Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 10:26 PM EDT

PDB ID	:	1HW9
Title	:	COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH SIMVASTATIN
Authors	:	Istvan, E.S.; Deisenhofer, J.
Deposited on	:	2001-01-09
Resolution	:	2.33 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:

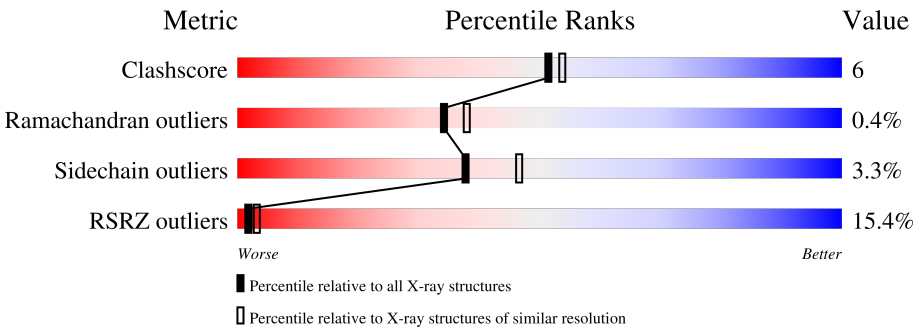
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.33 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	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	14% 75% 12% • 13%
1	B	467	14% 73% 11% • 15%
1	C	467	12% 73% 9% • 17%
1	D	467	12% 72% 10% • 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12185 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.

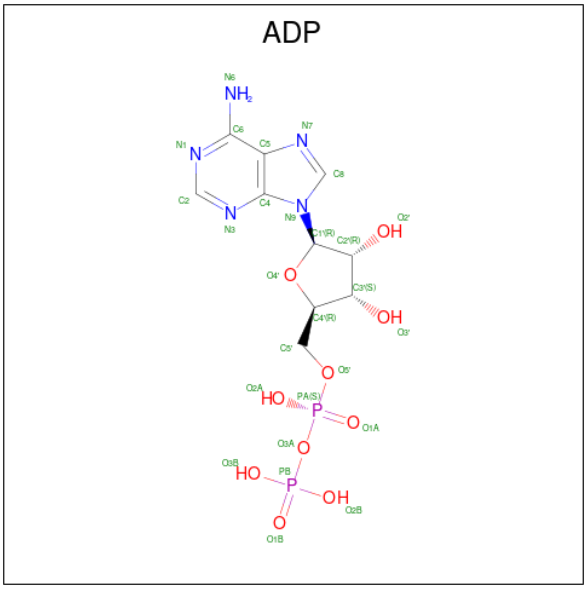
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3037	1892	533	582	30	0	0	0
1	B	398	2952	1838	518	567	29	0	0	0
1	C	389	2881	1792	504	556	29	0	0	0
1	D	388	2880	1792	504	555	29	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

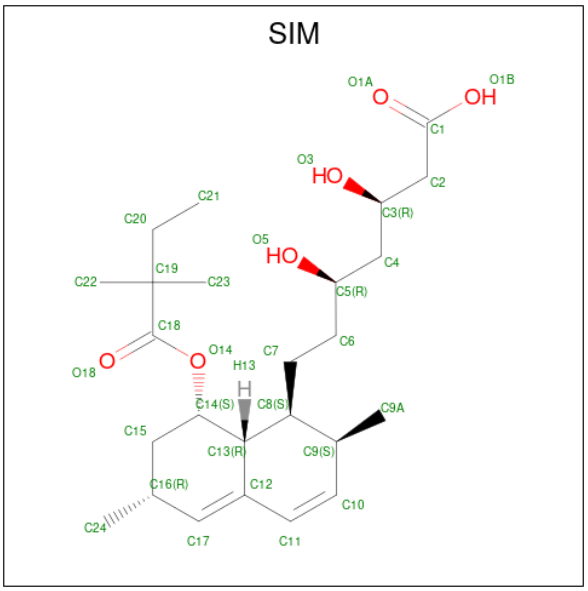
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	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
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	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	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 Simvastatin acid (three-letter code: SIM) (formula: $C_{25}H_{40}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 31 25 6	0	0
3	B	1	Total C O 31 25 6	0	0
3	C	1	Total C O 31 25 6	0	0
3	C	1	Total C O 31 25 6	0	0

- Molecule 4 is water.

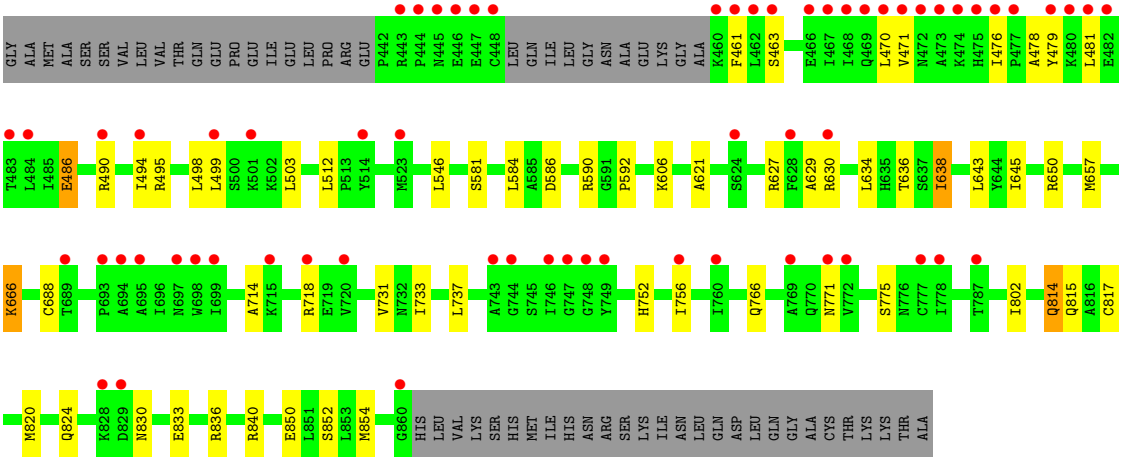
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	49	Total O 49 49	0	0
4	C	33	Total O 33 33	0	0
4	D	50	Total O 50 50	0	0

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.

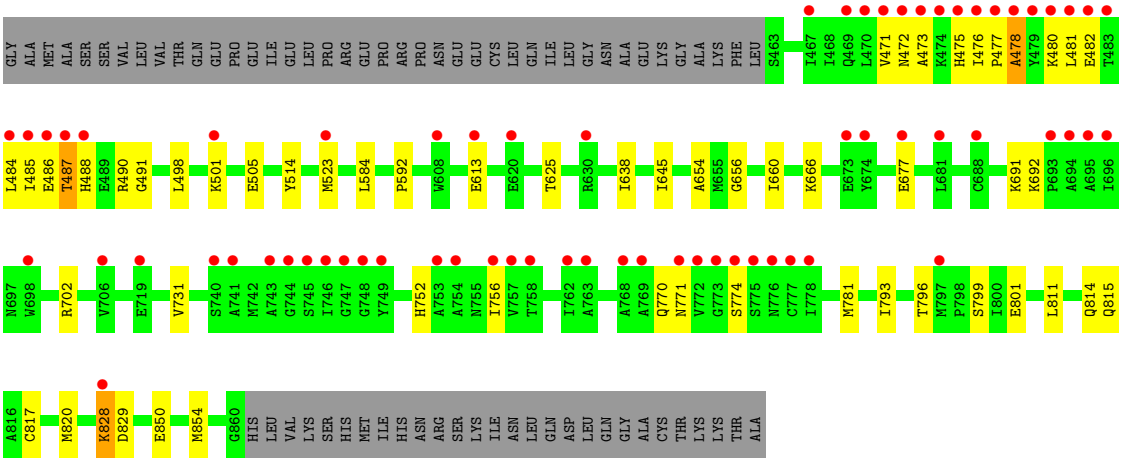
• Molecule 1: HMG-COA REDUCTASE

Chain A:



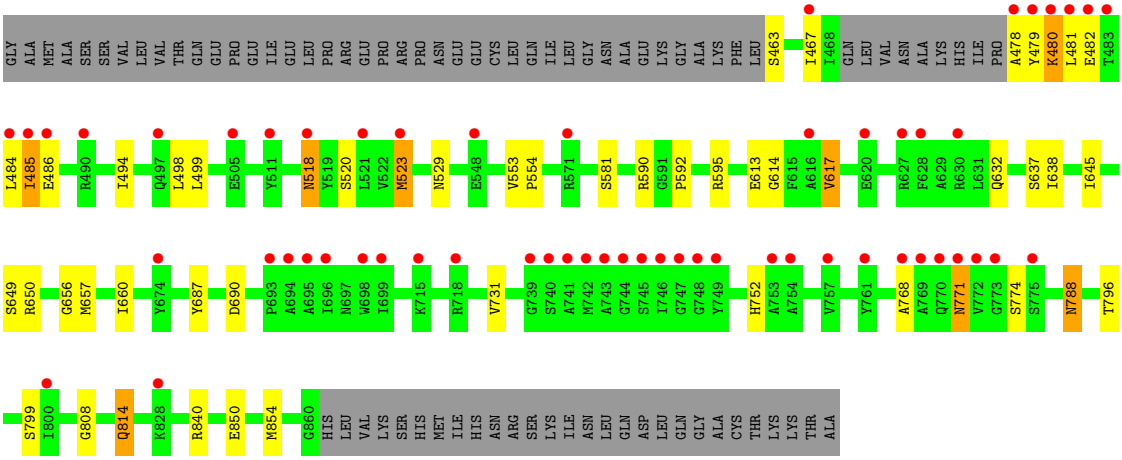
• Molecule 1: HMG-COA REDUCTASE

Chain B:



