



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 1HW9 / pdb_00001hw9
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

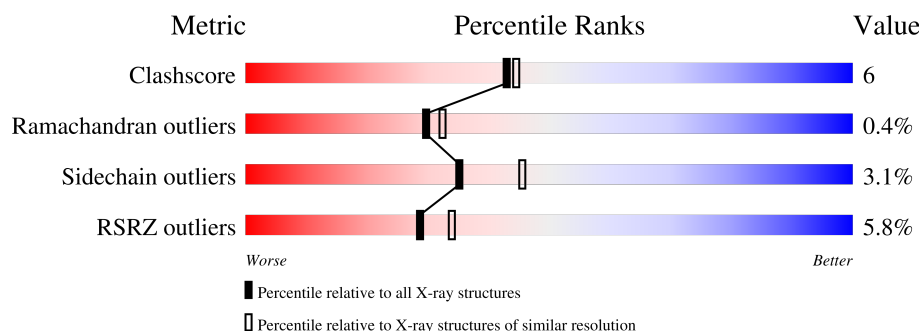
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	5% 72% 14% • 13%
1	B	467	6% 72% 12% • 15%
1	C	467	4% 70% 11% • 17%
1	D	467	4% 70% 12% • 17%

2 Entry composition

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.

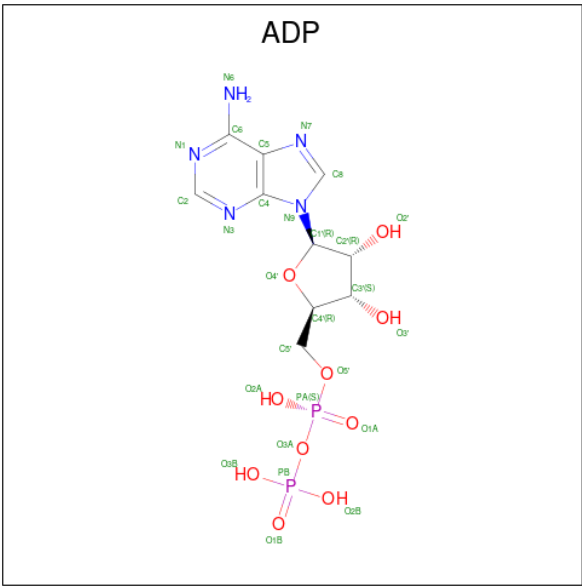
- Molecule 1 is a protein called HMG-COA REDUCTASE.

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

There are 20 discrepancies between the modelled and reference sequences:

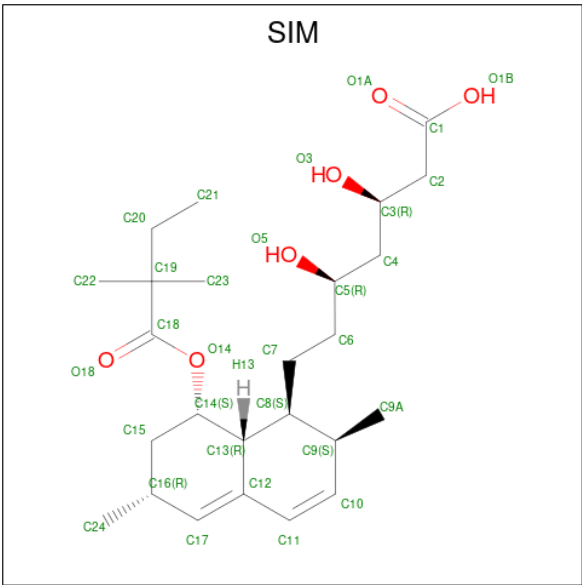
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: SIM) (formula: C₂₅H₄₀O₆).



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

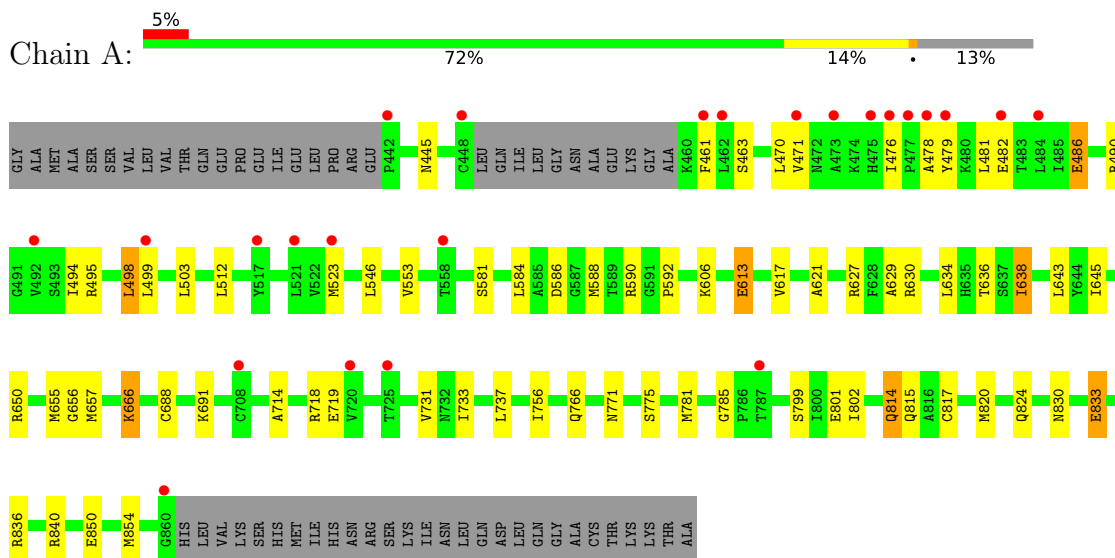
- Molecule 4 is water.

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

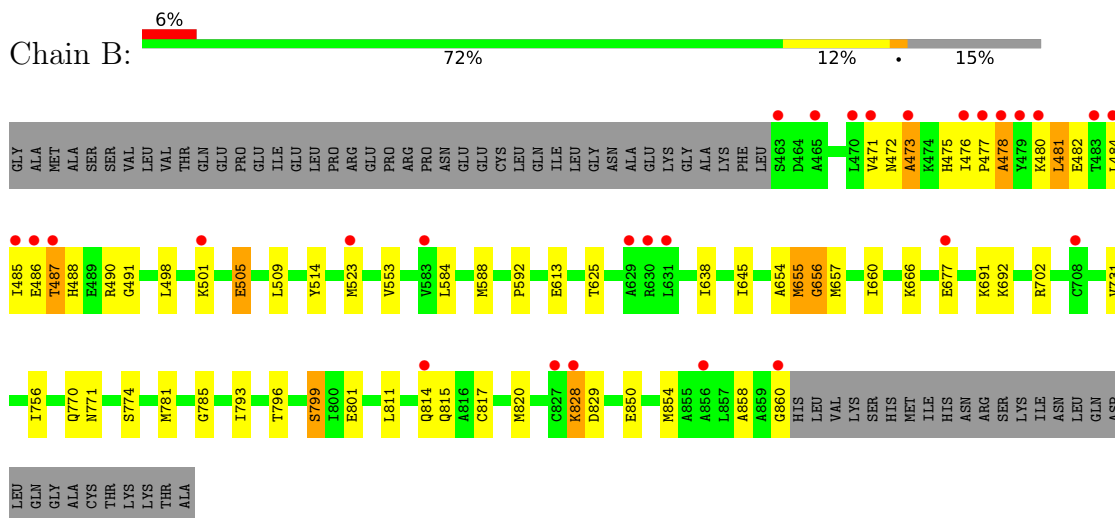
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HMG-COA REDUCTASE

