



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 05:40 AM EDT

PDB ID : 1HW8
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH COMPACTIN (ALSO KNOWN AS MEVASTATIN)
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

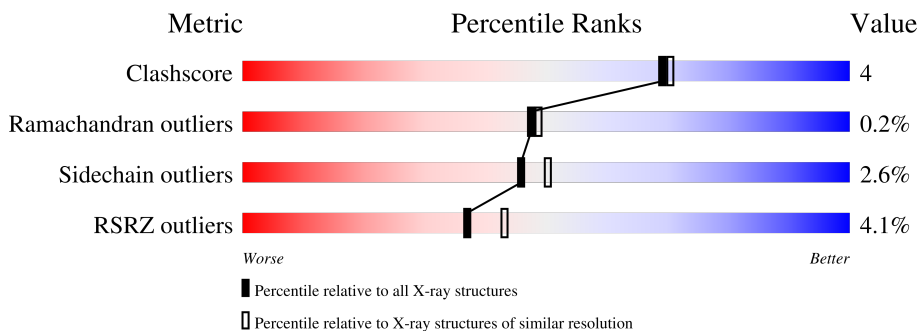
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	 7% 75% 11% 13%
1	B	467	 2% 81% 7% 12%
1	C	467	 3% 74% 5% 20%
1	D	467	 2% 74% 5% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	114	A	2	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12022 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.

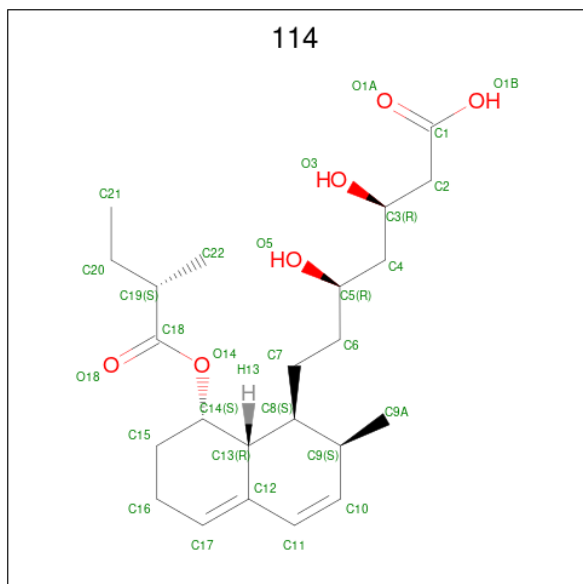
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3004	1867	527	580	30	0	0	0
1	B	410	3055	1904	536	585	30	0	0	0
1	C	373	2755	1711	487	528	29	0	0	0
1	D	372	2751	1709	486	527	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 (3R,5R)-3,5-dihydroxy-7-[(1S,2S,8S,8aR)-2-methyl-8-[[[(2S)-2-methylbutanoyl]oxy]-1,2,6,7,8,8a-hexahydronaphthalen-1-yl]heptanoic acid (three-letter code: 114) (formula: C₂₃H₃₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	23	6		
2	B	1	Total	C	O	0	0
			29	23	6		
2	C	1	Total	C	O	0	0
			29	23	6		
2	D	1	Total	C	O	0	0
			29	23	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