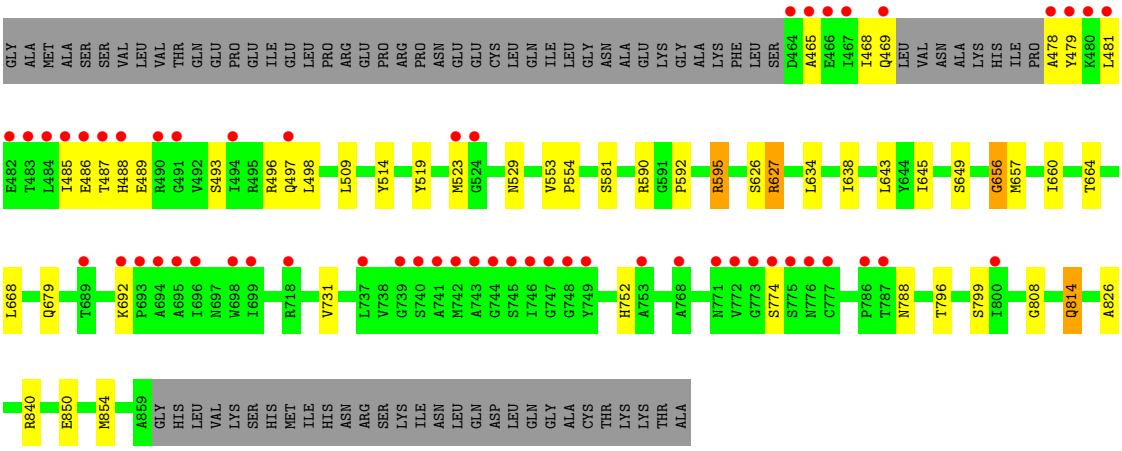
• Molecule 1: HMG-COA REDUCTASE

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	74.55Å 172.82Å 80.03Å 90.00° 117.56° 90.00°	Depositor
Resolution (Å)	43.43 – 2.33 52.40 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.43-2.33) 91.8 (52.40-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.248 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: SIM, 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	0.44	0/3081	0.63	0/4164
1	B	0.43	0/2994	0.63	0/4049
1	C	0.41	0/2920	0.62	0/3946
1	D	0.46	0/2919	0.63	1/3945 (0.0%)
All	All	0.44	0/11914	0.63	1/16104 (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	D	656	GLY	N-CA-C	5.09	125.82	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	3037	0	3072	37	0
1	B	2952	0	2989	39	0
1	C	2881	0	2911	31	0
1	D	2880	0	2911	34	0
2	A	27	0	12	0	0
2	B	54	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	0	0
2	D	27	0	12	2	0
3	A	31	0	39	0	0
3	B	31	0	39	0	0
3	C	62	0	78	1	0
4	A	44	0	0	0	0
4	B	49	0	0	0	0
4	C	33	0	0	0	0
4	D	50	0	0	0	0
All	All	12185	0	12099	136	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 (136) 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	1.46	0.98
1:C:485:ILE:HG22	1:C:486:GLU:H	1.45	0.82
1:B:817:CYS:HA	1:B:820:MET:HE3	1.69	0.75
1:A:479:TYR:HA	1:A:495:ARG:HH21	1.54	0.72
1:D:808:GLY:O	1:D:814:GLN:HG3	1.93	0.69
1:B:654:ALA:HB1	2:B:104:ADP:O1B	1.93	0.68
1:D:488:HIS:HD2	1:D:523:MET:HG3	1.58	0.68
1:A:584:LEU:HD11	1:D:638:ILE:HD11	1.75	0.67
1:B:485:ILE:HG22	1:B:486:GLU:H	1.60	0.67
1:A:714:ALA:HB1	1:A:718:ARG:NH1	2.09	0.66
1:D:519:TYR:O	1:D:523:MET:HG2	1.96	0.66
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.78	0.66
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.78	0.65
1:A:629:ALA:O	1:A:630:ARG:HD2	1.96	0.64
1:D:656:GLY:O	1:D:660:ILE:HG12	1.97	0.64
1:B:485:ILE:HG22	1:B:486:GLU:N	2.13	0.64
1:B:656:GLY:O	1:B:660:ILE:HG12	1.99	0.63
1:B:781:MET:HE2	1:B:793:ILE:HD12	1.82	0.62
1:D:638:ILE:HG22	1:D:643:LEU:HD13	1.81	0.62
1:C:808:GLY:O	1:C:814:GLN:HG3	2.00	0.61
1:B:850:GLU:O	1:B:854:MET:HG2	2.01	0.60
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.02	0.59
1:A:731:VAL:HG12	1:A:854:MET:CE	2.32	0.59
1:A:714:ALA:HB1	1:A:718:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ILE:HD11	1:C:494:ILE:HD12	1.85	0.58
1:C:850:GLU:O	1:C:854:MET:HG2	2.03	0.58
1:D:486:GLU:HG2	1:D:487:THR:H	1.67	0.58
1:A:606:LYS:HG3	1:A:636:THR:HG21	1.85	0.58
1:D:486:GLU:HG2	1:D:487:THR:N	2.20	0.57
1:B:584:LEU:HD22	1:C:638:ILE:HD12	1.86	0.57
1:D:581:SER:OG	1:D:840:ARG:HD2	2.05	0.57
1:C:480:LYS:O	1:C:484:LEU:HG	2.04	0.57
1:A:586:ASP:HB3	1:A:650:ARG:HE	1.70	0.56
1:C:581:SER:OG	1:C:840:ARG:HD2	2.05	0.56
1:D:850:GLU:O	1:D:854:MET:HG2	2.04	0.56
1:B:482:GLU:HG2	1:B:523:MET:HG2	1.88	0.56
1:A:756:ILE:HD12	1:A:756:ILE:N	2.21	0.55
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.88	0.55
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.89	0.55
1:C:482:GLU:HG2	1:C:523:MET:HG2	1.87	0.55
1:D:649:SER:HB3	1:D:660:ILE:HD12	1.89	0.55
1:D:485:ILE:HG22	1:D:486:GLU:N	2.23	0.55
1:A:581:SER:OG	1:A:840:ARG:HD2	2.07	0.54
1:A:731:VAL:HG12	1:A:854:MET:HE1	1.90	0.54
1:B:477:PRO:HG2	1:B:480:LYS:HZ3	1.73	0.54
1:A:817:CYS:HA	1:A:820:MET:HE3	1.89	0.53
1:D:493:SER:O	1:D:497:GLN:HG3	2.08	0.53
1:A:606:LYS:HG3	1:A:636:THR:CG2	2.39	0.53
1:C:656:GLY:O	1:C:660:ILE:HG12	2.09	0.52
1:B:475:HIS:O	1:B:476:ILE:HG13	2.10	0.52
1:B:828:LYS:CD	1:B:829:ASP:H	2.23	0.51
1:A:621:ALA:HB1	1:A:666:LYS:HE3	1.93	0.50
1:B:691:LYS:HE2	1:B:770:GLN:HG3	1.93	0.50
1:B:811:LEU:O	1:B:815:GLN:HG3	2.12	0.50
1:B:471:VAL:C	1:B:473:ALA:H	2.15	0.50
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.41	0.50
1:A:627:ARG:HD3	1:A:627:ARG:H	1.76	0.49
1:B:477:PRO:HG2	1:B:480:LYS:NZ	2.27	0.49
1:B:731:VAL:HG12	1:B:854:MET:CE	2.43	0.49
1:C:768:ALA:O	1:C:771:ASN:HB3	2.13	0.49
1:D:731:VAL:HG12	1:D:854:MET:HE3	1.95	0.48
1:C:731:VAL:HG12	1:C:854:MET:CE	2.43	0.48
1:A:592:PRO:HD2	1:A:645:ILE:O	2.13	0.48
1:C:479:TYR:HB3	1:C:529:ASN:OD1	2.13	0.48
1:C:485:ILE:HG22	1:C:486:GLU:N	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ILE:HG23	1:D:498:LEU:HD21	1.96	0.48
1:D:826:ALA:HB1	2:D:105:ADP:HN61	1.79	0.47
1:B:731:VAL:HG12	1:B:854:MET:HE3	1.96	0.47
1:C:731:VAL:HG12	1:C:854:MET:HE3	1.96	0.47
1:A:850:GLU:O	1:A:854:MET:HG2	2.15	0.47
1:B:477:PRO:O	1:B:478:ALA:CB	2.62	0.47
1:C:632:GLN:HE21	1:C:650:ARG:HG2	1.80	0.47
1:D:496:ARG:NH2	1:D:509:LEU:O	2.48	0.47
1:A:638:ILE:O	1:D:796:THR:HG21	2.15	0.47
1:A:771:ASN:ND2	1:A:775:SER:OG	2.48	0.47
1:B:592:PRO:HD2	1:B:645:ILE:O	2.14	0.47
1:C:463:SER:O	1:C:467:ILE:HG12	2.15	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.15	0.46
1:D:731:VAL:HG12	1:D:854:MET:CE	2.45	0.46
1:B:702:ARG:HD3	1:B:801:GLU:OE2	2.15	0.46
1:D:487:THR:HG22	1:D:489:GLU:H	1.80	0.46
1:B:828:LYS:HD3	1:B:829:ASP:H	1.81	0.46
1:B:482:GLU:HG3	1:B:488:HIS:HD2	1.81	0.46
1:D:479:TYR:HB3	1:D:529:ASN:OD1	2.16	0.45
1:B:476:ILE:HD13	1:B:484:LEU:CD2	2.46	0.45
1:B:498:LEU:O	1:B:501:LYS:HG2	2.17	0.45
1:D:488:HIS:CD2	1:D:523:MET:HG3	2.46	0.45
1:B:828:LYS:HD3	1:B:829:ASP:N	2.31	0.45
1:D:626:SER:HA	1:D:627:ARG:HH11	1.82	0.45
1:C:518:ASN:ND2	1:C:520:SER:OG	2.50	0.44
1:D:592:PRO:HD2	1:D:645:ILE:O	2.18	0.44
1:C:592:PRO:HD2	1:C:645:ILE:O	2.16	0.44
1:A:590:ARG:HA	1:A:590:ARG:HD3	1.84	0.44
1:A:815:GLN:HG2	1:A:824:GLN:CG	2.48	0.44
1:B:638:ILE:O	1:C:796:THR:HG21	2.18	0.44
1:C:480:LYS:NZ	1:C:480:LYS:HB3	2.33	0.44
1:B:477:PRO:HD2	1:B:480:LYS:HD2	2.00	0.43
1:C:614:GLY:O	1:C:617:VAL:HG13	2.18	0.43
1:A:471:VAL:HG13	1:A:476:ILE:O	2.17	0.43
1:C:478:ALA:O	1:C:481:LEU:HG	2.18	0.43
1:A:650:ARG:HH11	1:A:650:ARG:HG3	1.84	0.43
1:A:731:VAL:HG12	1:A:854:MET:HE3	2.00	0.43
1:D:485:ILE:HG22	1:D:486:GLU:H	1.83	0.43
1:A:490:ARG:O	1:A:494:ILE:HG12	2.19	0.43
1:D:478:ALA:O	1:D:481:LEU:HG	2.18	0.43
1:C:553:VAL:HA	1:C:554:PRO:HD2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:ASP:OD2	3:C:1:SIM:H41	2.18	0.42
1:A:546:LEU:HD11	1:A:581:SER:HB3	2.02	0.42
1:A:733:ILE:O	1:A:737:LEU:HB2	2.19	0.42
1:D:627:ARG:H	1:D:627:ARG:NH1	2.18	0.42
1:A:830:ASN:O	1:A:833:GLU:HB2	2.19	0.42
1:B:485:ILE:CG2	1:B:486:GLU:N	2.82	0.42
1:D:590:ARG:HD3	1:D:590:ARG:HA	1.85	0.42
1:D:774:SER:HA	1:D:799:SER:O	2.20	0.42
1:A:657:MET:CE	1:A:657:MET:HA	2.50	0.42
1:A:836:ARG:O	1:A:840:ARG:HG3	2.20	0.42
1:C:788:ASN:HD22	1:C:788:ASN:HA	1.65	0.42
1:C:649:SER:HB3	1:C:660:ILE:HD12	2.00	0.42
1:A:629:ALA:C	1:A:630:ARG:HD2	2.40	0.41
1:B:692:LYS:HE2	1:B:692:LYS:HB2	1.89	0.41
1:B:475:HIS:C	1:B:476:ILE:HG13	2.41	0.41
1:D:664:THR:O	1:D:668:LEU:HG	2.21	0.41
1:D:692:LYS:HE2	1:D:692:LYS:HB2	1.91	0.41
1:D:826:ALA:HB1	2:D:105:ADP:N6	2.35	0.41
1:A:814:GLN:H	1:A:814:GLN:NE2	2.19	0.41
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.84	0.41
1:A:478:ALA:O	1:A:481:LEU:HG	2.21	0.40
1:D:553:VAL:HA	1:D:554:PRO:HD2	1.95	0.40
1:C:613:GLU:O	1:C:617:VAL:HG12	2.21	0.40
1:C:637:SER:HB2	1:C:687:TYR:OH	2.21	0.40
1:C:774:SER:HA	1:C:799:SER:O	2.21	0.40
1:B:478:ALA:O	1:B:481:LEU:HG	2.22	0.40
1:B:487:THR:HG23	1:B:490:ARG:CB	2.50	0.40
1:B:756:ILE:HD12	1:B:756:ILE:N	2.36	0.40
1:B:774:SER:HA	1:B:799:SER:O	2.22	0.40
1:D:595:ARG:HD2	1:D:679:GLN:OE1	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	404/467 (86%)	381 (94%)	22 (5%)	1 (0%)	47	55
1	B	396/467 (85%)	373 (94%)	20 (5%)	3 (1%)	19	20
1	C	385/467 (82%)	364 (94%)	20 (5%)	1 (0%)	41	47
1	D	384/467 (82%)	365 (95%)	17 (4%)	2 (0%)	29	31
All	All	1569/1868 (84%)	1483 (94%)	79 (5%)	7 (0%)	34	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	D	465	ALA
1	B	478	ALA
1	B	514	TYR
1	C	485	ILE
1	D	514	TYR
1	B	472	ASN

