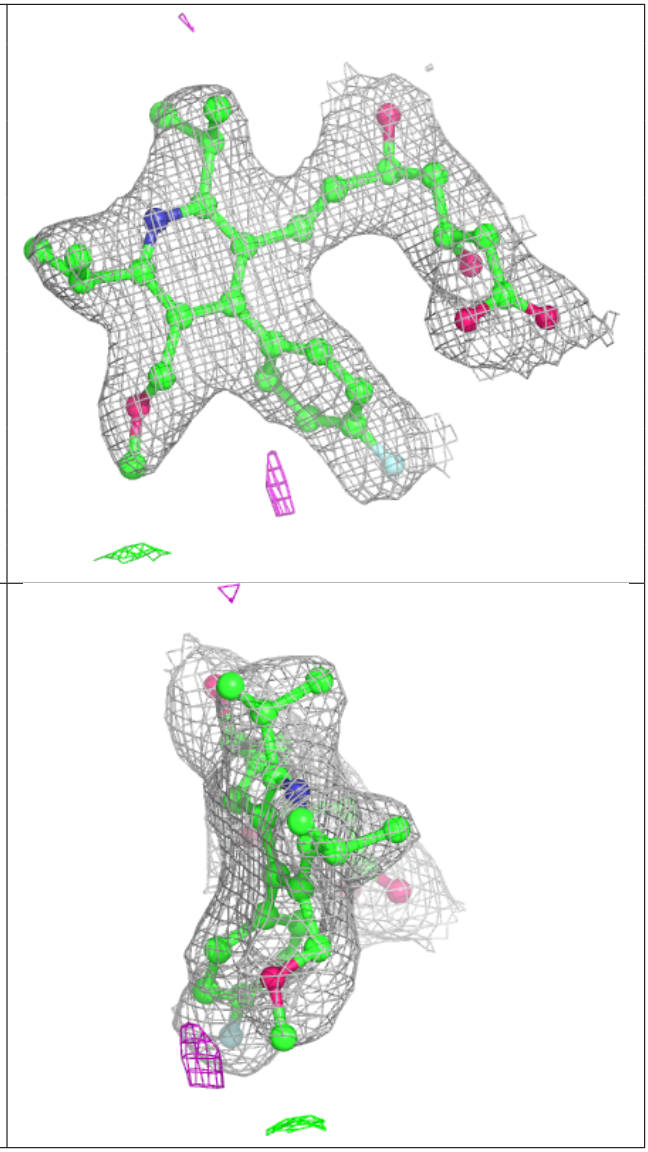
Electron density around ADP A 101:

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



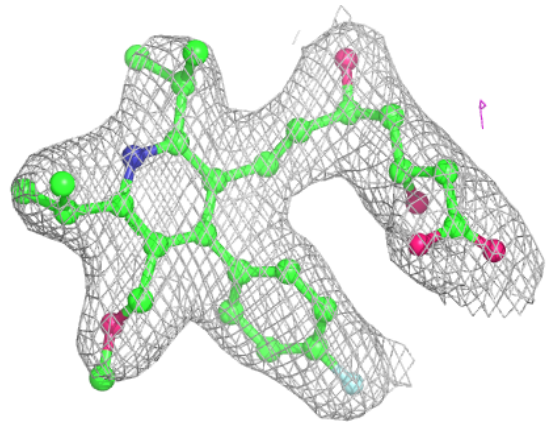
Electron density around 116 B 1:

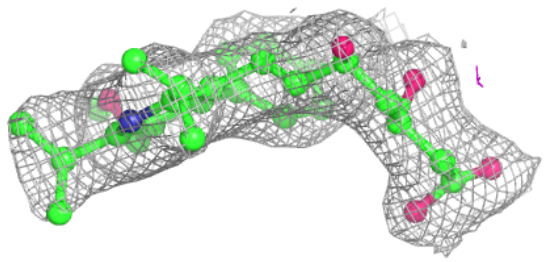
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

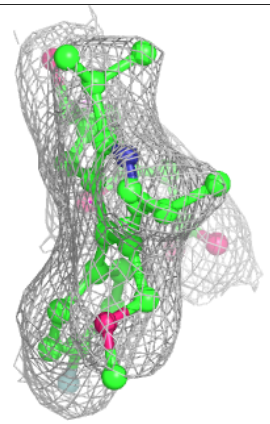


Electron density around 116 C 4:

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

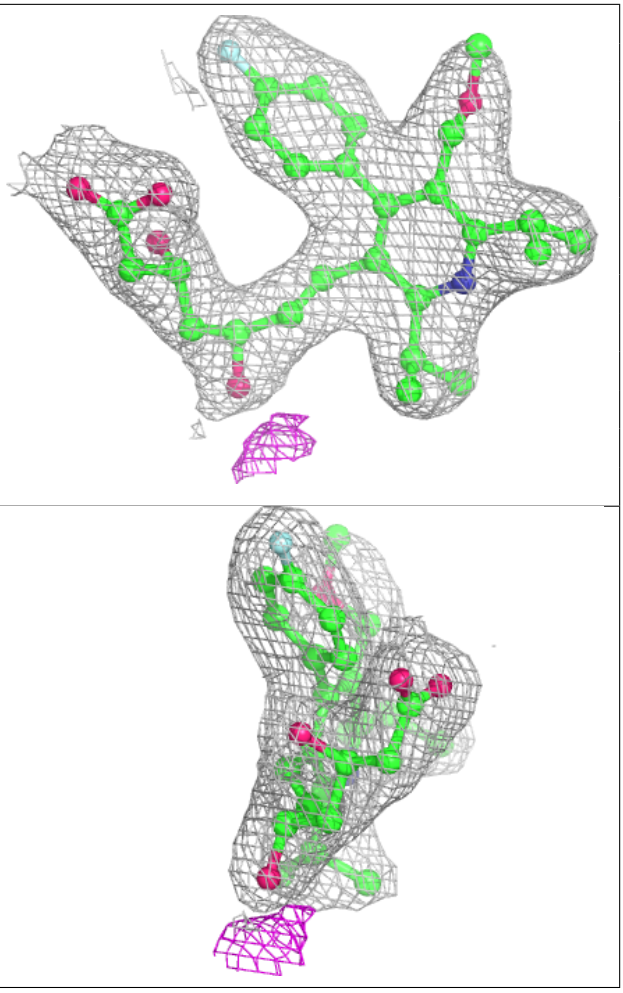






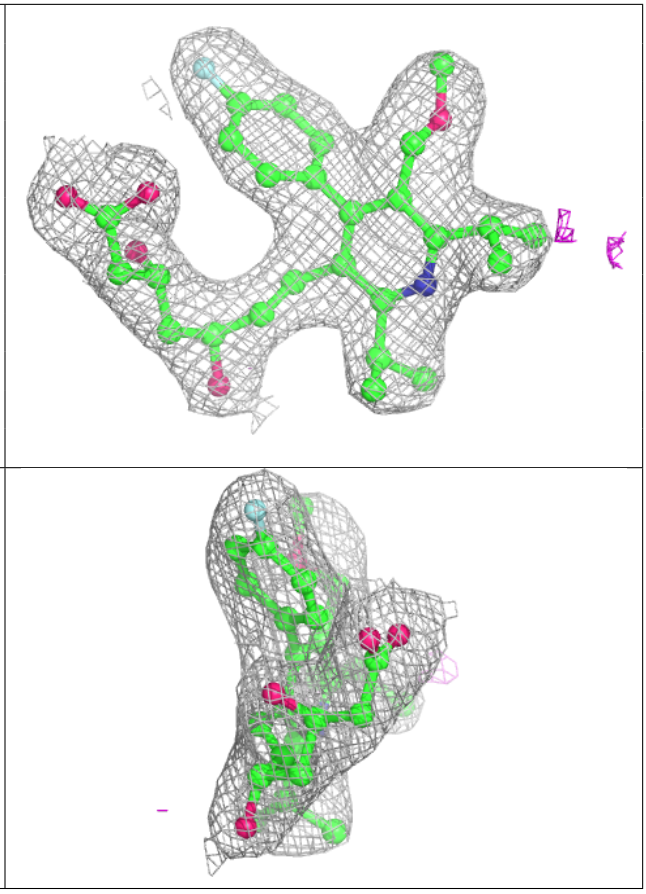
Electron density around 116 A 2:

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



Electron density around 116 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)



6.5 Other polymers (i)

There are no such residues in this entry.