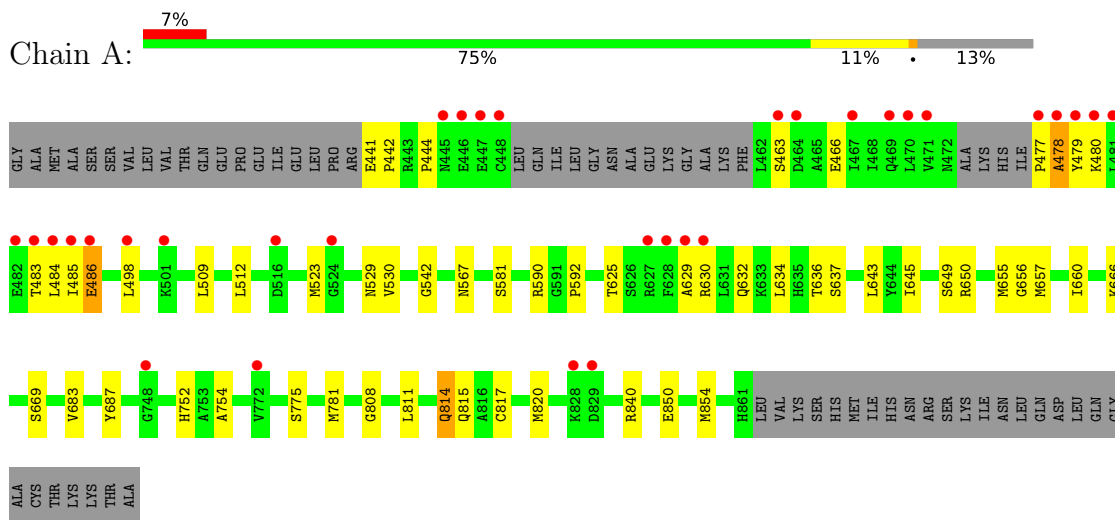
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	79	Total	O	0	0
			79	79		
4	C	67	Total	O	0	0
			67	67		
4	D	75	Total	O	0	0
			75	75		

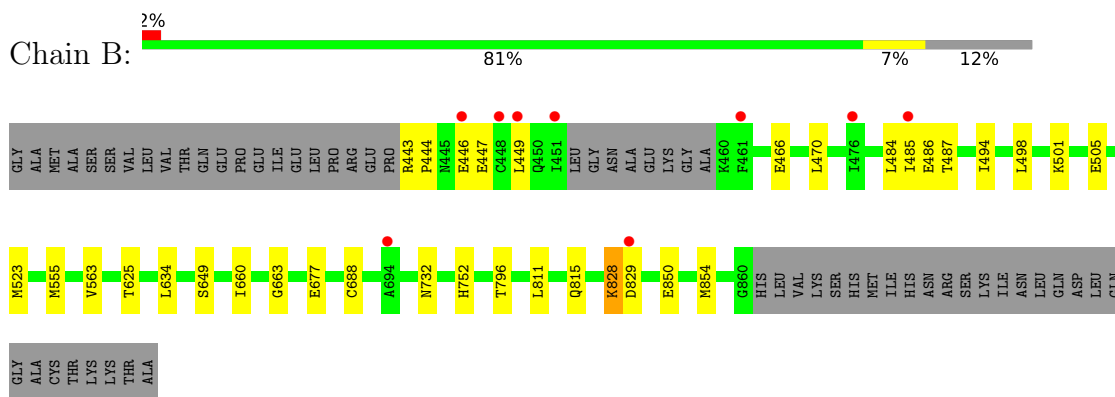
3 Residue-property plots [i](#)