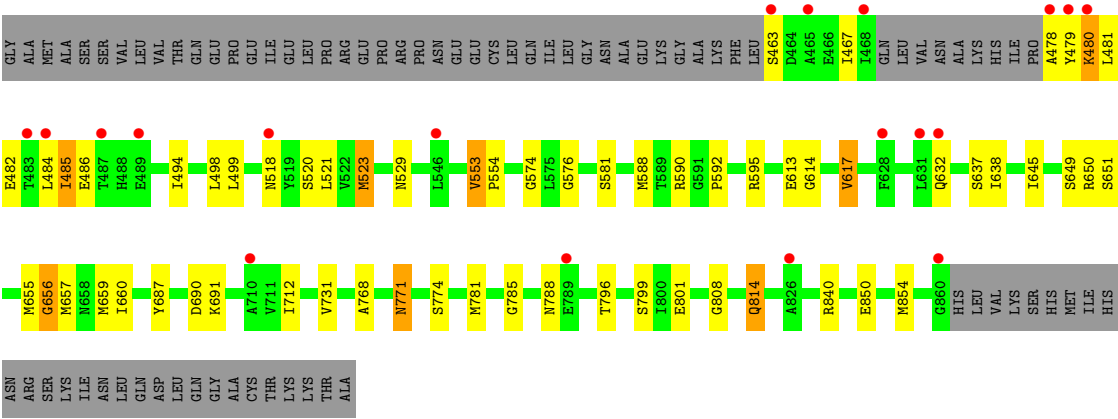


- Molecule 1: HMG-COA REDUCTASE

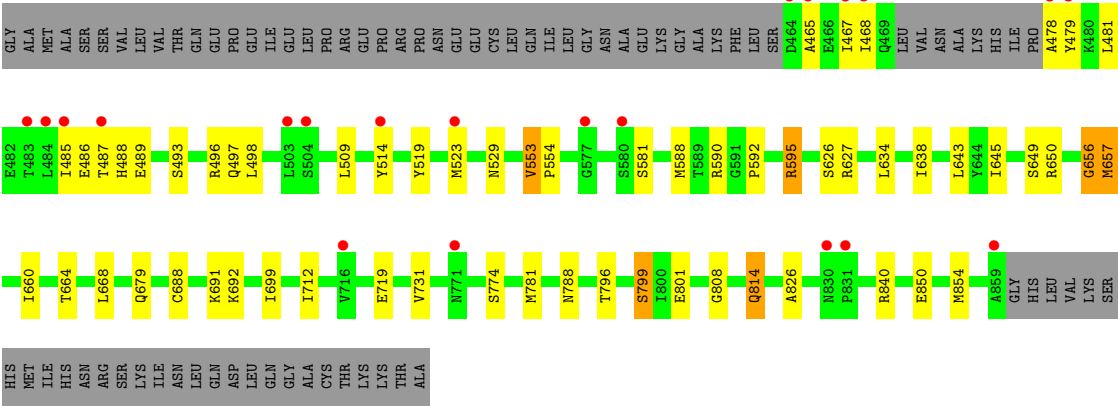


- Molecule 1: HMG-COA REDUCTASE





● Molecule 1: HMG-COA REDUCTASE



4 Data and refinement statistics

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 43.43 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.43-2.33) 92.2 (43.43-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.248 0.218 , (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)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.54	0/3081	1.00	9/4164 (0.2%)
1	B	0.53	0/2994	1.00	10/4049 (0.2%)
1	C	0.52	0/2920	0.95	8/3946 (0.2%)
1	D	0.56	0/2919	0.98	10/3945 (0.3%)
All	All	0.54	0/11914	0.99	37/16104 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	553	VAL	N-CA-C	10.88	118.75	107.76
1	A	553	VAL	N-CA-C	10.74	118.61	107.76
1	C	553	VAL	N-CA-C	10.59	118.46	107.76
1	B	553	VAL	N-CA-C	10.57	118.43	107.76
1	B	785	GLY	CA-C-N	8.35	127.93	119.24
1	B	785	GLY	C-N-CA	8.35	127.93	119.24
1	A	785	GLY	CA-C-N	7.81	127.72	119.05
1	A	785	GLY	C-N-CA	7.81	127.72	119.05
1	B	505	GLU	CA-C-N	7.62	128.31	119.47
1	B	505	GLU	C-N-CA	7.62	128.31	119.47
1	D	656	GLY	N-CA-C	7.61	125.82	115.32
1	B	656	GLY	N-CA-C	6.95	125.22	115.43
1	C	785	GLY	CA-C-N	6.87	126.11	118.97
1	C	785	GLY	C-N-CA	6.87	126.11	118.97
1	A	656	GLY	N-CA-C	6.86	125.11	115.43
1	C	656	GLY	N-CA-C	6.79	125.00	115.43
1	B	481	LEU	N-CA-C	6.69	118.57	111.28
1	D	719	GLU	N-CA-C	6.38	119.54	111.69
1	A	719	GLU	N-CA-C	6.16	119.27	111.69
1	D	650	ARG	N-CA-C	-5.91	102.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	MET	N-CA-C	-5.66	105.11	111.28
1	C	655	MET	N-CA-C	-5.59	105.28	111.71
1	B	473	ALA	N-CA-C	-5.50	105.36	113.61
1	C	691	LYS	N-CA-C	5.50	119.57	112.86
1	A	655	MET	N-CA-C	-5.47	105.32	111.28
1	D	712	ILE	CA-C-N	5.37	125.29	119.76
1	D	712	ILE	C-N-CA	5.37	125.29	119.76
1	D	799	SER	N-CA-C	5.29	119.30	109.56
1	A	691	LYS	N-CA-C	5.29	119.31	112.86
1	B	799	SER	N-CA-C	5.18	119.02	109.24
1	C	712	ILE	CA-C-N	5.11	125.03	119.76
1	C	712	ILE	C-N-CA	5.11	125.03	119.76
1	A	799	SER	N-CA-C	5.10	118.88	109.24
1	A	445	ASN	N-CA-C	5.09	117.57	111.71
1	D	691	LYS	N-CA-C	5.08	119.05	112.86
1	D	467	ILE	N-CA-C	-5.04	104.99	112.04
1	D	699	ILE	N-CA-C	5.02	116.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	3072	41	0
1	B	2952	0	2989	44	0
1	C	2881	0	2911	35	0
1	D	2880	0	2911	36	0
2	A	27	0	12	0	0
2	B	54	0	24	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	150	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 (150) 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	1.66	0.76
1:D:588:MET:HE1	1:D:801:GLU:HG2	1.68	0.76
1:C:588:MET:HE1	1:C:801:GLU:HG2	1.70	0.72
1:A:479:TYR:HA	1:A:495:ARG:HH21	1.54	0.72
1:C:651:SER:HA	1:C:659:MET:HE1	1.73	0.70
1:A:657:MET:HE3	1:A:657:MET:HA	1.74	0.69
1:A:731:VAL:HG12	1:A:854:MET:HE1	1.75	0.69
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:A:482:GLU:HG3	1:A:523:MET:HE2	1.80	0.63
1:D:638:ILE:HG22	1:D:643:LEU:HD13	1.81	0.62
1:A:817:CYS:HA	1:A:820:MET:HE3	1.82	0.61
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:B:655:MET:HE1	1:B:657:MET:HB2	1.83	0.59
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.02	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:731:VAL:HG12	1:A:854:MET:CE	2.32	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:A:781:MET:HE1	1:A:854:MET:HG3	1.87	0.56
1:C:581:SER:OG	1:C:840:ARG:HD2	2.05	0.56
1:B:588:MET:HE1	1:B:801:GLU:HG2	1.87	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:B:477:PRO:HG2	1:B:480:LYS:HZ3	1.72	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:B:471:VAL:C	1:B:473:ALA:H	2.15	0.54
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:B:781:MET:HE2	1:B:793:ILE:HD12	1.91	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:657:MET:HE3	1:B:657:MET:HA	1.91	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: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:C:781:MET:HE1	1:C:854:MET:HG3	1.95	0.49
1:C:731:VAL:HG12	1:C:854:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:588:MET:HE1	1:A:801:GLU:HG2	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:A:629:ALA:C	1:A:630:ARG:HD2	2.40	0.46
1:D:731:VAL:HG12	1:D:854:MET:CE	2.45	0.46
1:B:475:HIS:C	1:B:476:ILE:HG13	2.41	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:D:781:MET:HE1	1:D:854:MET:HG3	1.96	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:A:820:MET:HE2	1:B:509:LEU:HD21	1.98	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:B:858:ALA:C	1:B:860:GLY:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:692:LYS:HE2	1:B:692:LYS:HB2	1.89	0.41
1:C:574:GLY:C	1:C:576:GLY:H	2.27	0.41
1:C:731:VAL:HG12	1:C:854:MET:HE1	2.03	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:657:MET:HE2	1:D:657:MET:HA	2.01	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:A:613:GLU:CD	1:A:613:GLU:H	2.29	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:731:VAL:HG12	1:B:854:MET:HE1	2.02	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/467 (86%)	381 (94%)	22 (5%)	1 (0%)	43	50
1	B	396/467 (85%)	373 (94%)	20 (5%)	3 (1%)	16	16
1	C	385/467 (82%)	364 (94%)	20 (5%)	1 (0%)	36	41
1	D	384/467 (82%)	365 (95%)	17 (4%)	2 (0%)	24	26
All	All	1569/1868 (84%)	1483 (94%)	79 (5%)	7 (0%)	30	32

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

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%)	310 (95%)	16 (5%)	22	28
1	B	316/375 (84%)	309 (98%)	7 (2%)	45	58
1	C	308/375 (82%)	298 (97%)	10 (3%)	34	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	308/375 (82%)	302 (98%)	6 (2%)	50 63
All	All	1258/1500 (84%)	1219 (97%)	39 (3%)	35 45

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	PHE
1	A	463	SER
1	A	470	LEU
1	A	486	GLU
1	A	498	LEU
1	A	499	LEU
1	A	503	LEU
1	A	512	LEU
1	A	613	GLU
1	A	617	VAL
1	A	634	LEU
1	A	638	ILE
1	A	666	LYS
1	A	688	CYS
1	A	814	GLN
1	A	833	GLU
1	B	487	THR
1	B	505	GLU
1	B	613	GLU
1	B	677	GLU
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	521	LEU
1	C	523	MET
1	C	595	ARG
1	C	617	VAL
1	C	657	MET
1	C	771	ASN
1	C	814	GLN
1	D	595	ARG
1	D	634	LEU
1	D	657	MET

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Mol	Chain	Res	Type
1	D	688	CYS
1	D	788	ASN
1	D	814	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	552	GLN
1	A	635	HIS
1	A	736	ASN
1	A	771	ASN
1	A	788	ASN
1	A	814	GLN
1	B	488	HIS
1	B	771	ASN
1	B	776	ASN
1	C	518	ASN
1	C	552	GLN
1	C	632	GLN
1	C	635	HIS
1	C	672	HIS
1	C	770	GLN
1	C	771	ASN
1	C	788	ASN
1	C	819	GLN
1	D	488	HIS
1	D	497	GLN
1	D	552	GLN
1	D	635	HIS
1	D	771	ASN
1	D	788	ASN
1	D	819	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	103	-	28,29,29	1.55	5 (17%)	43,45,45	0.84	0
2	ADP	B	104	-	28,29,29	2.04	5 (17%)	43,45,45	0.76	0
3	SIM	C	2	-	32,32,32	2.00	10 (31%)	38,46,46	1.45	7 (18%)
2	ADP	B	101	-	28,29,29	1.59	5 (17%)	43,45,45	0.76	0
2	ADP	D	105	-	28,29,29	1.87	5 (17%)	43,45,45	0.78	1 (2%)
3	SIM	A	4	-	32,32,32	2.13	11 (34%)	38,46,46	1.50	7 (18%)
2	ADP	A	102	-	28,29,29	1.54	4 (14%)	43,45,45	0.69	0
3	SIM	B	3	-	32,32,32	2.08	12 (37%)	38,46,46	1.46	8 (21%)
3	SIM	C	1	-	32,32,32	2.08	10 (31%)	38,46,46	1.50	6 (15%)