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%)	312 (96%)	14 (4%)	29	36
1	B	316/375 (84%)	308 (98%)	8 (2%)	47	58
1	C	308/375 (82%)	296 (96%)	12 (4%)	32	41
1	D	308/375 (82%)	300 (97%)	8 (3%)	46	56
All	All	1258/1500 (84%)	1216 (97%)	42 (3%)	38	46

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	PHE

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Mol	Chain	Res	Type
1	A	463	SER
1	A	470	LEU
1	A	486	GLU
1	A	499	LEU
1	A	503	LEU
1	A	512	LEU
1	A	634	LEU
1	A	638	ILE
1	A	666	LYS
1	A	688	CYS
1	A	752	HIS
1	A	814	GLN
1	A	852	SER
1	B	487	THR
1	B	505	GLU
1	B	613	GLU
1	B	677	GLU
1	B	752	HIS
1	B	771	ASN
1	B	814	GLN
1	B	828	LYS
1	C	480	LYS
1	C	498	LEU
1	C	499	LEU
1	C	518	ASN
1	C	523	MET
1	C	595	ARG
1	C	617	VAL
1	C	657	MET
1	C	752	HIS
1	C	771	ASN
1	C	788	ASN
1	C	814	GLN
1	D	469	GLN
1	D	595	ARG
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
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 (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	HIS
1	A	771	ASN
1	A	788	ASN
1	A	814	GLN
1	B	488	HIS
1	B	635	HIS
1	B	771	ASN
1	B	776	ASN
1	C	518	ASN
1	C	552	GLN
1	C	635	HIS
1	C	771	ASN
1	C	788	ASN
1	C	819	GLN
1	D	488	HIS
1	D	552	GLN
1	D	771	ASN
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	$\#\|Z\| > 2$
3	SIM	C	1	-	32,32,32	2.07	11 (34%)	37,46,46	1.53	6 (16%)
2	ADP	B	101	-	24,29,29	1.42	4 (16%)	29,45,45	0.80	1 (3%)
2	ADP	B	104	-	24,29,29	1.58	5 (20%)	29,45,45	0.76	1 (3%)
2	ADP	D	105	-	24,29,29	1.45	3 (12%)	29,45,45	0.78	1 (3%)
3	SIM	B	3	-	32,32,32	2.06	11 (34%)	37,46,46	1.49	8 (21%)
3	SIM	A	4	-	32,32,32	2.12	11 (34%)	37,46,46	1.54	7 (18%)
3	SIM	C	2	-	32,32,32	1.98	10 (31%)	37,46,46	1.47	7 (18%)
2	ADP	C	103	-	24,29,29	1.28	3 (12%)	29,45,45	0.95	2 (6%)
2	ADP	A	102	-	24,29,29	1.29	2 (8%)	29,45,45	0.75	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
3	SIM	C	1	-	-	3/26/55/55	0/2/2/2
2	ADP	B	101	-	-	2/12/32/32	0/3/3/3
2	ADP	B	104	-	-	1/12/32/32	0/3/3/3
2	ADP	D	105	-	-	5/12/32/32	0/3/3/3
3	SIM	B	3	-	-	1/26/55/55	0/2/2/2
3	SIM	A	4	-	-	5/26/55/55	0/2/2/2
3	SIM	C	2	-	-	2/26/55/55	0/2/2/2
2	ADP	C	103	-	-	5/12/32/32	0/3/3/3
2	ADP	A	102	-	-	2/12/32/32	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIM	C16-C17	4.65	1.55	1.50
3	C	2	SIM	C16-C17	4.62	1.55	1.50
3	C	1	SIM	O1A-C1	4.51	1.37	1.22
3	C	2	SIM	O1A-C1	4.40	1.36	1.22
3	B	3	SIM	O1A-C1	4.32	1.36	1.22
3	C	1	SIM	C16-C17	4.30	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	SIM	C13-C12	4.16	1.57	1.52
3	A	4	SIM	O1A-C1	3.97	1.35	1.22
3	C	1	SIM	C13-C12	3.94	1.57	1.52
3	A	4	SIM	C9-C8	3.82	1.58	1.54
3	A	4	SIM	C13-C12	3.82	1.57	1.52
3	B	3	SIM	C16-C17	3.80	1.54	1.50
3	A	4	SIM	C19-C18	3.75	1.58	1.52
3	C	2	SIM	C13-C12	3.74	1.57	1.52
3	C	1	SIM	C19-C18	3.60	1.58	1.52
2	C	103	ADP	C8-N7	-3.48	1.28	1.34
3	B	3	SIM	C19-C18	3.47	1.58	1.52
2	B	104	ADP	O4'-C1'	3.46	1.45	1.41
2	D	105	ADP	C8-N7	-3.44	1.28	1.34
3	B	3	SIM	C9-C8	3.41	1.58	1.54
3	C	2	SIM	C19-C18	3.36	1.58	1.52
2	A	102	ADP	C8-N7	-3.28	1.28	1.34
2	B	104	ADP	C8-N7	-3.26	1.28	1.34
2	B	101	ADP	C8-N7	-3.23	1.28	1.34
3	B	3	SIM	C9-C10	3.21	1.55	1.50
2	B	101	ADP	O4'-C4'	3.11	1.51	1.45
3	C	1	SIM	C9-C10	3.05	1.55	1.50
3	C	1	SIM	O14-C18	3.04	1.39	1.34
3	C	1	SIM	C13-C8	3.01	1.58	1.54
3	B	3	SIM	C13-C8	2.98	1.58	1.54
2	B	104	ADP	O4'-C4'	2.98	1.51	1.45
3	C	2	SIM	C9-C10	2.98	1.55	1.50
2	D	105	ADP	O4'-C4'	2.91	1.51	1.45
3	A	4	SIM	C9-C10	2.85	1.54	1.50
3	A	4	SIM	C13-C8	2.82	1.58	1.54
3	A	4	SIM	O1B-C1	-2.81	1.21	1.30
3	C	1	SIM	C9-C8	2.70	1.57	1.54
2	B	101	ADP	O4'-C1'	2.64	1.44	1.41
3	C	2	SIM	O1B-C1	-2.55	1.22	1.30
3	A	4	SIM	O14-C18	2.51	1.38	1.34
3	C	2	SIM	C9-C8	2.49	1.57	1.54
3	C	2	SIM	C13-C8	2.49	1.58	1.54
2	B	104	ADP	C2'-C3'	2.46	1.60	1.53
2	D	105	ADP	O4'-C1'	2.45	1.44	1.41
3	B	3	SIM	O1B-C1	-2.39	1.22	1.30
2	A	102	ADP	O4'-C4'	2.36	1.50	1.45
3	C	1	SIM	O1B-C1	-2.24	1.23	1.30
3	C	1	SIM	C11-C12	-2.22	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	SIM	C15-C14	2.22	1.56	1.52
3	A	4	SIM	C15-C14	2.21	1.56	1.52
3	B	3	SIM	C17-C12	2.19	1.37	1.34
2	C	103	ADP	C2'-C3'	2.19	1.59	1.53
3	B	3	SIM	C15-C14	2.15	1.56	1.52
3	B	3	SIM	O14-C18	2.12	1.38	1.34
3	C	2	SIM	C11-C12	-2.11	1.37	1.43
2	B	101	ADP	C2'-C3'	2.08	1.59	1.53
2	B	104	ADP	O2'-C2'	2.06	1.47	1.43
3	A	4	SIM	C11-C12	-2.04	1.37	1.43
3	C	1	SIM	C7-C8	2.03	1.57	1.53
2	C	103	ADP	O4'-C4'	2.01	1.49	1.45

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	SIM	C13-C8-C9	-4.43	108.35	110.70
3	A	4	SIM	C13-C8-C9	-4.08	108.53	110.70
3	C	2	SIM	C8-C9-C10	-3.69	108.63	110.90
3	B	3	SIM	C13-C8-C9	-3.59	108.80	110.70
3	A	4	SIM	C24-C16-C17	-3.55	108.00	111.19
3	B	3	SIM	C24-C16-C17	-3.27	108.25	111.19
3	C	1	SIM	O1A-C1-C2	-3.26	112.33	122.80
3	C	2	SIM	O1A-C1-C2	-3.21	112.50	122.80
3	C	2	SIM	O1B-C1-C2	3.20	124.34	114.07
3	B	3	SIM	O1A-C1-C2	-3.17	112.64	122.80
3	C	1	SIM	O1B-C1-C2	3.16	124.20	114.07
3	B	3	SIM	O1B-C1-C2	3.15	124.18	114.07
3	C	1	SIM	C24-C16-C17	-3.07	108.43	111.19
3	A	4	SIM	O1B-C1-C2	3.03	123.77	114.07
3	C	2	SIM	C13-C8-C9	-3.01	109.10	110.70
3	C	1	SIM	C8-C9-C10	-2.91	109.11	110.90
3	A	4	SIM	C8-C9-C10	-2.89	109.12	110.90
3	A	4	SIM	O1A-C1-C2	-2.89	113.55	122.80
3	C	2	SIM	C9A-C9-C10	-2.83	106.39	110.85
3	C	2	SIM	C24-C16-C17	-2.81	108.67	111.19
3	A	4	SIM	C9A-C9-C10	-2.75	106.52	110.85
3	C	1	SIM	C9A-C9-C10	-2.71	106.57	110.85
3	C	2	SIM	C14-O14-C18	2.64	121.58	117.38
3	B	3	SIM	C8-C9-C10	-2.56	109.33	110.90
3	B	3	SIM	C9A-C9-C10	-2.41	107.04	110.85
3	A	4	SIM	C14-O14-C18	2.29	121.03	117.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3	SIM	C7-C8-C13	2.28	115.59	112.50
2	D	105	ADP	C5-C6-N6	2.19	123.67	120.35
2	B	101	ADP	C5-C6-N6	2.18	123.66	120.35
2	B	104	ADP	C5-C6-N6	2.16	123.64	120.35
2	A	102	ADP	C5-C6-N6	2.16	123.63	120.35
2	C	103	ADP	C3'-C2'-C1'	2.16	104.22	100.98
2	C	103	ADP	C5-C6-N6	2.09	123.53	120.35
3	B	3	SIM	O14-C14-C15	2.07	112.37	108.08