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

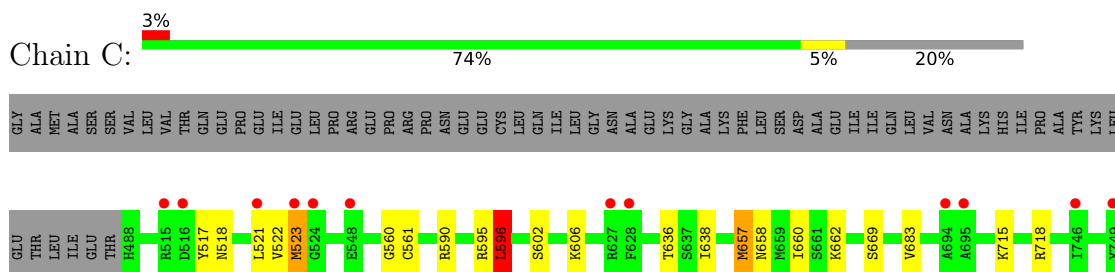
• Molecule 1: HMG-COA REDUCTASE

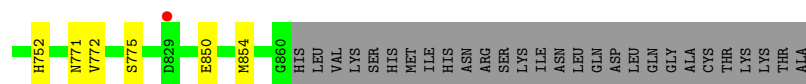


• Molecule 1: HMG-COA REDUCTASE

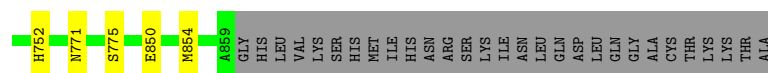
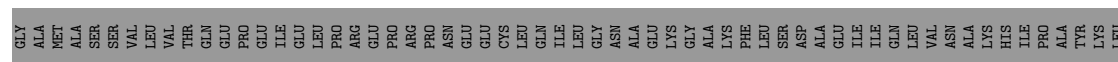
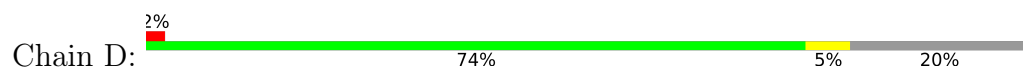


• Molecule 1: HMG-COA REDUCTASE





● Molecule 1: HMG-COA REDUCTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.83Å 173.00Å 75.18Å 90.00° 118.38° 90.00°	Depositor
Resolution (Å)	43.13 – 2.10 52.54 – 2.09	Depositor EDS
% Data completeness (in resolution range)	92.7 (43.13-2.10) 88.2 (52.54-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.223 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.028 for h,-k,-h-l 0.029 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12022	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 114, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/3046	0.68	0/4117
1	B	0.52	0/3098	0.68	0/4187
1	C	0.50	0/2794	0.67	1/3776 (0.0%)
1	D	0.53	0/2790	0.70	1/3771 (0.0%)
All	All	0.51	0/11728	0.68	2/15851 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	LEU	CA-CB-CG	-6.27	100.89	115.30
1	D	596	LEU	CA-CB-CG	-6.14	101.18	115.30

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	3004	0	3026	38	0
1	B	3055	0	3094	18	0
1	C	2755	0	2784	20	0
1	D	2751	0	2781	13	0
2	A	29	0	35	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	35	0	0
2	C	29	0	35	2	0
2	D	29	0	35	1	0
3	B	27	0	12	3	0
3	D	27	0	12	1	0
4	A	66	0	0	0	0
4	B	79	0	0	0	0
4	C	67	0	0	1	0
4	D	75	0	0	0	0
All	All	12022	0	11849	87	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 4.