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	-	-	5/16/32/32	0/3/3/3
2	ADP	B	104	-	-	3/16/32/32	0/3/3/3
3	SIM	C	2	-	-	2/26/55/55	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	101	-	-	2/16/32/32	0/3/3/3
2	ADP	D	105	-	-	5/16/32/32	0/3/3/3
3	SIM	A	4	-	-	5/26/55/55	0/2/2/2
2	ADP	A	102	-	-	2/16/32/32	0/3/3/3
3	SIM	B	3	-	-	1/26/55/55	0/2/2/2
3	SIM	C	1	-	-	4/26/55/55	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	ADP	PA-O3A	7.79	1.67	1.59
2	D	105	ADP	PA-O3A	6.83	1.66	1.59
2	C	103	ADP	PA-O3A	4.86	1.64	1.59
3	A	4	SIM	C16-C17	4.86	1.55	1.50
3	C	2	SIM	C16-C17	4.83	1.55	1.50
2	A	102	ADP	PA-O3A	4.81	1.64	1.59
3	C	1	SIM	O1A-C1	4.59	1.37	1.22
2	B	101	ADP	PA-O3A	4.51	1.64	1.59
3	C	1	SIM	C16-C17	4.49	1.55	1.50
3	C	2	SIM	O1A-C1	4.47	1.36	1.22
3	B	3	SIM	O1A-C1	4.39	1.36	1.22
3	B	3	SIM	C13-C12	4.16	1.57	1.52
3	A	4	SIM	O1A-C1	4.04	1.35	1.22
3	B	3	SIM	C16-C17	3.97	1.54	1.50
3	C	1	SIM	C13-C12	3.94	1.57	1.52
3	A	4	SIM	C9-C8	3.87	1.58	1.54
3	A	4	SIM	C13-C12	3.82	1.57	1.52
3	C	2	SIM	C13-C12	3.74	1.57	1.52
3	A	4	SIM	C19-C18	3.70	1.58	1.52
3	C	1	SIM	C19-C18	3.55	1.58	1.52
3	B	3	SIM	C9-C8	3.45	1.58	1.54
3	B	3	SIM	C19-C18	3.42	1.58	1.52
3	C	2	SIM	C19-C18	3.31	1.58	1.52
2	D	105	ADP	C1'-N9	3.20	1.55	1.46
2	B	101	ADP	O4'-C4'	3.13	1.51	1.45
3	B	3	SIM	C9-C10	3.00	1.55	1.50
2	B	104	ADP	O4'-C4'	3.00	1.51	1.45
2	C	103	ADP	C1'-N9	2.95	1.54	1.46
2	B	101	ADP	C1'-N9	2.94	1.54	1.46
3	C	1	SIM	O14-C18	2.94	1.39	1.34
2	D	105	ADP	O4'-C4'	2.93	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIM	O1B-C1	-2.88	1.21	1.30
2	A	102	ADP	C1'-N9	2.88	1.54	1.46
3	C	1	SIM	C9-C10	2.85	1.55	1.50
3	C	1	SIM	C13-C8	2.84	1.58	1.54
3	B	3	SIM	C13-C8	2.81	1.58	1.54
2	B	104	ADP	C1'-N9	2.79	1.54	1.46
3	C	2	SIM	C9-C10	2.78	1.55	1.50
3	C	1	SIM	C9-C8	2.73	1.57	1.54
2	B	101	ADP	C8-N9	-2.73	1.32	1.37
3	A	4	SIM	C9-C10	2.66	1.54	1.50
3	A	4	SIM	C13-C8	2.66	1.58	1.54
3	C	2	SIM	O1B-C1	-2.62	1.22	1.30
2	B	104	ADP	C8-N9	-2.59	1.33	1.37
2	A	102	ADP	C8-N9	-2.54	1.33	1.37
2	D	105	ADP	C8-N9	-2.53	1.33	1.37
3	C	2	SIM	C9-C8	2.52	1.57	1.54
2	B	104	ADP	C2'-C3'	2.47	1.60	1.53
2	C	103	ADP	C8-N9	-2.47	1.33	1.37
3	B	3	SIM	O1B-C1	-2.46	1.22	1.30
3	A	4	SIM	O14-C18	2.42	1.38	1.34
2	A	102	ADP	O4'-C4'	2.37	1.50	1.45
3	C	1	SIM	C11-C12	-2.36	1.36	1.43
3	C	2	SIM	C13-C8	2.34	1.58	1.54
3	C	1	SIM	O1B-C1	-2.31	1.23	1.30
3	C	2	SIM	C11-C12	-2.24	1.37	1.43
3	B	3	SIM	C17-C12	2.20	1.37	1.34
3	C	2	SIM	C15-C14	2.20	1.56	1.52
2	C	103	ADP	C2'-C3'	2.20	1.59	1.53
3	A	4	SIM	C15-C14	2.19	1.56	1.52
3	A	4	SIM	C11-C12	-2.16	1.37	1.43
3	B	3	SIM	C15-C14	2.13	1.56	1.52
2	B	101	ADP	C2'-C3'	2.09	1.59	1.53
3	B	3	SIM	C11-C12	-2.08	1.37	1.43
3	B	3	SIM	O14-C18	2.05	1.38	1.34
2	C	103	ADP	O4'-C4'	2.02	1.49	1.45
2	D	105	ADP	C2'-C3'	2.01	1.58	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	SIM	C8-C9-C10	-3.68	108.63	110.88
3	B	3	SIM	C13-C8-C9	-3.59	108.80	110.70
3	C	1	SIM	O1A-C1-C2	-3.42	112.33	122.84
3	C	2	SIM	O1A-C1-C2	-3.37	112.50	122.84
3	A	4	SIM	C24-C16-C17	-3.36	108.00	111.11
3	C	2	SIM	O1B-C1-C2	3.32	124.34	114.00
3	B	3	SIM	O1A-C1-C2	-3.32	112.64	122.84
3	C	1	SIM	O1B-C1-C2	3.28	124.20	114.00
3	B	3	SIM	O1B-C1-C2	3.27	124.18	114.00
3	A	4	SIM	O1B-C1-C2	3.14	123.77	114.00
3	B	3	SIM	C24-C16-C17	-3.09	108.25	111.11
3	A	4	SIM	O1A-C1-C2	-3.03	113.55	122.84
3	C	2	SIM	C13-C8-C9	-3.01	109.10	110.70
3	C	1	SIM	C24-C16-C17	-2.90	108.43	111.11
3	C	1	SIM	C8-C9-C10	-2.89	109.11	110.88
3	A	4	SIM	C8-C9-C10	-2.88	109.12	110.88
3	C	2	SIM	C14-O14-C18	2.65	121.58	117.39
3	C	2	SIM	C24-C16-C17	-2.64	108.67	111.11
3	C	2	SIM	C9A-C9-C10	-2.56	106.39	110.73
3	B	3	SIM	C8-C9-C10	-2.54	109.33	110.88
3	A	4	SIM	C9A-C9-C10	-2.49	106.52	110.73
3	C	1	SIM	C9A-C9-C10	-2.45	106.57	110.73
3	A	4	SIM	C14-O14-C18	2.30	121.03	117.39
2	D	105	ADP	O4'-C1'-N9	2.30	112.50	108.09
3	B	3	SIM	C7-C8-C13	2.28	115.59	112.50
3	B	3	SIM	C9A-C9-C10	-2.18	107.04	110.73
3	B	3	SIM	O14-C14-C15	2.04	112.37	108.11

There are no chirality outliers.

All (29) torsion outliers are listed below:

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

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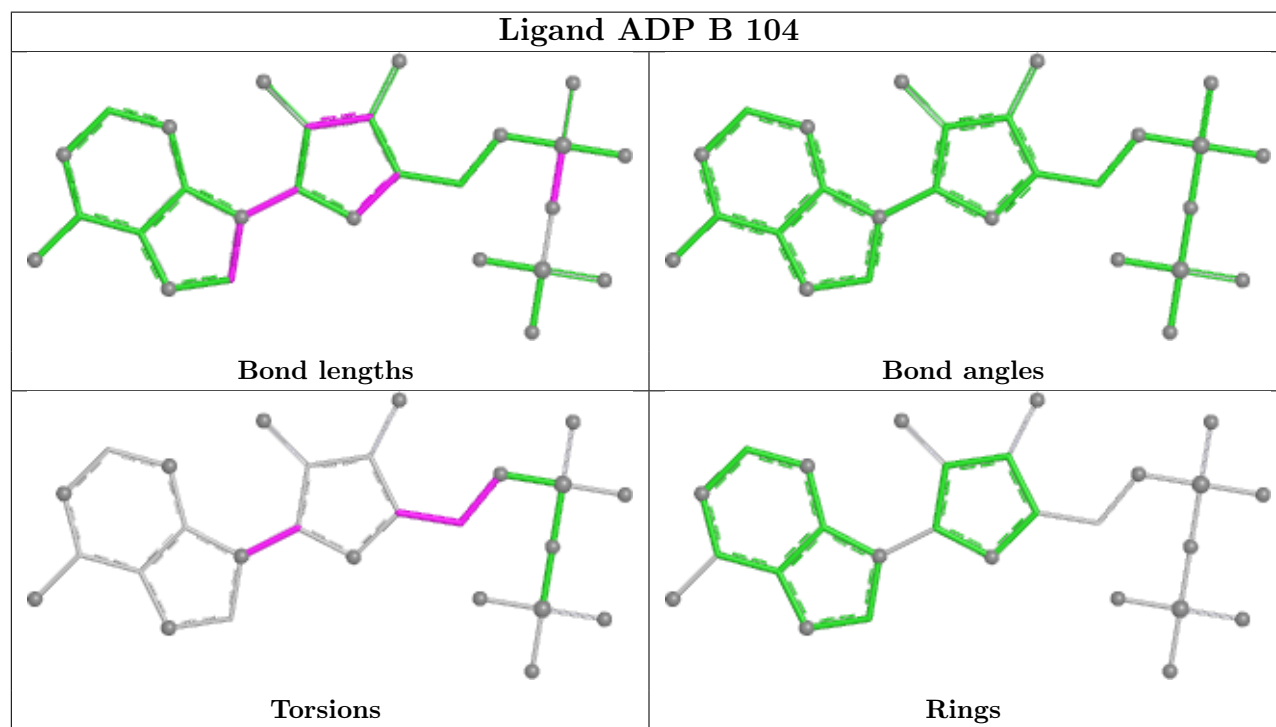
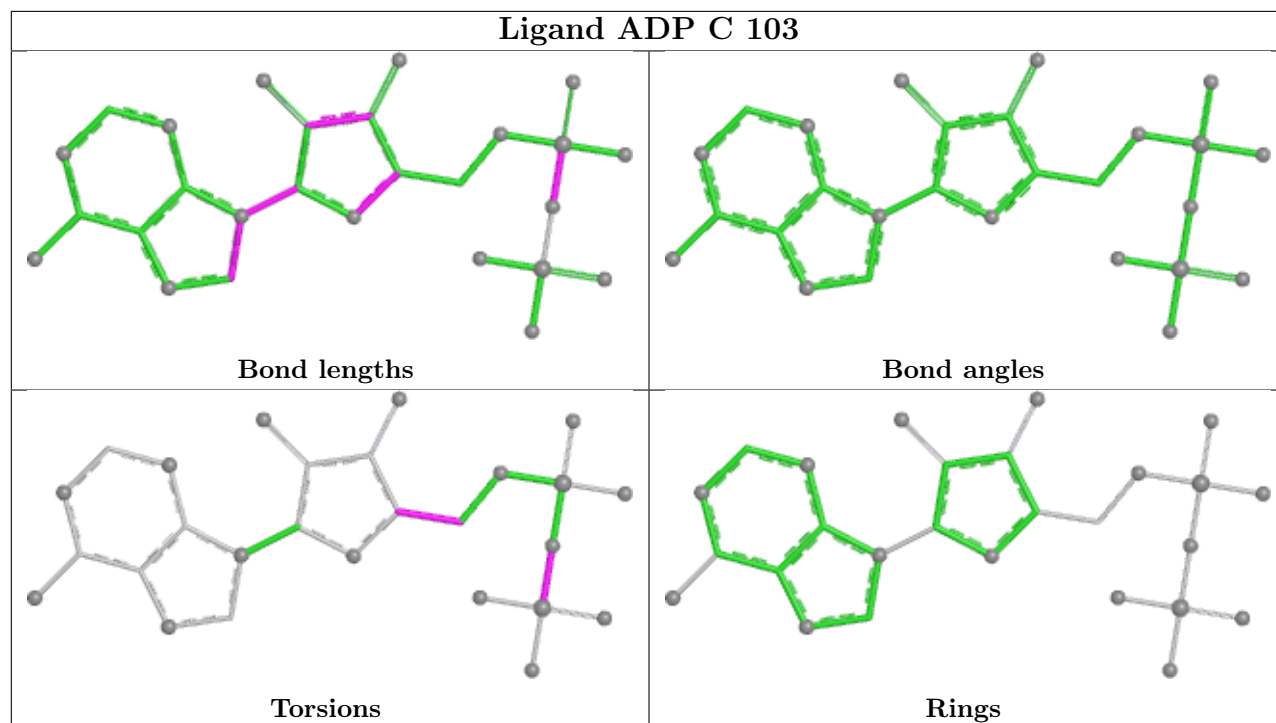
Mol	Chain	Res	Type	Atoms
2	B	104	ADP	C4'-C5'-O5'-PA
2	A	102	ADP	C3'-C4'-C5'-O5'
3	B	3	SIM	C23-C19-C20-C21
3	C	1	SIM	C23-C19-C20-C21
3	A	4	SIM	O14-C18-C19-C20
2	C	103	ADP	PA-O3A-PB-O1B
3	A	4	SIM	O14-C18-C19-C22
3	A	4	SIM	O14-C18-C19-C23
3	C	1	SIM	O14-C18-C19-C23
3	A	4	SIM	O1B-C1-C2-C3
2	D	105	ADP	PA-O3A-PB-O1B
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	C	1	SIM	O14-C18-C19-C22
3	C	1	SIM	C3-C4-C5-C6
2	B	104	ADP	O4'-C1'-N9-C8
3	A	4	SIM	O1A-C1-C2-C3
2	B	104	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

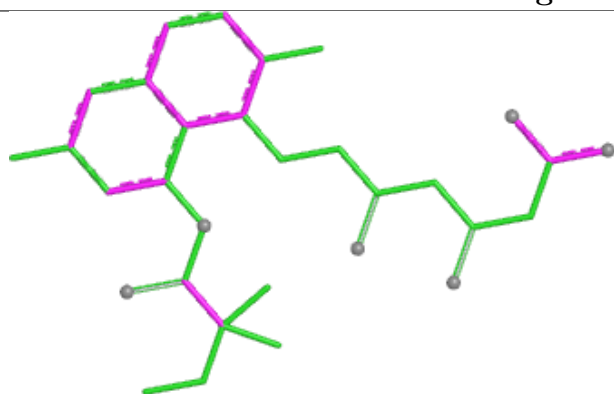
3 monomers are involved in 4 short contacts:

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

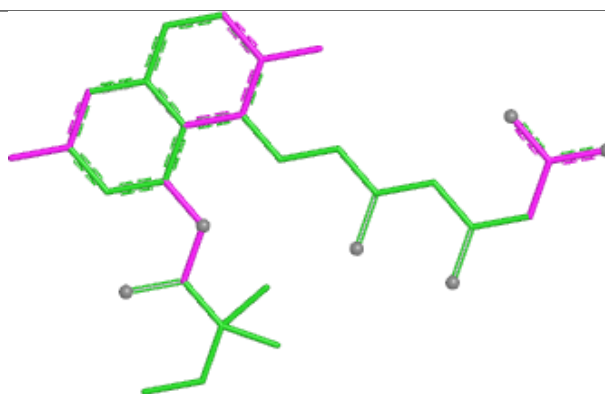
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