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	101	ADP	O4'-C4'-C5'-O5'
2	B	101	ADP	C3'-C4'-C5'-O5'
2	C	103	ADP	O4'-C4'-C5'-O5'
2	D	105	ADP	PA-O3A-PB-O3B
2	C	103	ADP	C3'-C4'-C5'-O5'
3	C	2	SIM	C22-C19-C20-C21
2	D	105	ADP	C4'-C5'-O5'-PA
2	A	102	ADP	PA-O3A-PB-O2B
3	C	2	SIM	O14-C18-C19-C22
2	B	104	ADP	C4'-C5'-O5'-PA
2	D	105	ADP	C3'-C4'-C5'-O5'
3	A	4	SIM	O14-C18-C19-C23
3	C	1	SIM	O14-C18-C19-C23
3	A	4	SIM	O14-C18-C19-C20
2	A	102	ADP	C3'-C4'-C5'-O5'
3	A	4	SIM	O1B-C1-C2-C3
2	C	103	ADP	PA-O3A-PB-O1B
3	B	3	SIM	C23-C19-C20-C21
3	C	1	SIM	C23-C19-C20-C21
3	A	4	SIM	O14-C18-C19-C22
3	C	1	SIM	O14-C18-C19-C22
2	D	105	ADP	PA-O3A-PB-O1B
2	C	103	ADP	PA-O3A-PB-O2B
2	C	103	ADP	PA-O3A-PB-O3B
2	D	105	ADP	PA-O3A-PB-O2B
3	A	4	SIM	O1A-C1-C2-C3

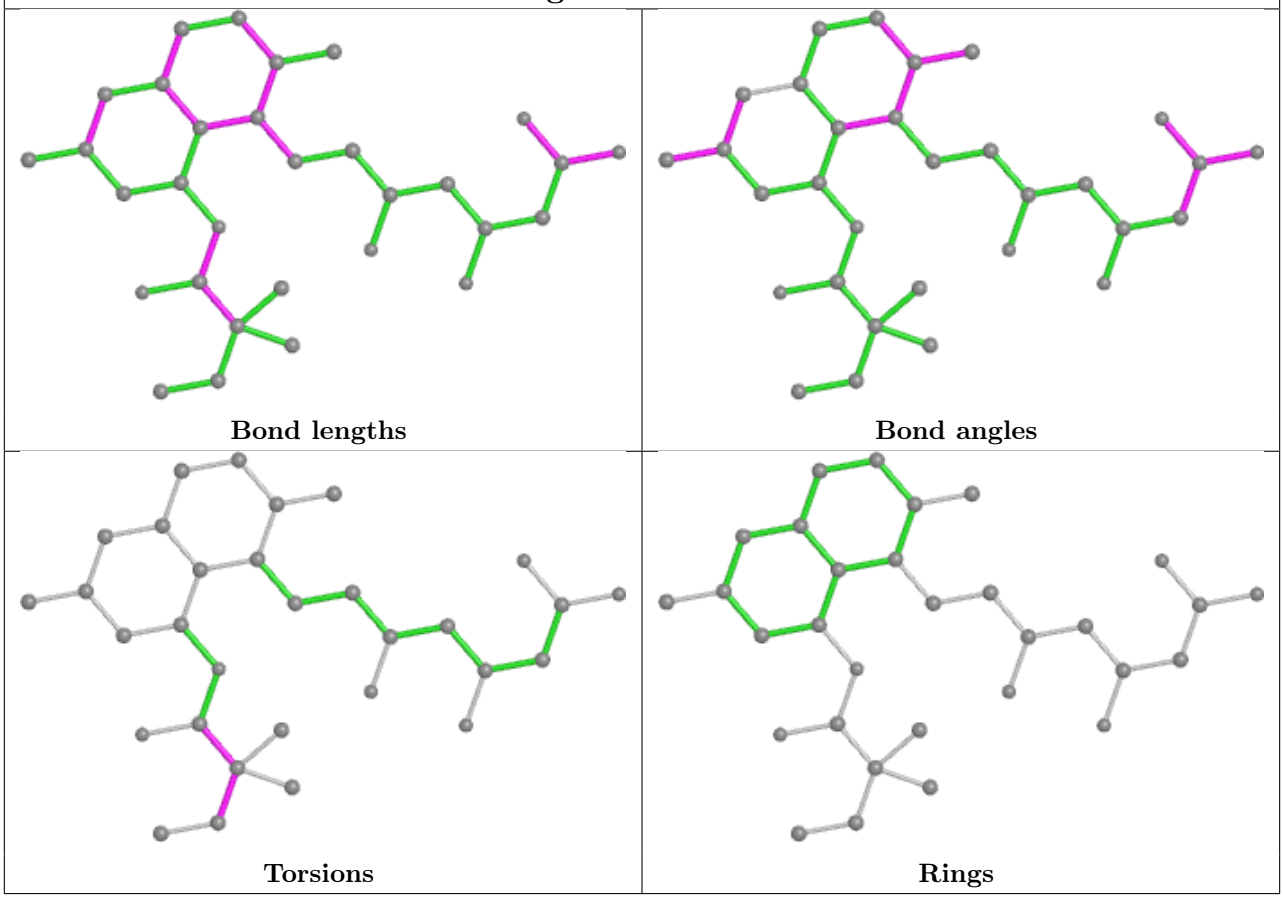
There are no ring outliers.

3 monomers are involved in 4 short contacts:

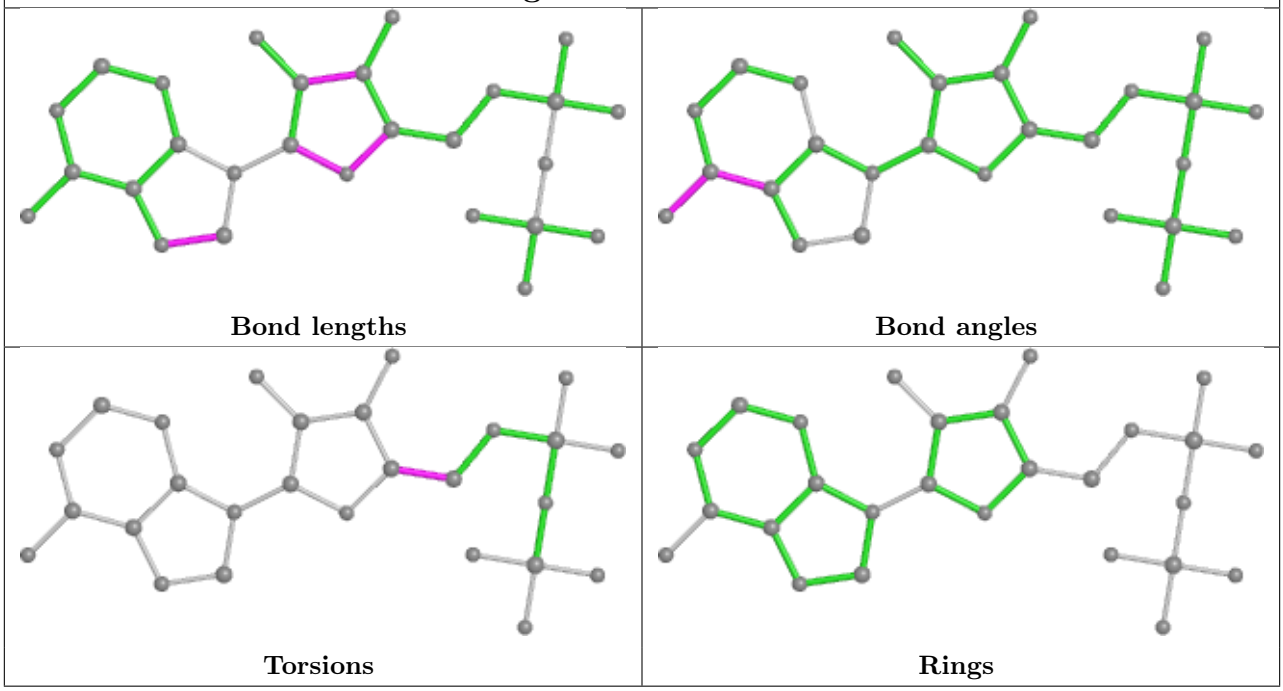
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	SIM	1	0
2	B	104	ADP	1	0
2	D	105	ADP	2	0

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.