All (87) 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:828:LYS:HD2	1:B:828:LYS:H	1.19	1.08
1:B:828:LYS:HD2	1:B:828:LYS:N	1.99	0.74
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.71	0.73
1:A:529:ASN:ND2	3:B:101:ADP:H2	1.88	0.72
1:A:581:SER:OG	1:A:840:ARG:HD2	1.94	0.67
1:B:828:LYS:H	1:B:828:LYS:CD	1.90	0.66
1:A:683:VAL:HG11	2:A:2:114:H221	1.77	0.66
1:A:529:ASN:HD22	3:B:101:ADP:H2	1.40	0.66
1:A:655:MET:SD	1:A:657:MET:HG2	2.36	0.66
1:D:596:LEU:HD13	1:D:602:SER:HA	1.81	0.63
1:D:595:ARG:HD2	1:D:679:GLN:OE1	1.98	0.63
1:C:518:ASN:HD21	1:C:521:LEU:HD13	1.64	0.60
1:A:542:GLY:H	1:A:567:ASN:ND2	2.00	0.59
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.34	0.58
1:A:529:ASN:ND2	3:B:101:ADP:C2	2.72	0.57
1:A:625:THR:CG2	1:A:666:LYS:HG3	2.33	0.57
1:A:590:ARG:NH2	1:A:657:MET:HE3	2.20	0.56
1:A:817:CYS:HA	1:A:820:MET:HE3	1.87	0.56
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.88	0.56
1:A:656:GLY:O	1:A:660:ILE:HG12	2.07	0.55
1:C:850:GLU:O	1:C:854:MET:HG2	2.07	0.54
1:A:811:LEU:HB2	1:A:814:GLN:HG2	1.91	0.53
1:A:632:GLN:NE2	1:A:650:ARG:HG2	2.23	0.53
1:C:658:ASN:O	1:C:662:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLY:H	1:A:567:ASN:HD22	1.57	0.52
1:A:683:VAL:CG1	2:A:2:114:H221	2.39	0.52
1:D:850:GLU:O	1:D:854:MET:HG2	2.09	0.52
1:B:446:GLU:O	1:B:449:LEU:HG	2.09	0.52
1:B:649:SER:HB3	1:B:660:ILE:CD1	2.40	0.51
1:C:596:LEU:HD13	1:C:602:SER:HA	1.92	0.51
1:A:625:THR:HG22	1:A:666:LYS:HG3	1.92	0.50
1:C:518:ASN:ND2	1:C:521:LEU:HD13	2.27	0.50
1:A:781:MET:CE	1:A:854:MET:HG3	2.42	0.50
1:D:606:LYS:HG3	1:D:636:THR:OG1	2.12	0.50
1:D:715:LYS:HG3	1:D:718:ARG:NH2	2.26	0.49
1:A:485:ILE:CG2	1:A:486:GLU:N	2.76	0.49
1:C:523:MET:HE1	4:C:1172:HOH:O	2.13	0.49
1:A:477:PRO:O	1:A:478:ALA:HB3	2.13	0.49
1:A:441:GLU:N	1:A:442:PRO:CD	2.76	0.48
1:A:754:ALA:HA	1:A:775:SER:OG	2.14	0.48
1:C:606:LYS:HG3	1:C:636:THR:OG1	2.14	0.48
1:B:485:ILE:HD13	1:B:494:ILE:HD12	1.94	0.47
1:C:683:VAL:HG11	2:C:4:114:H221	1.95	0.47
1:C:715:LYS:HG3	1:C:718:ARG:NH2	2.29	0.47
1:D:683:VAL:HG11	2:D:3:114:H221	1.95	0.47
1:A:480:LYS:O	1:A:483:THR:HG22	2.15	0.47
1:B:498:LEU:O	1:B:501:LYS:HG2	2.14	0.47
1:C:715:LYS:HB3	1:C:715:LYS:NZ	2.30	0.47
1:D:715:LYS:HB3	1:D:715:LYS:NZ	2.29	0.47
1:A:484:LEU:HD22	1:A:485:ILE:HD12	1.97	0.46
1:B:850:GLU:O	1:B:854:MET:HG2	2.16	0.46
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.75	0.45
1:C:517:TYR:HE2	1:C:522:VAL:HG21	1.82	0.45
1:B:811:LEU:O	1:B:815:GLN:HG3	2.17	0.45
1:A:850:GLU:O	1:A:854:MET:HG2	2.17	0.45
1:A:629:ALA:O	1:A:630:ARG:HD2	2.16	0.45
1:B:466:GLU:O	1:B:470:LEU:HD13	2.16	0.45
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.82	0.44
1:C:657:MET:HA	1:C:657:MET:CE	2.47	0.44
1:D:771:ASN:OD1	1:D:775:SER:OG	2.34	0.44
1:B:447:GLU:C	1:B:449:LEU:H	2.20	0.44
1:A:592:PRO:HD2	1:A:645:ILE:O	2.17	0.44
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.61	0.43
1:A:479:TYR:HB3	1:A:529:ASN:HD21	1.84	0.43
1:B:732:ASN:HA	1:B:854:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:GLY:O	1:C:561:CYS:HB2	2.18	0.43
1:A:629:ALA:C	1:A:630:ARG:HD2	2.39	0.43
1:C:590:ARG:HB2	1:C:660:ILE:HG22	2.00	0.43
1:B:677:GLU:H	1:B:677:GLU:CD	2.21	0.43
1:C:772:VAL:HG23	1:D:771:ASN:ND2	2.34	0.43
1:A:630:ARG:O	1:A:632:GLN:NE2	2.52	0.43
1:C:771:ASN:OD1	1:C:775:SER:OG	2.36	0.43
1:A:463:SER:OG	1:A:466:GLU:HG3	2.19	0.43
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.72	0.42
1:A:649:SER:HB3	1:A:660:ILE:HD12	2.01	0.41
1:D:493:SER:O	1:D:497:GLN:HG3	2.19	0.41
1:C:523:MET:HA	1:C:523:MET:CE	2.50	0.41
1:D:656:GLY:HA2	3:D:102:ADP:O1B	2.21	0.41
1:A:781:MET:HE3	1:A:854:MET:HG3	2.01	0.41
1:B:625:THR:HG21	1:B:663:GLY:HA2	2.01	0.41
1:A:811:LEU:O	1:A:815:GLN:HG3	2.21	0.41
1:A:637:SER:HB2	1:A:687:TYR:OH	2.21	0.41
1:A:808:GLY:O	1:A:814:GLN:HG3	2.22	0.40
1:B:796:THR:HG21	1:C:638:ILE:O	2.20	0.40
1:B:443:ARG:HA	1:B:444:PRO:HD3	1.95	0.40
1:D:560:GLY:O	1:D:561:CYS:HB2	2.20	0.40
1:C:683:VAL:CG1	2:C:4:114:H221	2.52	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	398/467 (85%)	381 (96%)	14 (4%)	3 (1%)	19 15
1	B	406/467 (87%)	389 (96%)	17 (4%)	0	100 100
1	C	371/467 (79%)	359 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	370/467 (79%)	356 (96%)	14 (4%)	0	100	100
All	All	1545/1868 (83%)	1485 (96%)	57 (4%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	ALA
1	A	486	GLU
1	A	444	PRO