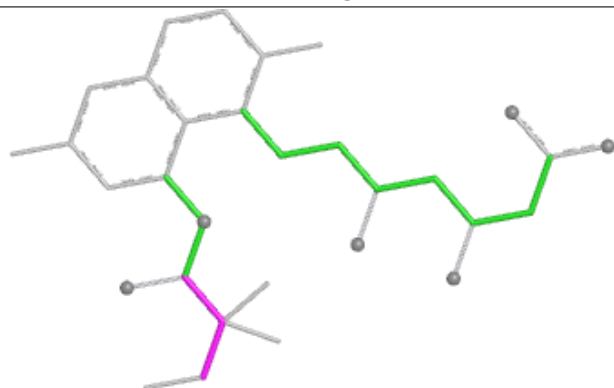
Ligand SIM C 2



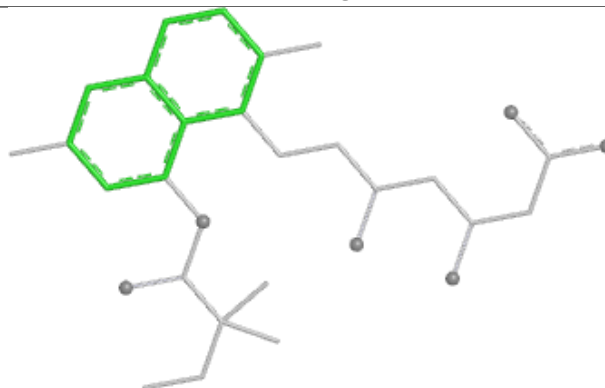
Bond lengths



Bond angles

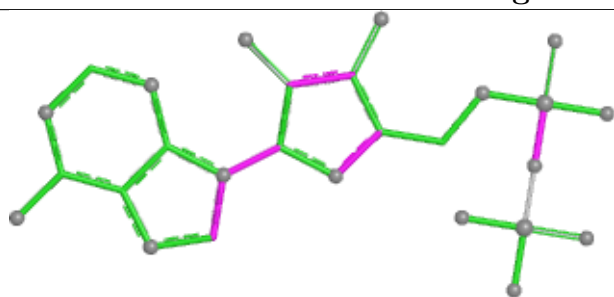


Torsions

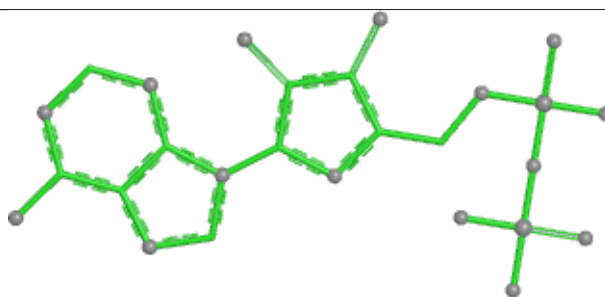


Rings

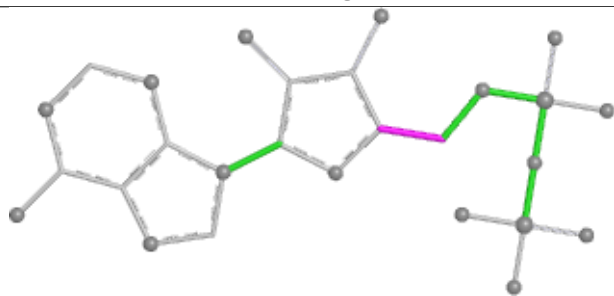
Ligand ADP B 101



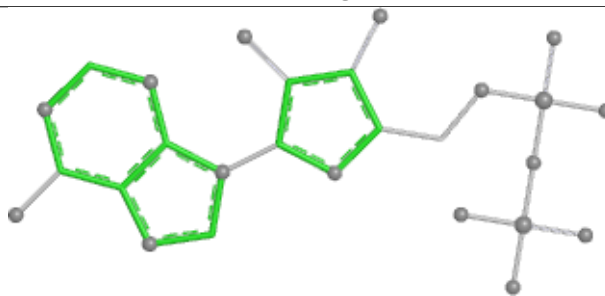
Bond lengths



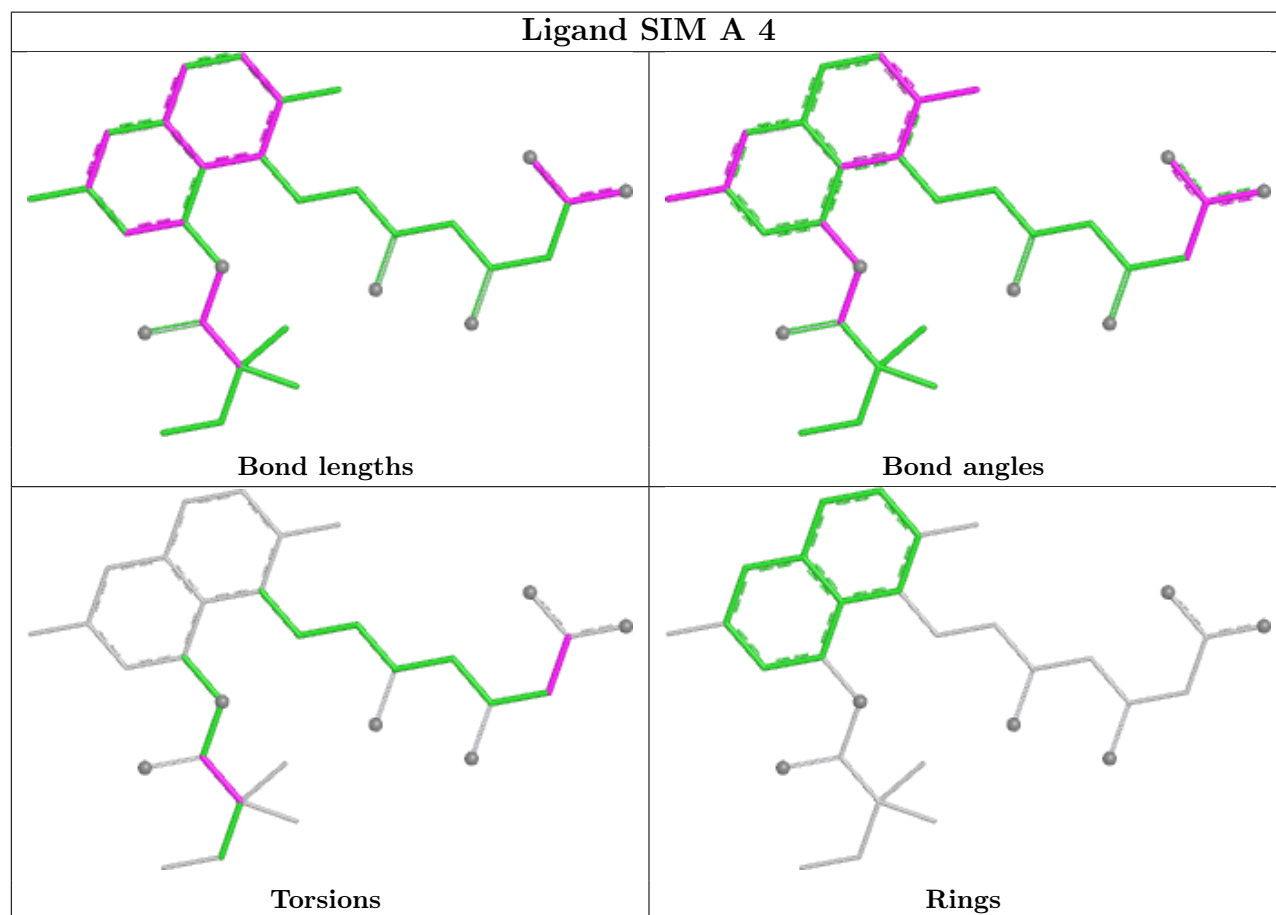
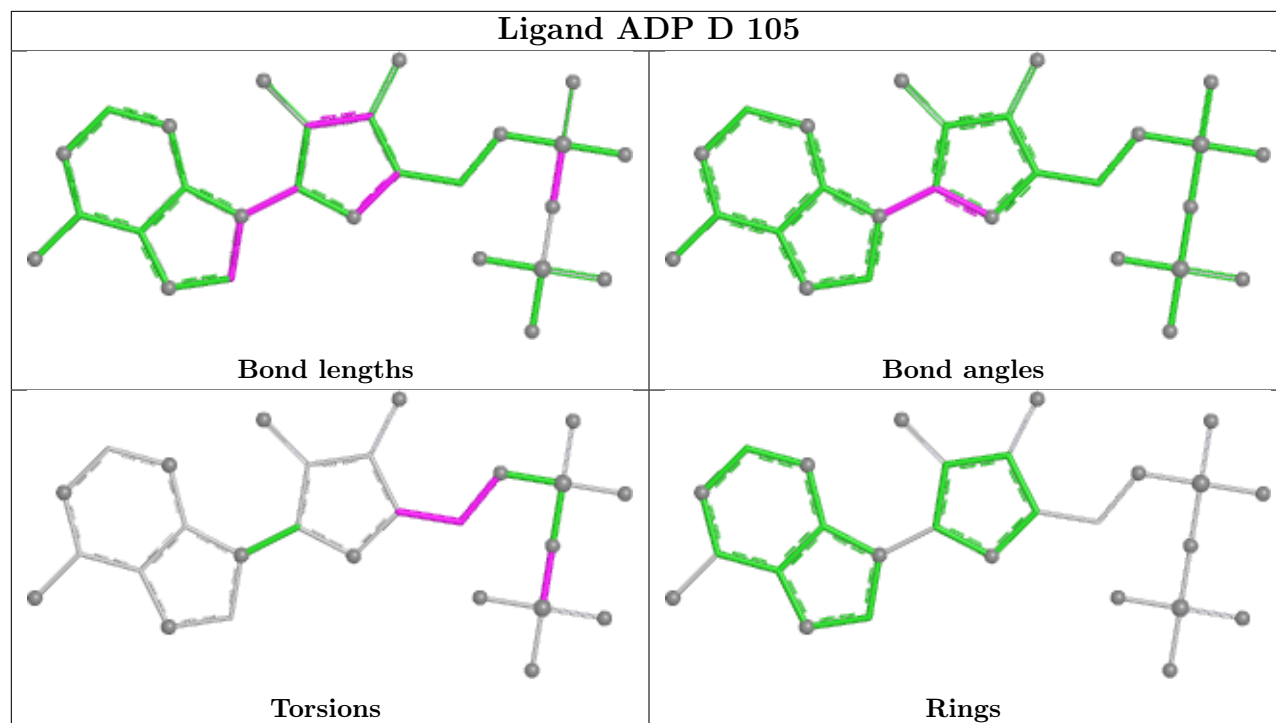
Bond angles

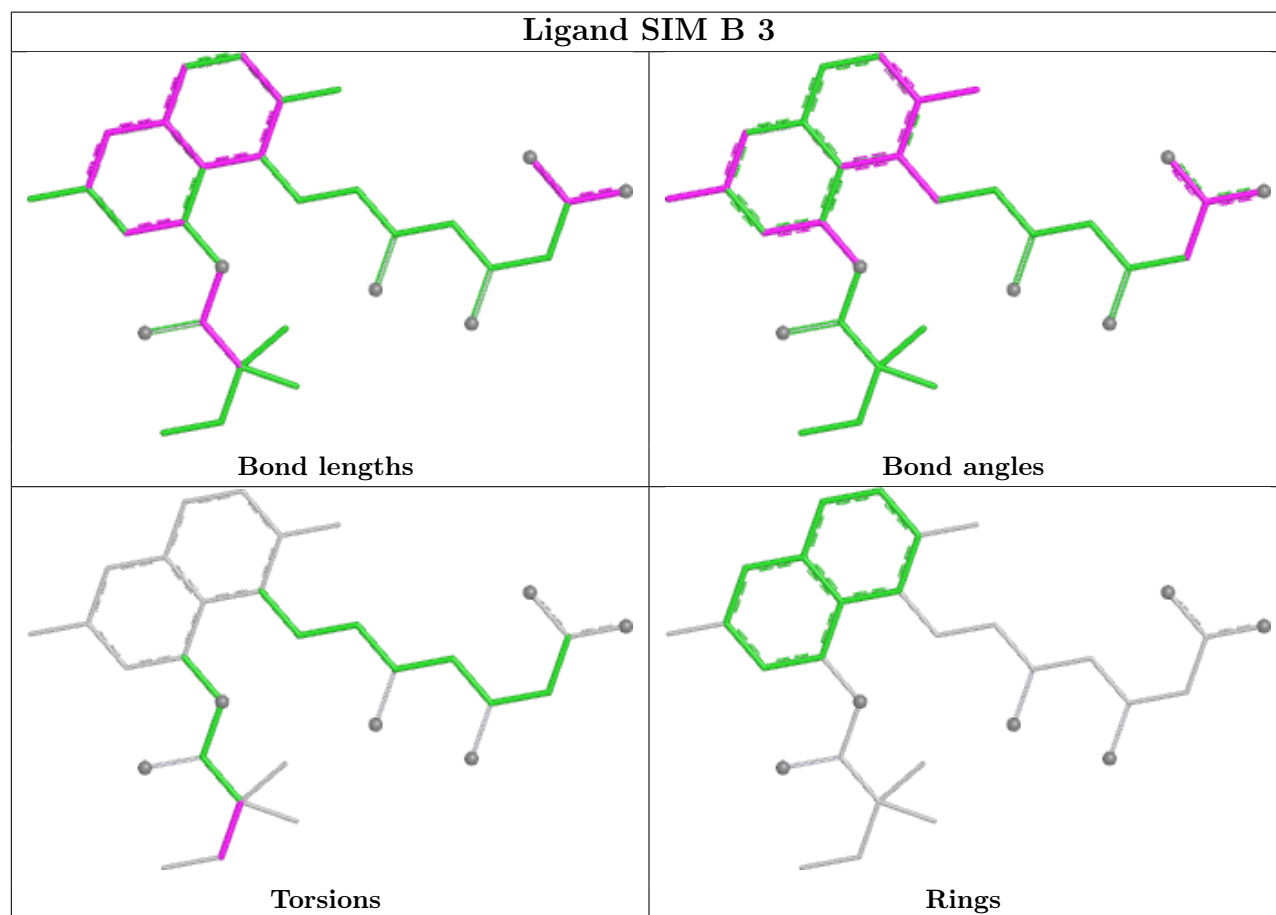
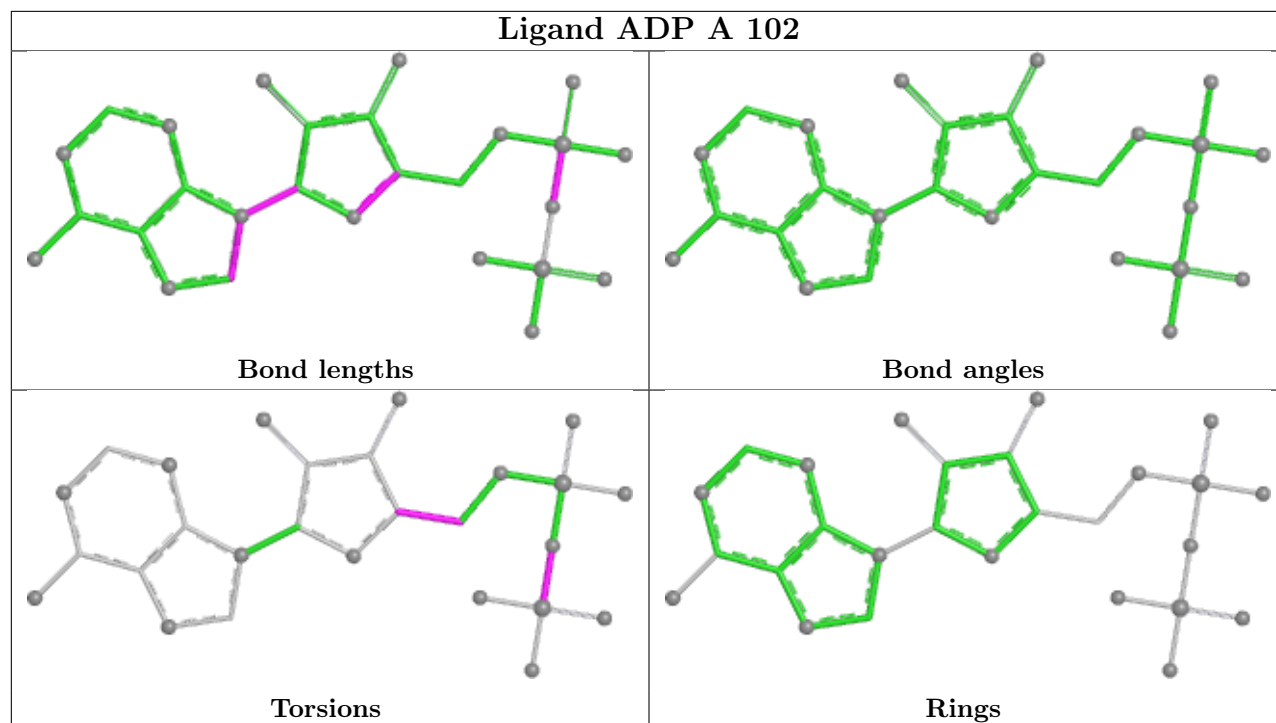