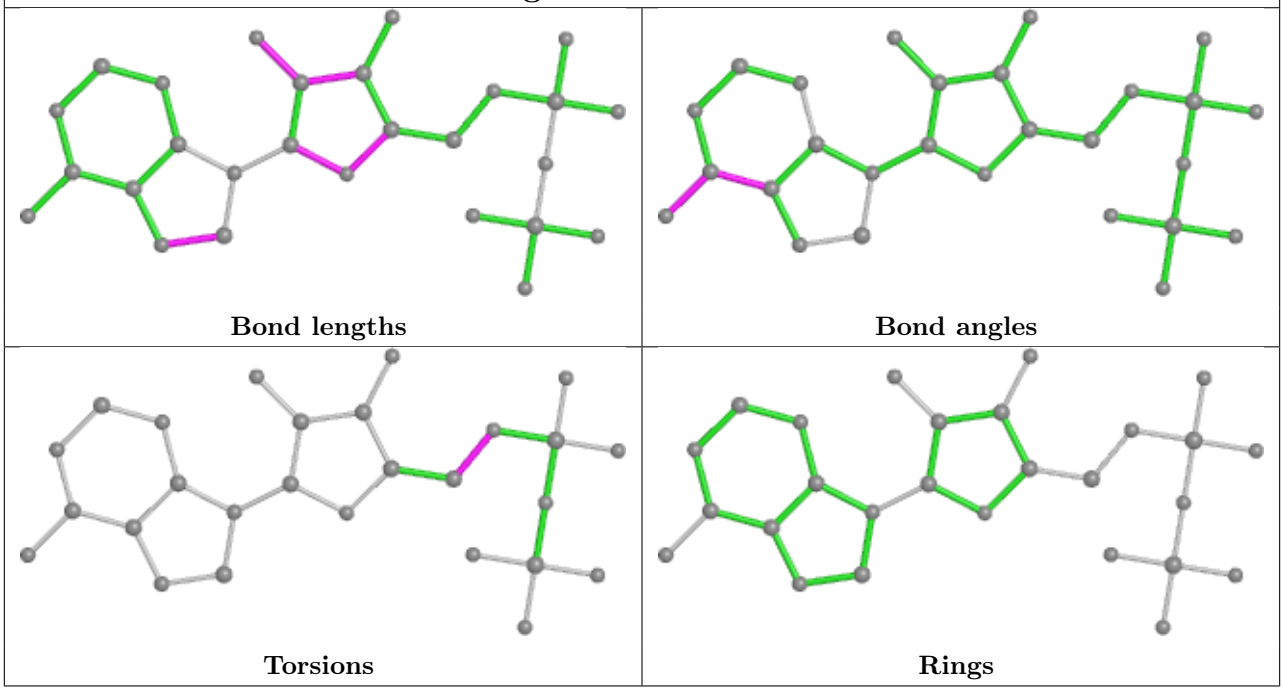
Ligand SIM C 1



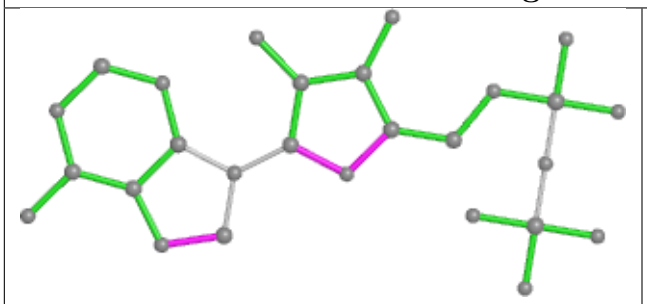
Ligand ADP B 101



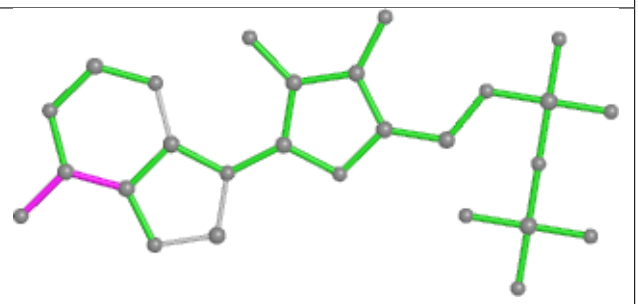
Ligand ADP B 104



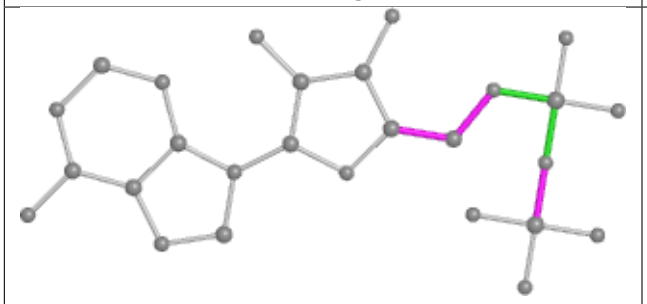
Ligand ADP D 105



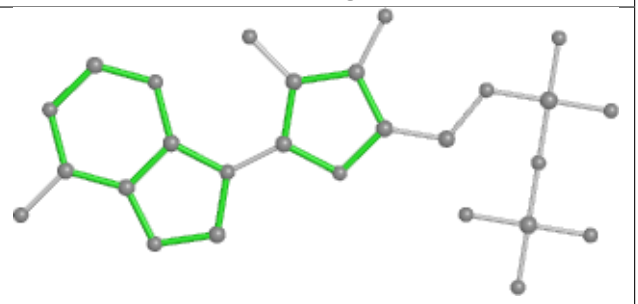
Bond lengths



Bond angles

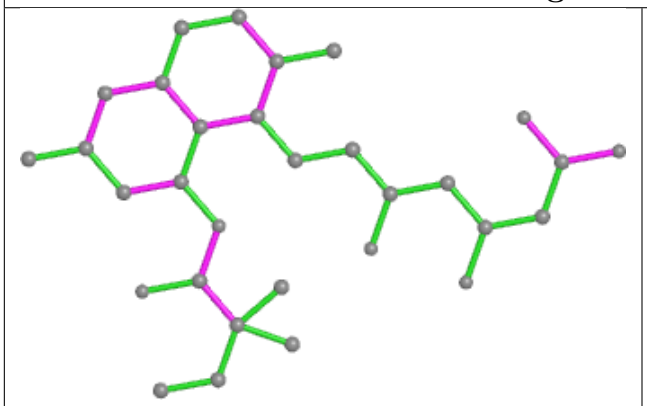


Torsions

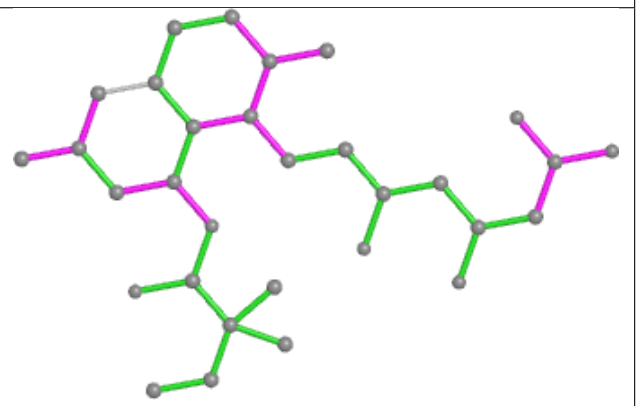


Rings

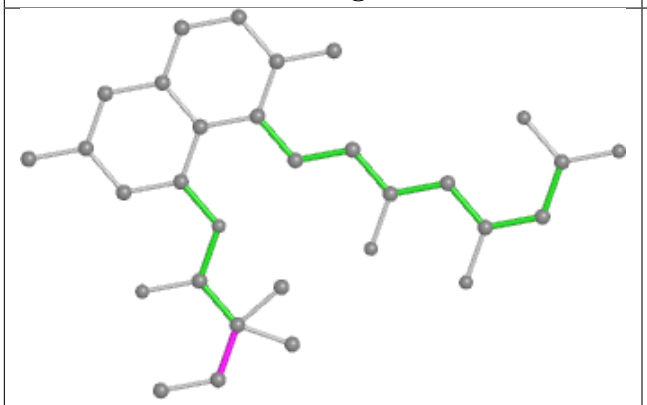
Ligand SIM B 3



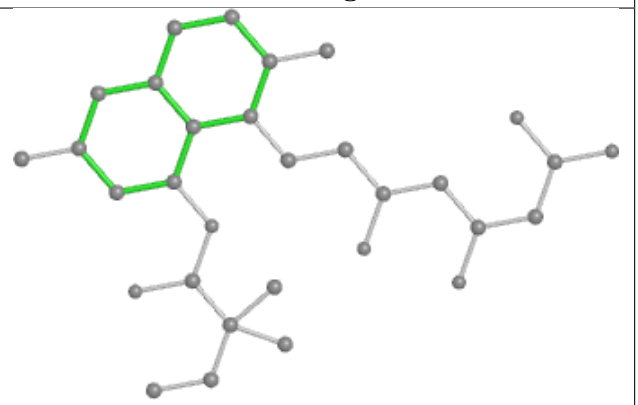
Bond lengths



Bond angles

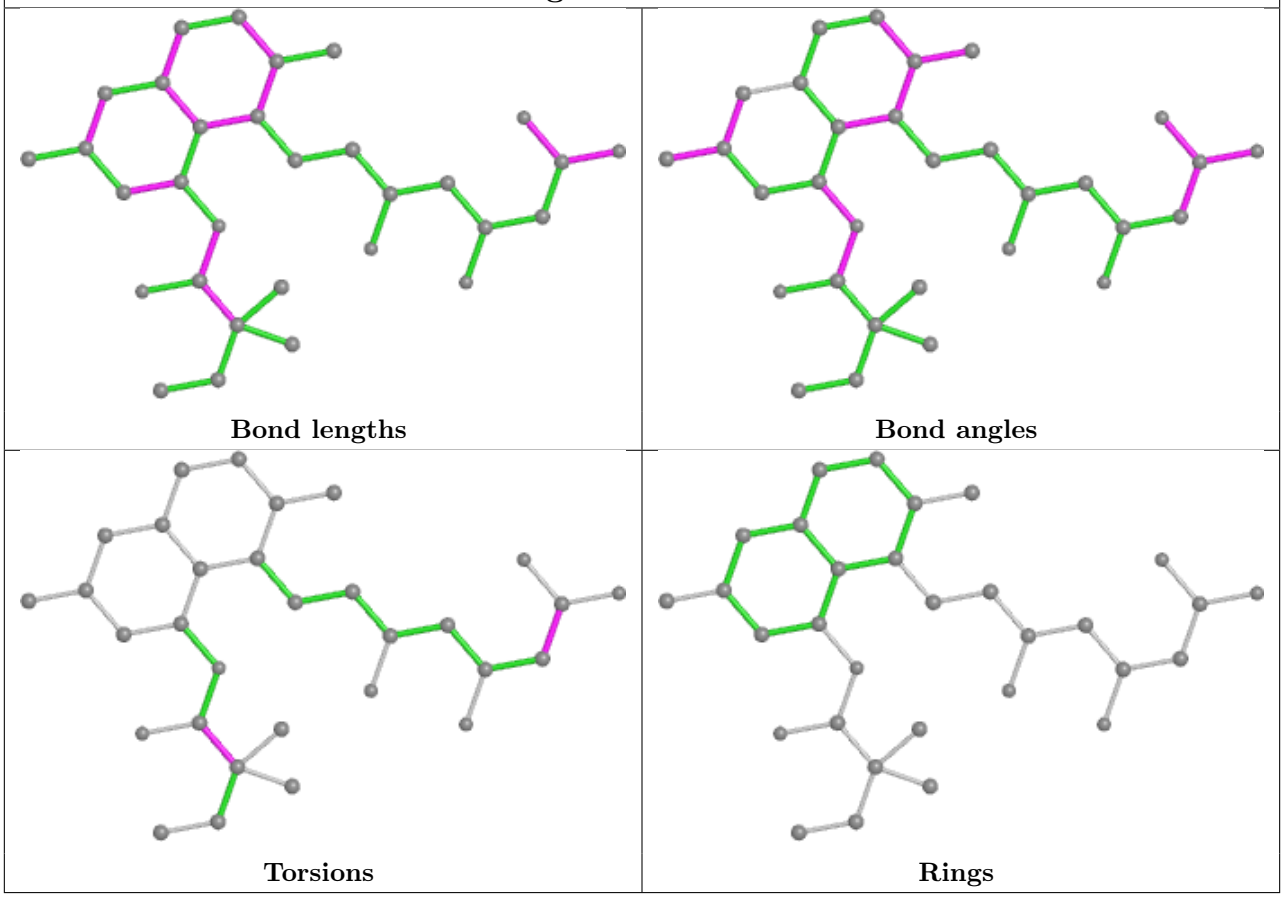


Torsions

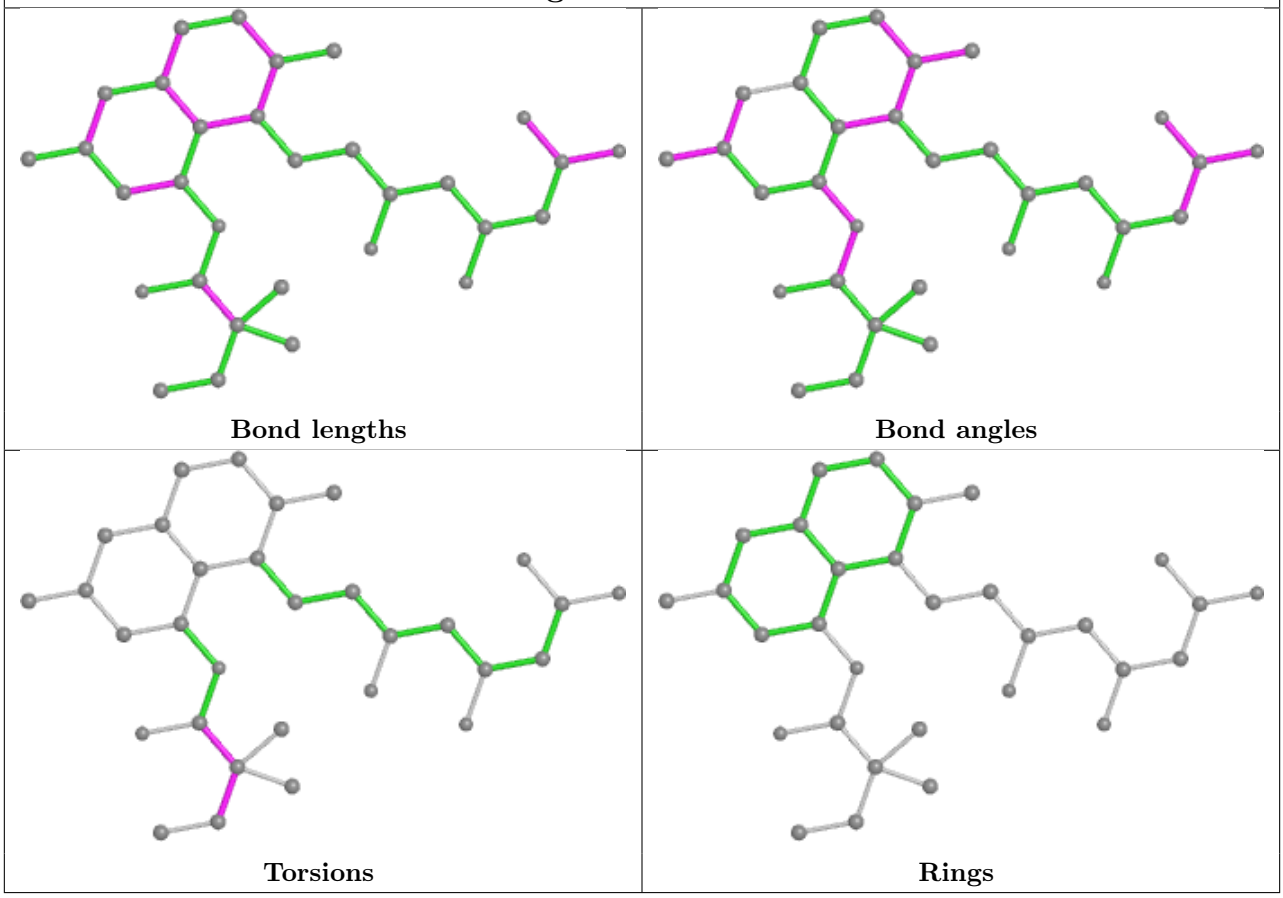


Rings

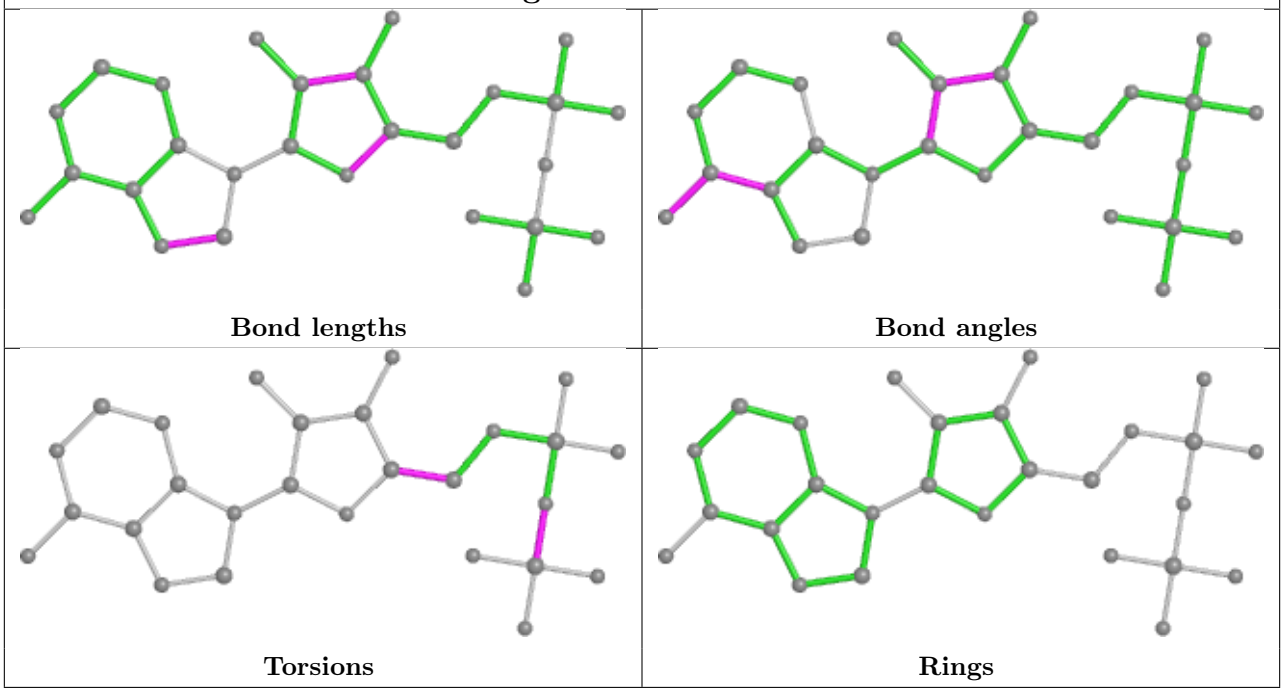
Ligand SIM A 4



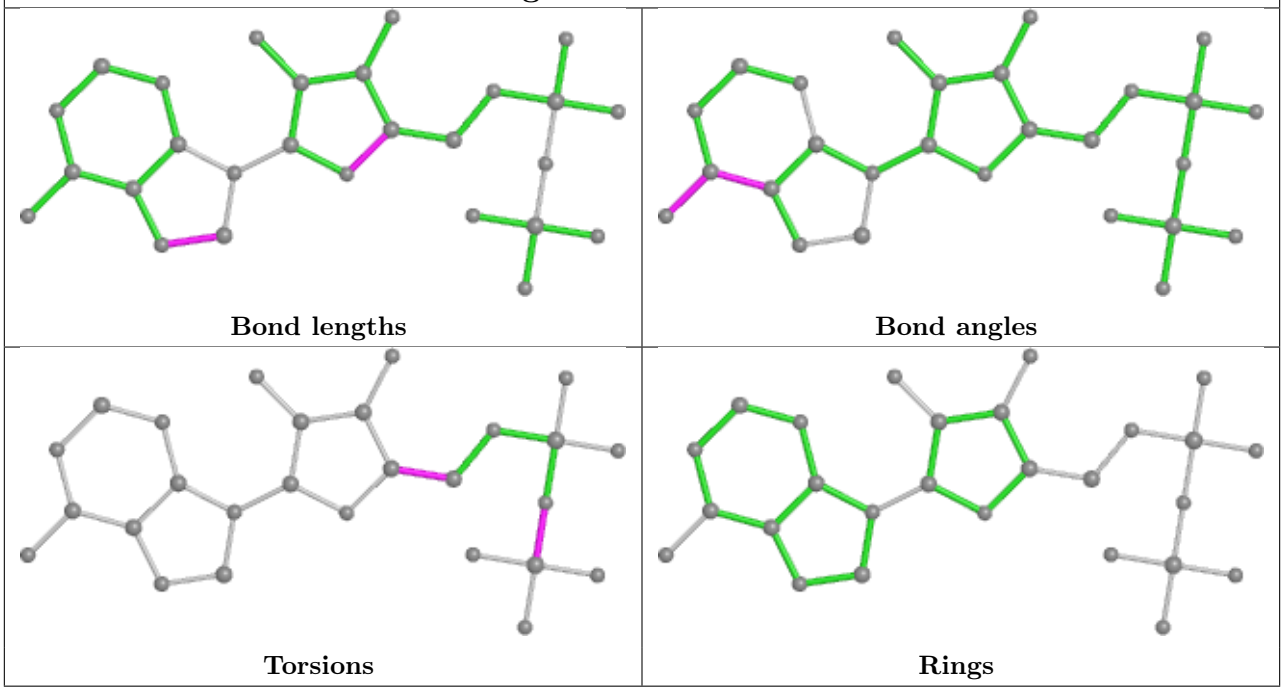
Ligand SIM C 2



Ligand ADP C 103



Ligand ADP A 102



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	408/467 (87%)	0.89	64 (15%)	2	3	36, 57, 100, 101	0
1	B	398/467 (85%)	0.91	67 (16%)	1	2	38, 57, 91, 101	0
1	C	389/467 (83%)	0.79	57 (14%)	2	4	39, 58, 86, 101	0
1	D	388/467 (83%)	0.75	55 (14%)	2	4	36, 54, 83, 101	0
All	All	1583/1868 (84%)	0.84	243 (15%)	2	3	36, 57, 96, 101	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	8.9
1	A	475	HIS	8.4
1	A	473	ALA	8.0
1	D	484	LEU	7.8
1	A	484	LEU	7.3
1	D	479	TYR	7.3
1	A	476	ILE	7.0
1	D	467	ILE	6.9
1	B	476	ILE	6.8
1	C	484	LEU	6.1
1	D	485	ILE	6.1
1	B	471	VAL	6.0
1	A	471	VAL	5.9
1	A	448	CYS	5.9
1	A	479	TYR	5.8
1	C	483	THR	5.8
1	B	483	THR	5.7
1	D	478	ALA	5.5
1	B	485	ILE	5.5
1	C	627	ARG	5.4
1	A	472	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	446	GLU	5.3
1	B	478	ALA	5.2
1	C	479	TYR	5.2
1	B	486	GLU	5.1
1	D	466	GLU	5.0
1	A	462	LEU	5.0
1	C	480	LYS	4.9
1	B	479	TYR	4.9
1	D	490	ARG	4.9
1	A	470	LEU	4.7
1	B	477	PRO	4.7
1	C	486	GLU	4.7
1	D	494	ILE	4.7
1	B	475	HIS	4.6
1	C	694	ALA	4.6
1	B	484	LEU	4.6
1	D	745	SER	4.5
1	A	523	MET	4.3
1	D	523	MET	4.3
1	D	694	ALA	4.3
1	D	480	LYS	4.2
1	B	746	ILE	4.2
1	D	469	GLN	4.1
1	A	481	LEU	4.1
1	D	743	ALA	4.0
1	A	461	PHE	4.0
1	C	628	PHE	4.0
1	C	773	GLY	4.0
1	A	445	ASN	4.0
1	D	746	ILE	3.9
1	A	772	VAL	3.9
1	B	630	ARG	3.9
1	B	481	LEU	3.9
1	A	746	ILE	3.9
1	A	693	PRO	3.9