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	323/375 (86%)	316 (98%)	7 (2%)	52	57
1	B	328/375 (88%)	318 (97%)	10 (3%)	41	44
1	C	294/375 (78%)	288 (98%)	6 (2%)	55	60
1	D	294/375 (78%)	285 (97%)	9 (3%)	40	43
All	All	1239/1500 (83%)	1207 (97%)	32 (3%)	46	50

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

Mol	Chain	Res	Type
1	A	498	LEU
1	A	509	LEU
1	A	512	LEU
1	A	634	LEU
1	A	669	SER
1	A	752	HIS
1	A	814	GLN
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	505	GLU

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Mol	Chain	Res	Type
1	B	523	MET
1	B	634	LEU
1	B	688	CYS
1	B	752	HIS
1	B	828	LYS
1	B	829	ASP
1	C	523	MET
1	C	595	ARG
1	C	596	LEU
1	C	657	MET
1	C	669	SER
1	C	752	HIS
1	D	500	SER
1	D	509	LEU
1	D	595	ARG
1	D	596	LEU
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	660	ILE
1	D	752	HIS

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

Mol	Chain	Res	Type
1	A	488	HIS
1	A	518	ASN
1	A	529	ASN
1	A	567	ASN
1	A	632	GLN
1	B	472	ASN
1	B	488	HIS
1	B	510	GLN
1	B	635	HIS
1	D	642	ASN
1	D	672	HIS
1	D	788	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	ADP	D	102	-	24,29,29	1.42	3 (12%)	29,45,45	0.81	1 (3%)
2	114	A	2	-	30,30,30	1.87	7 (23%)	38,41,41	1.26	5 (13%)
2	114	D	3	-	30,30,30	1.87	7 (23%)	38,41,41	1.28	4 (10%)
2	114	B	1	-	30,30,30	1.82	9 (30%)	38,41,41	1.33	7 (18%)
3	ADP	B	101	-	24,29,29	1.27	2 (8%)	29,45,45	0.77	1 (3%)
2	114	C	4	-	30,30,30	1.81	6 (20%)	38,41,41	1.37	7 (18%)