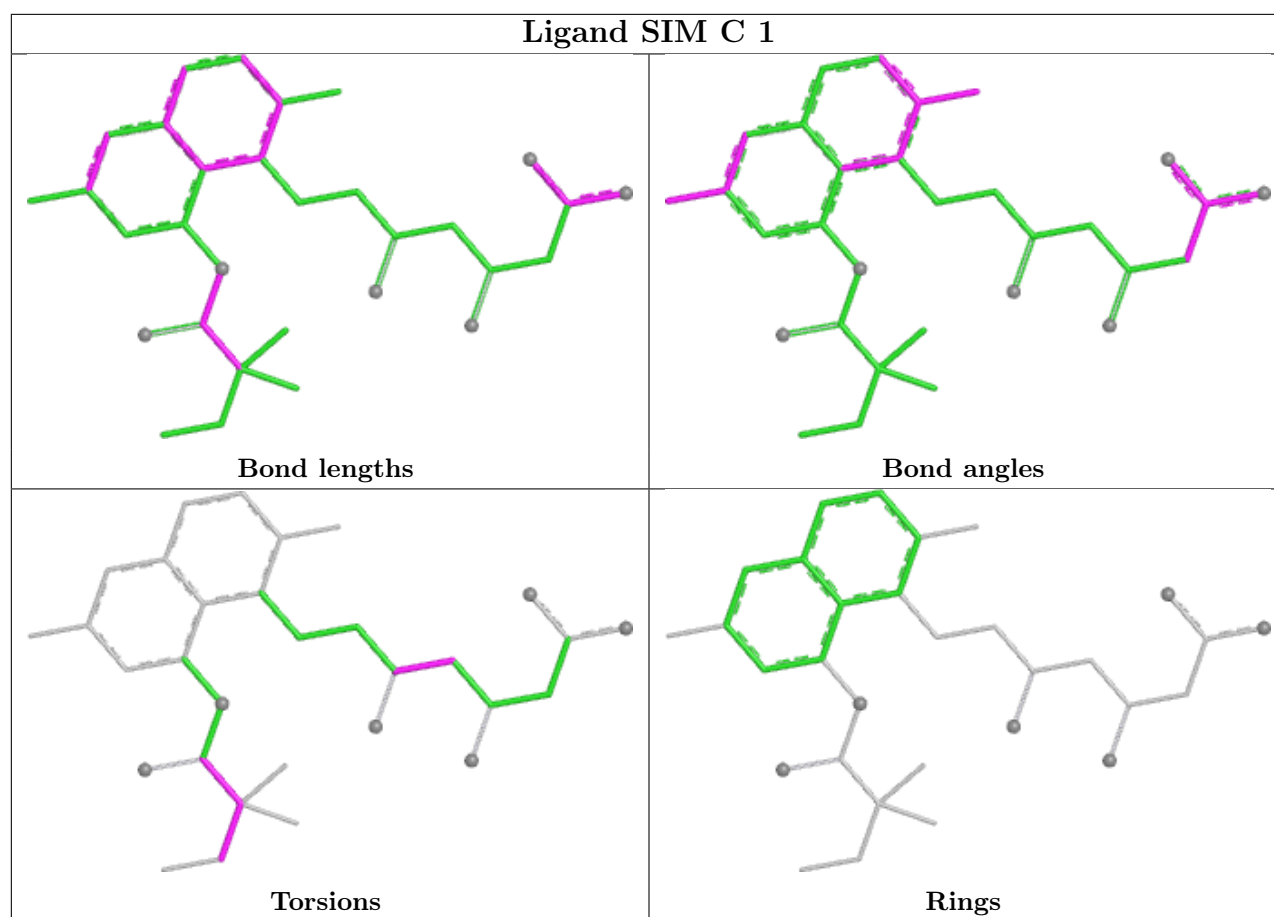
Torsions



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	408/467 (87%)	0.53	24 (5%)	28 33	36, 57, 100, 101	0
1	B	398/467 (85%)	0.62	28 (7%)	22 26	38, 57, 91, 101	0
1	C	389/467 (83%)	0.57	19 (4%)	35 41	39, 58, 86, 101	0
1	D	388/467 (83%)	0.49	21 (5%)	31 37	36, 54, 83, 101	0
All	All	1583/1868 (84%)	0.55	92 (5%)	29 34	36, 57, 96, 101	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	ALA	4.8
1	D	859	ALA	4.8
1	D	483	THR	4.5
1	B	476	ILE	4.5
1	A	442	PRO	4.2
1	B	860	GLY	4.2
1	A	476	ILE	3.9
1	A	461	PHE	3.8
1	B	630	ARG	3.8
1	A	860	GLY	3.7
1	D	479	TYR	3.7
1	D	465	ALA	3.7
1	D	487	THR	3.6
1	B	483	THR	3.6
1	B	484	LEU	3.6
1	B	708	CYS	3.6
1	C	487	THR	3.5
1	C	860	GLY	3.4
1	C	463	SER	3.3
1	C	468	ILE	3.3
1	B	629	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	473	ALA	3.1
1	B	471	VAL	3.1
1	A	499	LEU	3.1
1	A	523	MET	3.1
1	C	480	LYS	3.0
1	C	631	LEU	2.9
1	A	479	TYR	2.9
1	A	462	LEU	2.9
1	C	478	ALA	2.9
1	B	631	LEU	2.8
1	B	523	MET	2.8
1	B	479	TYR	2.8
1	C	479	TYR	2.8
1	B	487	THR	2.7
1	C	518	ASN	2.7
1	B	827	CYS	2.7
1	D	467	ILE	2.7
1	B	486	GLU	2.7
1	B	814	GLN	2.6
1	B	677	GLU	2.6
1	A	478	ALA	2.6
1	A	725	THR	2.6
1	D	523	MET	2.5
1	C	628	PHE	2.5
1	D	468	ILE	2.5
1	D	580	SER	2.5
1	D	503	LEU	2.4
1	A	787	THR	2.4
1	D	504	SER	2.4
1	D	830	ASN	2.4
1	A	473	ALA	2.4
1	A	708	CYS	2.4
1	C	484	LEU	2.4
1	A	477	PRO	2.3
1	D	831	PRO	2.3
1	C	465	ALA	2.3
1	C	710	ALA	2.3
1	A	482	GLU	2.3
1	A	448	CYS	2.3
1	D	771	ASN	2.3
1	D	514	TYR	2.3
1	D	478	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	492	VAL	2.3
1	C	483	THR	2.2
1	C	632	GLN	2.2
1	C	489	GLU	2.2
1	A	558	THR	2.2
1	B	465	ALA	2.2
1	B	463	SER	2.2
1	A	471	VAL	2.2
1	D	716	VAL	2.2
1	A	521	LEU	2.2
1	C	546	LEU	2.2
1	D	577	GLY	2.2
1	A	517	TYR	2.1
1	D	485	ILE	2.1
1	D	464	ASP	2.1
1	B	828	LYS	2.1
1	C	826	ALA	2.1
1	B	485	ILE	2.1
1	B	856	ALA	2.1
1	D	484	LEU	2.1
1	A	720	VAL	2.1
1	C	789	GLU	2.1
1	B	583	VAL	2.1
1	B	480	LYS	2.0
1	B	477	PRO	2.0
1	A	475	HIS	2.0
1	A	484	LEU	2.0
1	B	470	LEU	2.0
1	B	501	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