1	A	447	GLU	3.9
1	D	695	ALA	3.8
1	A	483	THR	3.8
1	B	772	VAL	3.7
1	B	469	GLN	3.7
1	B	677	GLU	3.7
1	A	480	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	524	GLY	3.7
1	A	748	GLY	3.6
1	A	699	ILE	3.6
1	D	464	ASP	3.6
1	C	769	ALA	3.6
1	D	486	GLU	3.6
1	B	693	PRO	3.6
1	C	746	ILE	3.6
1	D	786	PRO	3.6
1	D	740	SER	3.5
1	B	694	ALA	3.5
1	B	698	TRP	3.5
1	B	523	MET	3.5
1	C	743	ALA	3.4
1	B	743	ALA	3.4
1	B	608	TRP	3.4
1	A	460	LYS	3.4
1	A	514	TYR	3.4
1	A	698	TRP	3.4
1	D	487	THR	3.4
1	B	754	ALA	3.3
1	D	772	VAL	3.3
1	A	769	ALA	3.3
1	C	772	VAL	3.3
1	C	828	LYS	3.3
1	A	466	GLU	3.3
1	B	776	ASN	3.2
1	B	777	CYS	3.2
1	B	613	GLU	3.2
1	B	758	THR	3.2
1	A	482	GLU	3.2
1	D	693	PRO	3.2
1	C	698	TRP	3.2
1	A	777	CYS	3.2
1	D	771	ASN	3.2
1	A	628	PHE	3.2
1	B	487	THR	3.2
1	C	481	LEU	3.2
1	C	741	ALA	3.1
1	D	465	ALA	3.1
1	B	501	LYS	3.1
1	B	828	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	696	ILE	3.1
1	B	695	ALA	3.1
1	A	499	LEU	3.0
1	B	773	GLY	3.0
1	C	770	GLN	3.0
1	C	695	ALA	3.0
1	B	472	ASN	3.0
1	B	771	ASN	3.0
1	B	757	VAL	3.0
1	A	694	ALA	3.0
1	C	715	LYS	3.0
1	D	747	GLY	3.0
1	B	470	LEU	3.0
1	B	748	GLY	3.0
1	C	693	PRO	3.0
1	A	689	THR	3.0
1	C	630	ARG	3.0
1	C	740	SER	2.9
1	D	774	SER	2.9
1	A	828	LYS	2.9
1	B	480	LYS	2.9
1	C	745	SER	2.9
1	C	482	GLU	2.9
1	D	748	GLY	2.9
1	B	474	LYS	2.9
1	D	491	GLY	2.9
1	C	771	ASN	2.9
1	B	769	ALA	2.9
1	A	747	GLY	2.8
1	A	743	ALA	2.8
1	D	698	TRP	2.8
1	B	775	SER	2.8
1	A	756	ILE	2.8
1	C	757	VAL	2.8
1	B	749	TYR	2.8
1	C	518	ASN	2.8
1	B	756	ILE	2.7
1	D	482	GLU	2.7
1	B	473	ALA	2.7
1	A	771	ASN	2.7
1	C	753	ALA	2.7
1	C	699	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	753	ALA	2.7
1	C	754	ALA	2.7
1	C	761	TYR	2.7
1	B	673	GLU	2.7
1	A	494	ILE	2.7
1	B	778	ILE	2.7
1	D	768	ALA	2.7
1	C	744	GLY	2.7
1	A	477	PRO	2.6
1	C	548	GLU	2.6
1	A	718	ARG	2.6
1	A	467	ILE	2.6
1	B	488	HIS	2.6
1	D	749	TYR	2.6
1	D	741	ALA	2.6
1	A	469	GLN	2.6
1	C	523	MET	2.6
1	B	744	GLY	2.6
1	B	741	ALA	2.6
1	A	715	LYS	2.6
1	A	444	PRO	2.6
1	A	778	ILE	2.6
1	B	774	SER	2.5
1	C	775	SER	2.5
1	C	505	GLU	2.5
1	A	749	TYR	2.5
1	A	630	ARG	2.5
1	A	468	ILE	2.5
1	D	699	ILE	2.5
1	D	744	GLY	2.5
1	D	481	LEU	2.5
1	B	745	SER	2.5
1	A	787	THR	2.5