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	ADP	D	102	-	-	5/12/32/32	0/3/3/3
2	114	A	2	-	1/1/10/13	5/23/50/50	0/2/2/2
2	114	D	3	-	-	0/23/50/50	0/2/2/2
2	114	B	1	-	-	2/23/50/50	0/2/2/2
3	ADP	B	101	-	-	2/12/32/32	0/3/3/3
2	114	C	4	-	-	2/23/50/50	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	114	O1A-C1	4.54	1.37	1.22
2	D	3	114	C9-C8	4.49	1.59	1.54
2	C	4	114	O1A-C1	4.38	1.36	1.22
2	B	1	114	C9-C8	4.24	1.58	1.54
2	D	3	114	O1A-C1	4.18	1.36	1.22
2	D	3	114	C13-C12	4.14	1.57	1.52
2	B	1	114	O1A-C1	4.11	1.35	1.22
2	C	4	114	C9-C8	4.02	1.58	1.54
2	A	2	114	C9-C8	3.83	1.58	1.54
2	C	4	114	C13-C12	3.83	1.57	1.52
2	A	2	114	C13-C12	3.64	1.57	1.52
3	B	101	ADP	C8-N7	-3.50	1.28	1.34
2	B	1	114	C13-C12	3.44	1.57	1.52
3	D	102	ADP	C8-N7	-3.32	1.28	1.34
3	D	102	ADP	O4'-C4'	3.14	1.52	1.45
2	C	4	114	C9-C10	3.14	1.55	1.50
2	C	4	114	C13-C8	2.75	1.58	1.54
2	A	2	114	C9-C10	2.72	1.54	1.50
2	D	3	114	C9-C10	2.71	1.54	1.50
2	B	1	114	C13-C8	2.57	1.58	1.54
2	A	2	114	C13-C8	2.48	1.58	1.54
3	B	101	ADP	O4'-C4'	2.42	1.50	1.45
2	D	3	114	O1B-C1	-2.39	1.22	1.30
2	D	3	114	C11-C12	-2.27	1.36	1.43
2	B	1	114	C9-C10	2.26	1.53	1.50
2	B	1	114	C15-C14	2.23	1.56	1.52
2	D	3	114	C13-C8	2.19	1.57	1.54
2	B	1	114	O14-C18	2.15	1.39	1.34
2	A	2	114	C15-C14	2.11	1.56	1.52
2	A	2	114	O1B-C1	-2.11	1.23	1.30
2	C	4	114	C11-C12	-2.03	1.37	1.43
2	B	1	114	C11-C10	2.03	1.37	1.33
3	D	102	ADP	C2'-C3'	2.02	1.58	1.53
2	B	1	114	C11-C12	-2.02	1.37	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	114	C7-C8-C9	3.64	115.21	112.87
2	B	1	114	O1A-C1-C2	-3.24	112.40	122.80
2	C	4	114	O1B-C1-C2	3.15	124.16	114.07
2	C	4	114	O1A-C1-C2	-3.12	112.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	114	O1B-C1-C2	3.07	123.91	114.07
2	A	2	114	O1A-C1-C2	-3.06	112.98	122.80
2	A	2	114	O1B-C1-C2	3.03	123.79	114.07
2	D	3	114	O1A-C1-C2	-3.03	113.09	122.80
2	D	3	114	O1B-C1-C2	2.89	123.33	114.07
2	D	3	114	C9A-C9-C10	-2.87	106.33	110.85
2	C	4	114	C7-C8-C9	2.82	114.68	112.87
2	A	2	114	C9A-C9-C10	-2.71	106.57	110.85
2	C	4	114	C13-C8-C9	-2.69	109.27	110.70
2	B	1	114	C7-C8-C9	2.62	114.56	112.87
2	C	4	114	C9A-C9-C10	-2.56	106.81	110.85
2	B	1	114	C7-C8-C13	2.44	115.82	112.50
2	C	4	114	O14-C14-C15	2.41	112.90	108.46
2	B	1	114	C9A-C9-C10	-2.37	107.11	110.85
2	A	2	114	C7-C8-C9	2.33	114.36	112.87
2	B	1	114	C13-C8-C9	2.29	111.91	110.70
2	B	1	114	C15-C16-C17	2.17	115.46	111.85
2	A	2	114	C15-C16-C17	2.15	115.44	111.85
3	D	102	ADP	C5-C6-N6	2.12	123.57	120.35
2	C	4	114	C15-C16-C17	2.12	115.38	111.85
3	B	101	ADP	C5-C6-N6	2.06	123.49	120.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	114	C19

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	114	C22-C19-C20-C21
3	B	101	ADP	O4'-C4'-C5'-O5'
3	B	101	ADP	C3'-C4'-C5'-O5'
3	D	102	ADP	PA-O3A-PB-O3B
3	D	102	ADP	C3'-C4'-C5'-O5'
2	A	2	114	C18-C19-C20-C21
2	C	4	114	C18-C19-C20-C21
2	A	2	114	C22-C19-C20-C21
3	D	102	ADP	O4'-C4'-C5'-O5'
2	A	2	114	O14-C18-C19-C20
2	B	1	114	C18-C19-C20-C21
2	A	2	114	O18-C18-C19-C20