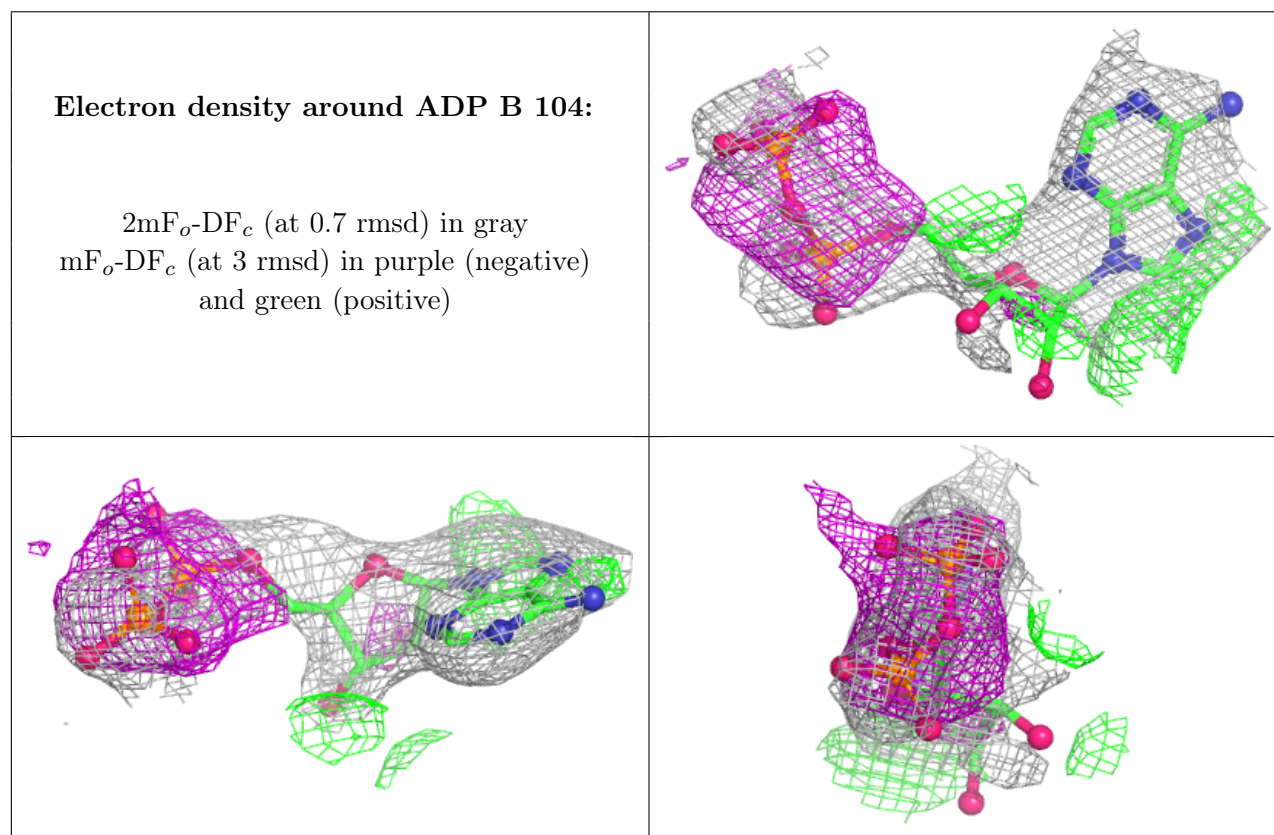
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

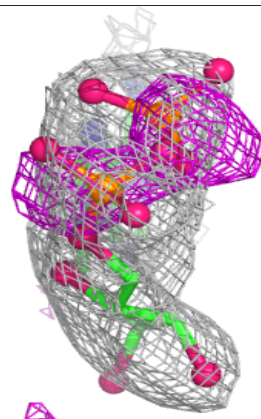
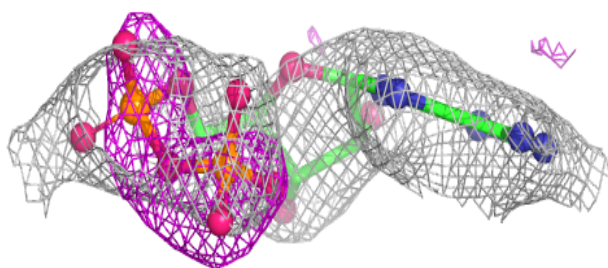
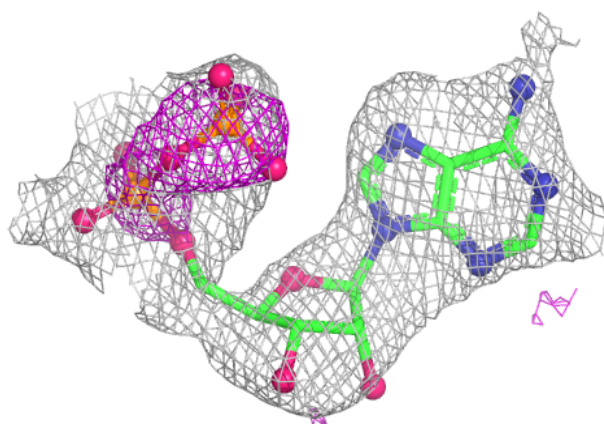
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	B	104	27/27	0.59	0.20	99,100,100,100	0
2	ADP	B	101	27/27	0.70	0.14	99,100,100,100	0
2	ADP	A	102	27/27	0.72	0.14	100,100,100,100	0
2	ADP	C	103	27/27	0.72	0.13	99,100,100,100	0
2	ADP	D	105	27/27	0.72	0.17	99,100,100,100	0
3	SIM	B	3	31/31	0.91	0.13	50,59,63,63	0
3	SIM	A	4	31/31	0.92	0.12	59,64,67,67	0
3	SIM	C	2	31/31	0.92	0.11	51,60,63,64	0
3	SIM	C	1	31/31	0.93	0.10	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.

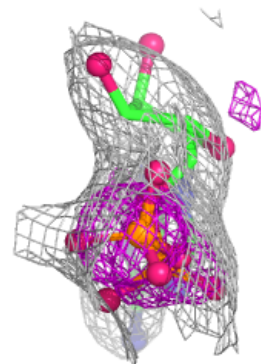
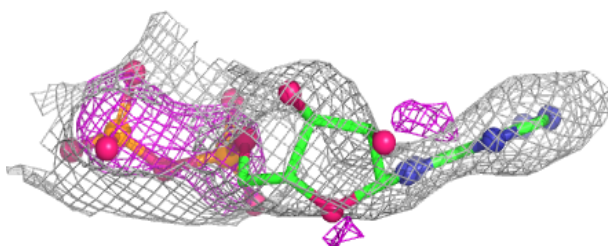
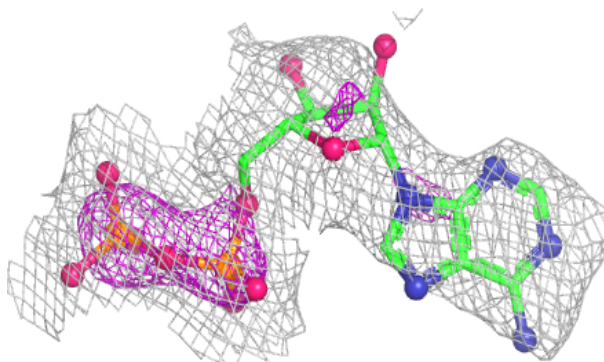


Electron density around ADP B 101:

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

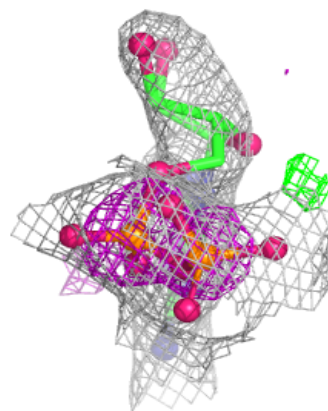
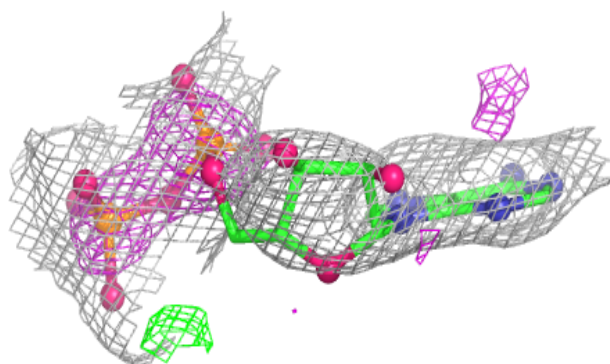
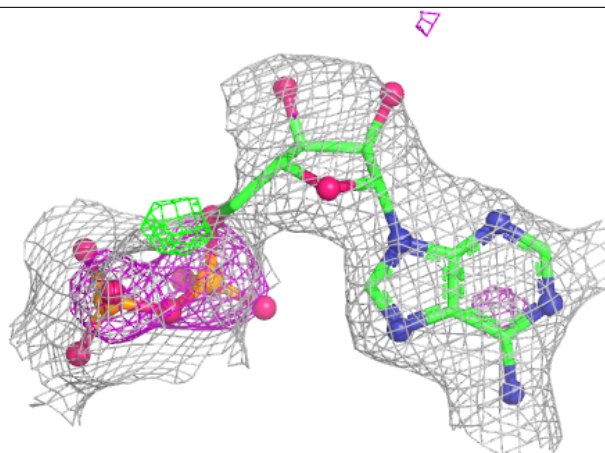
**Electron density around ADP A 102:**