1	A	474	LYS	2.5
1	B	740	SER	2.4
1	A	720	VAL	2.4
1	C	478	ALA	2.4
1	C	749	TYR	2.4
1	D	777	CYS	2.4
1	A	760	ILE	2.4
1	C	748	GLY	2.4
1	B	688	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	689	THR	2.4
1	D	742	MET	2.4
1	B	768	ALA	2.3
1	C	718	ARG	2.3
1	C	742	MET	2.3
1	C	620	GLU	2.3
1	A	860	GLY	2.3
1	B	747	GLY	2.3
1	D	488	HIS	2.3
1	A	501	LYS	2.3
1	B	762	ILE	2.3
1	A	744	GLY	2.2
1	B	719	GLU	2.2
1	C	485	ILE	2.2
1	C	616	ALA	2.2
1	D	776	ASN	2.2
1	B	706	VAL	2.2
1	A	624	SER	2.2
1	D	718	ARG	2.2
1	C	768	ALA	2.2
1	C	800	ILE	2.2
1	D	739	GLY	2.2
1	B	620	GLU	2.2
1	A	443	ARG	2.2
1	D	692	LYS	2.2
1	D	773	GLY	2.2
1	A	697	ASN	2.2
1	B	674	TYR	2.2
1	D	753	ALA	2.2
1	D	800	ILE	2.2
1	B	797	MET	2.2
1	C	674	TYR	2.2
1	B	696	ILE	2.2
1	C	467	ILE	2.2
1	C	696	ILE	2.2
1	A	695	ALA	2.1
1	A	829	ASP	2.1
1	B	467	ILE	2.1
1	C	747	GLY	2.1
1	B	763	ALA	2.1
1	A	463	SER	2.1
1	C	571	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	681	LEU	2.1
1	C	521	LEU	2.1
1	D	787	THR	2.1
1	D	775	SER	2.1
1	B	482	GLU	2.0
1	A	490	ARG	2.0
1	D	497	GLN	2.0
1	C	490	ARG	2.0
1	D	737	LEU	2.0
1	C	739	GLY	2.0
1	C	511	TYR	2.0
1	C	497	GLN	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.

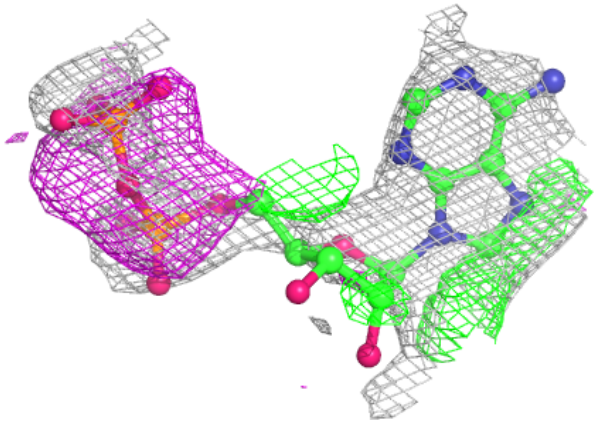
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	104	27/27	0.55	0.38	99,100,100,100	0
2	ADP	D	105	27/27	0.69	0.30	99,100,100,100	0
2	ADP	B	101	27/27	0.76	0.32	99,100,100,100	0
2	ADP	C	103	27/27	0.81	0.39	99,100,100,100	0
2	ADP	A	102	27/27	0.83	0.36	100,100,100,100	0
3	SIM	A	4	31/31	0.91	0.19	59,64,67,67	0
3	SIM	B	3	31/31	0.93	0.17	50,59,63,63	0
3	SIM	C	2	31/31	0.93	0.18	51,60,63,64	0
3	SIM	C	1	31/31	0.94	0.20	52,60,62,63	0

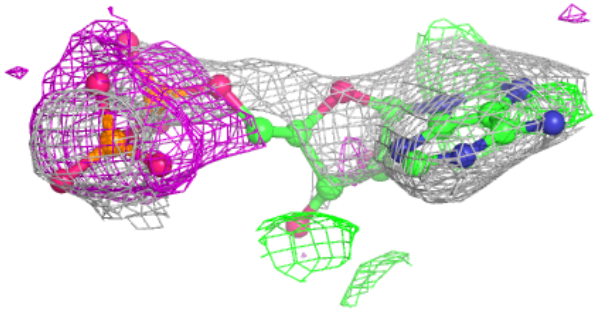
The following is a graphical depiction of the model fit to experimental electron density of all

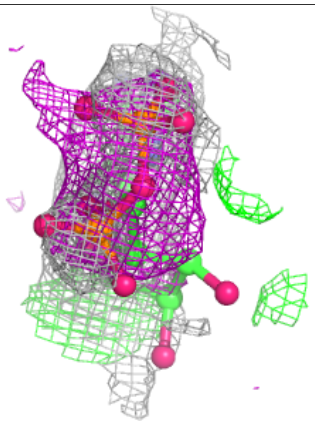
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

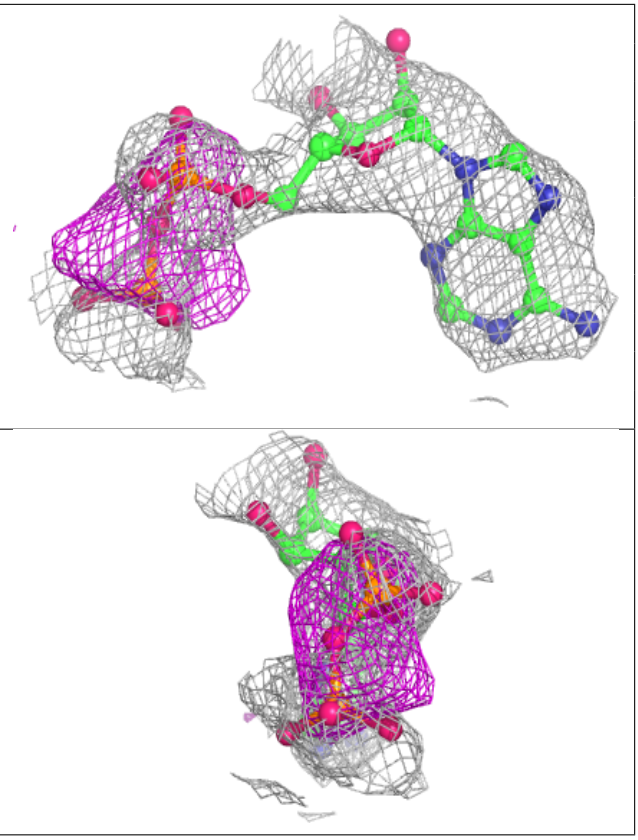






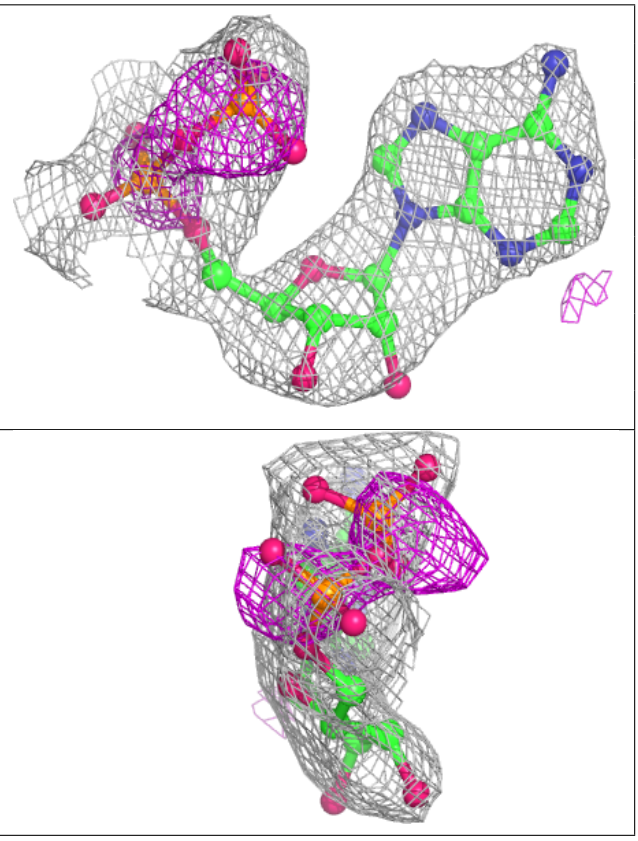
Electron density around ADP D 105:

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



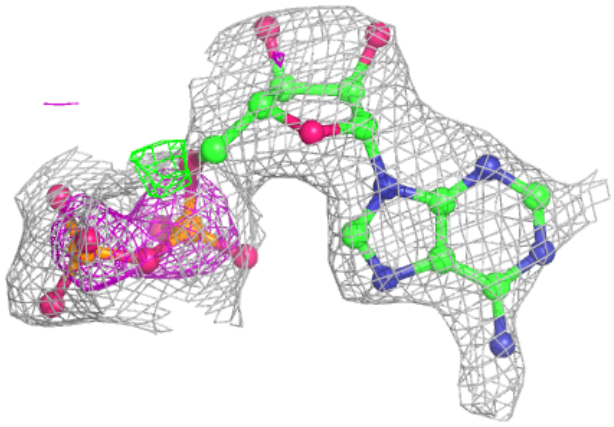
Electron density around ADP B 101:

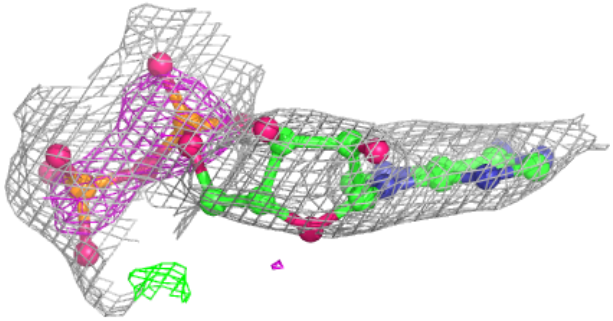
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

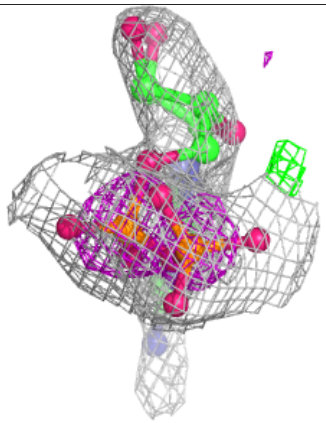


Electron density around ADP C 103:

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

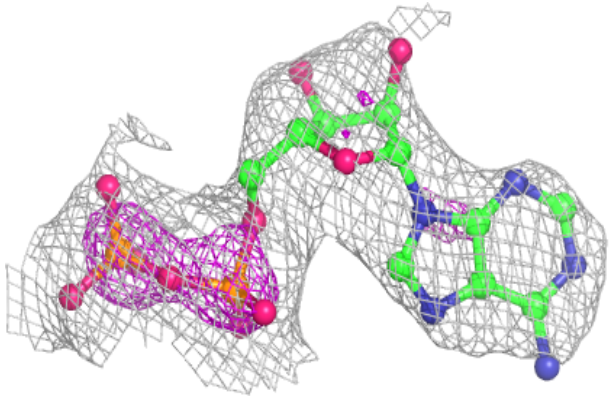


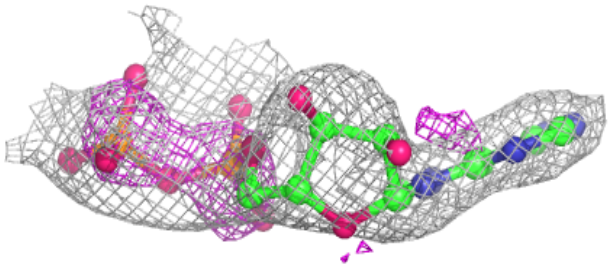


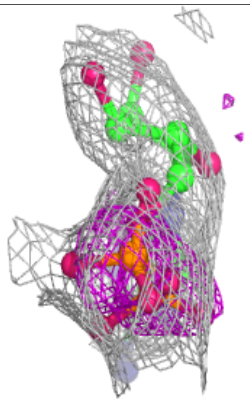


Electron density around ADP A 102:

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

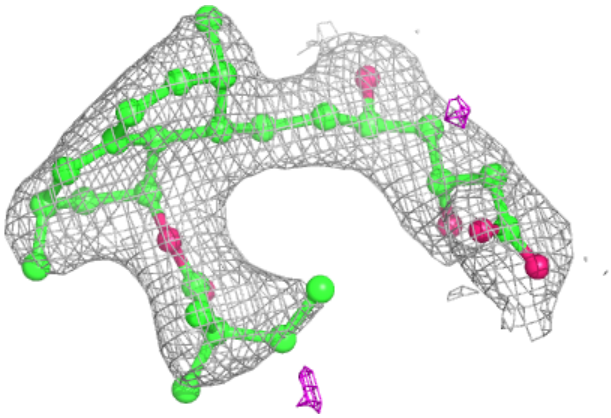


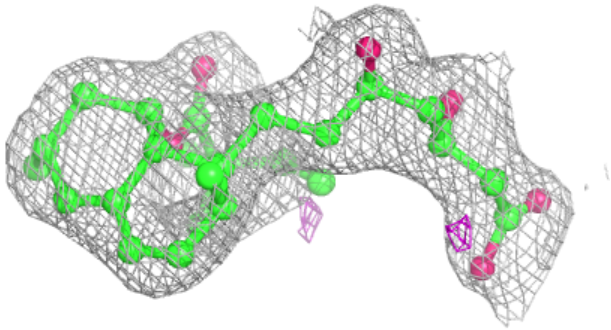


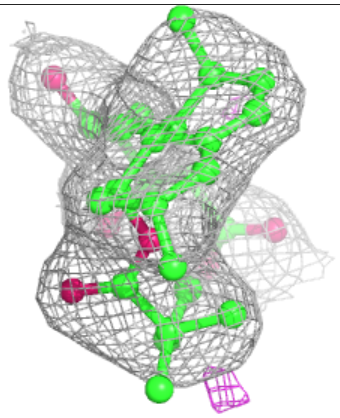


Electron density around SIM A 4:

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

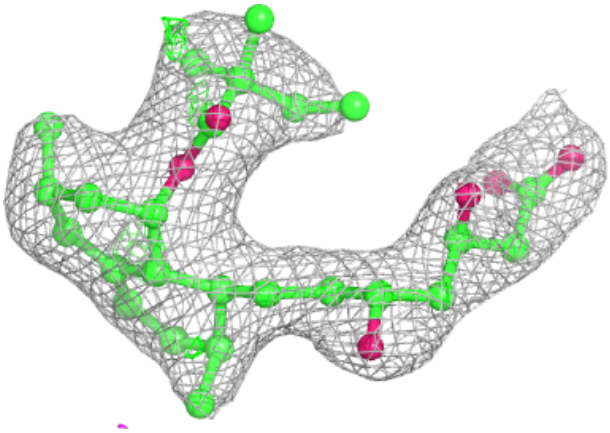


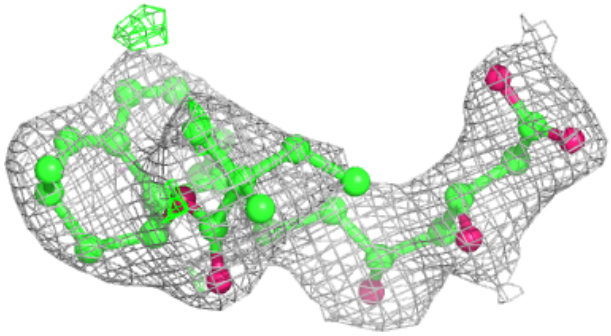


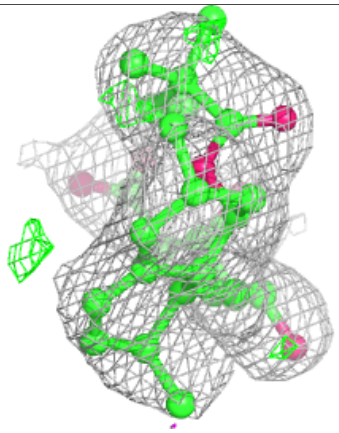


Electron density around SIM B 3:

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

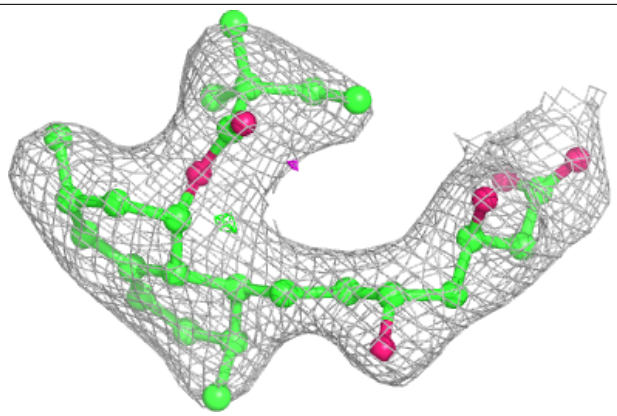


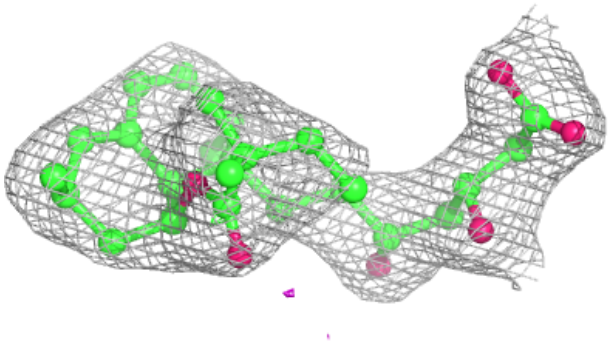


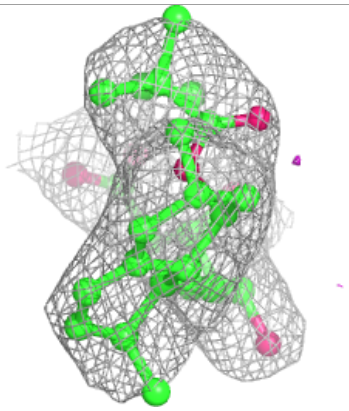


Electron density around SIM C 2:

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

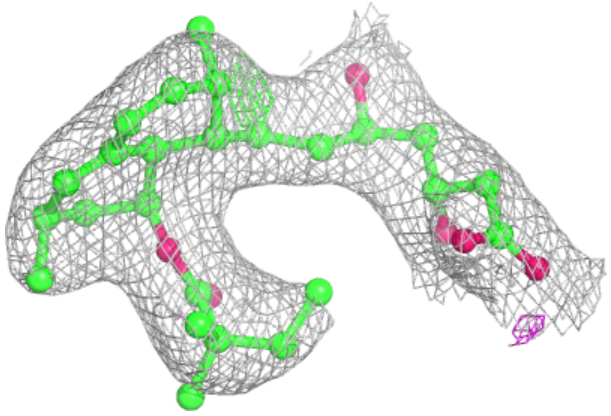


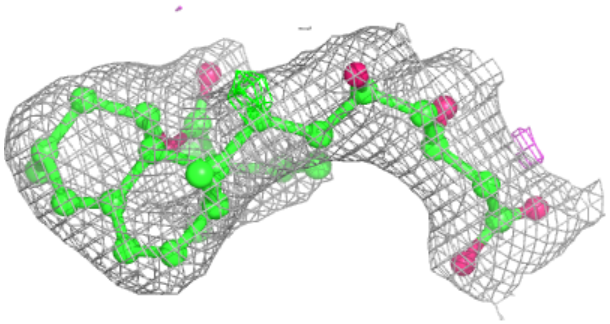


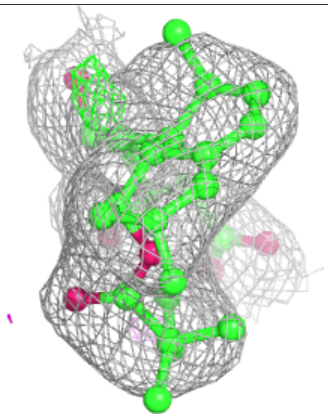


Electron density around SIM C 1:

$2mF_o$-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.