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

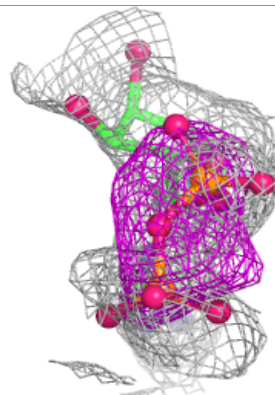
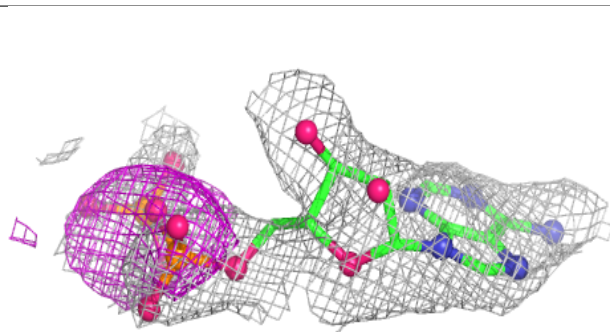
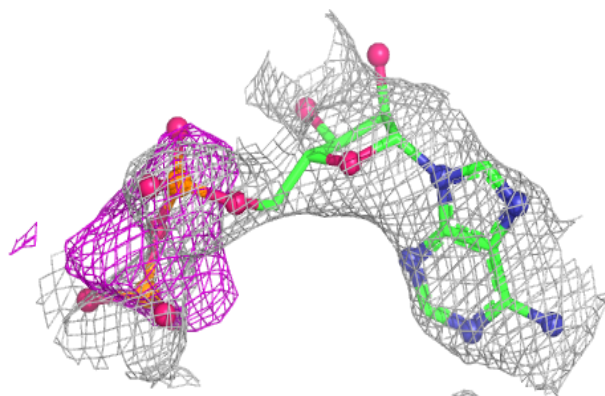


Electron density around ADP C 103:

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

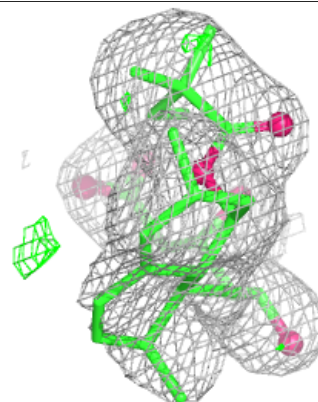
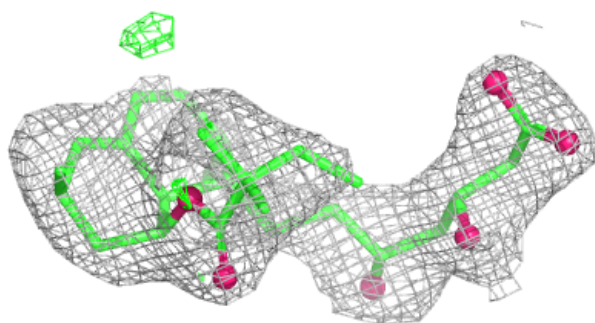
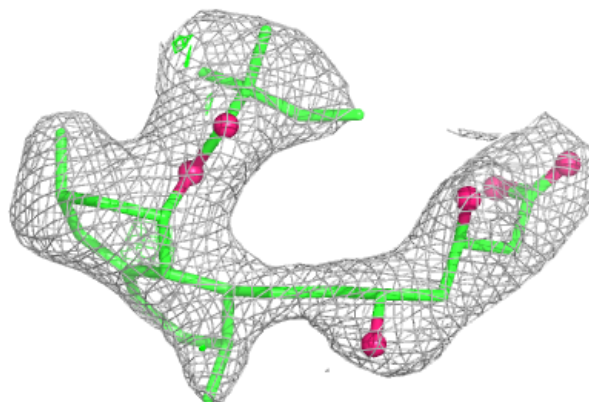
**Electron density around ADP D 105:**

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

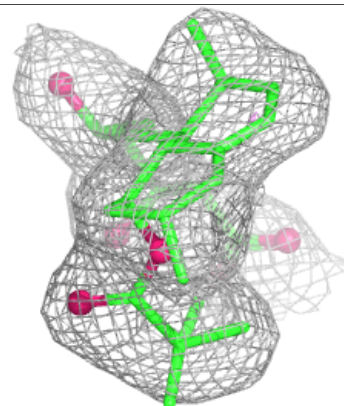
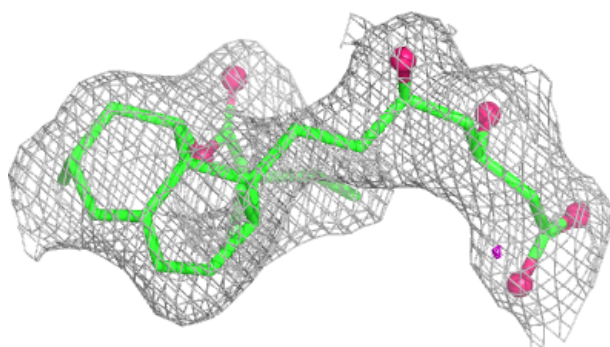
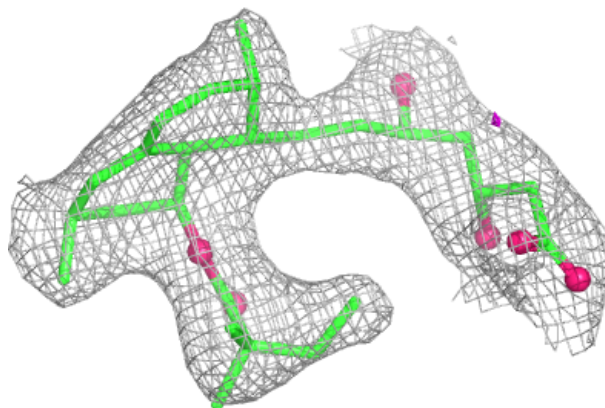


Electron density around SIM B 3:

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

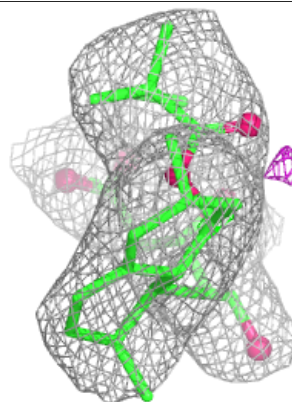
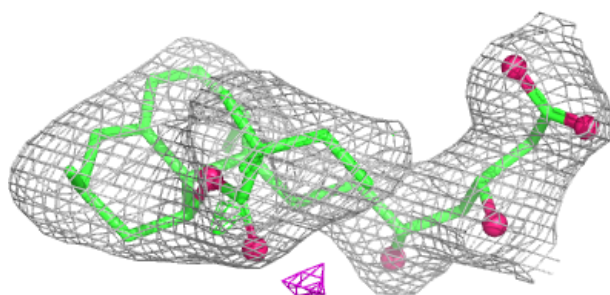
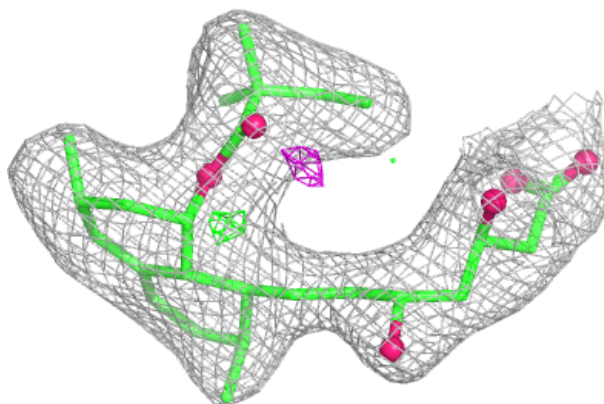
**Electron density around SIM A 4:**

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

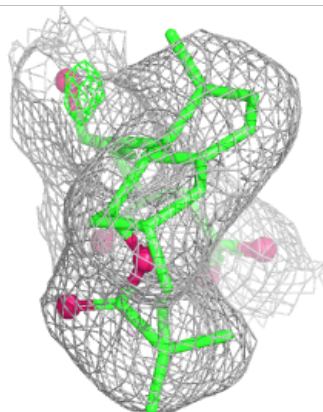
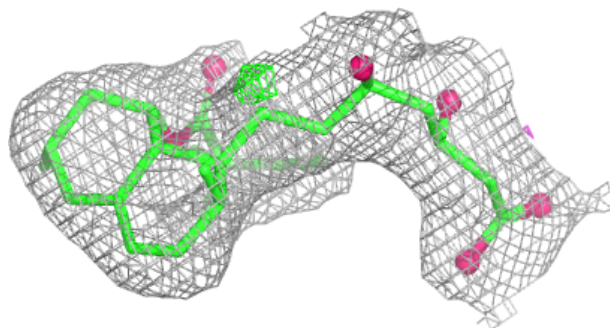
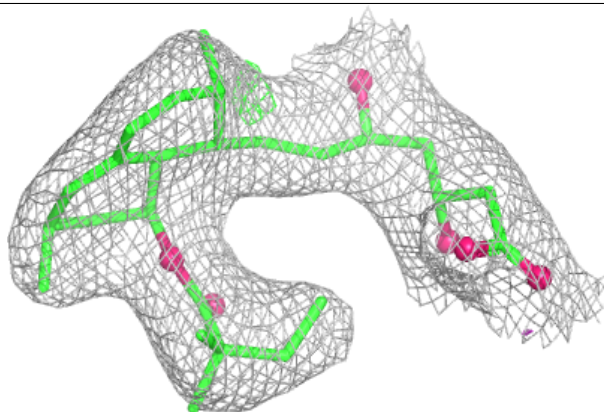


Electron density around SIM C 2:

$2mF_o-DF_c$ (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.