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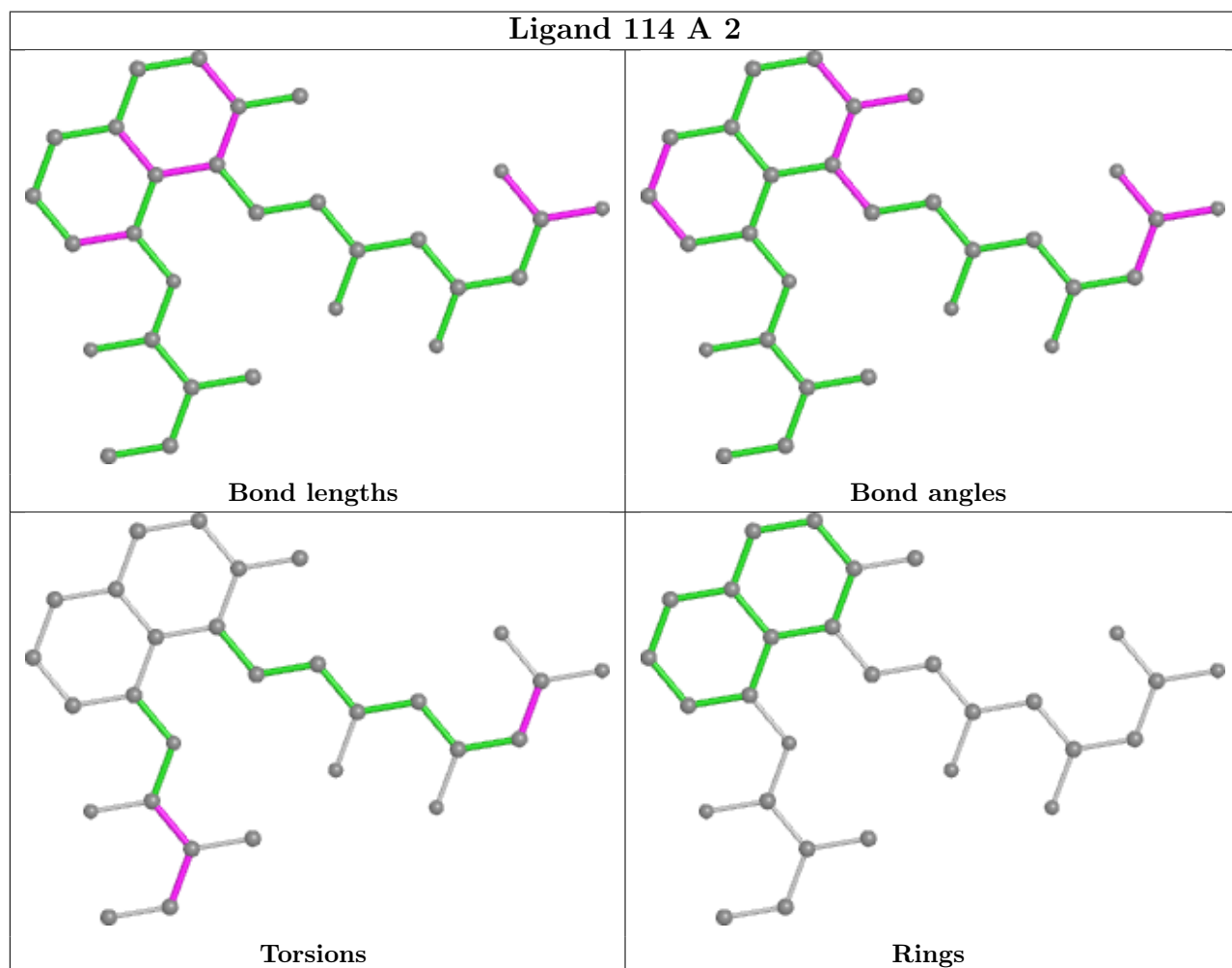
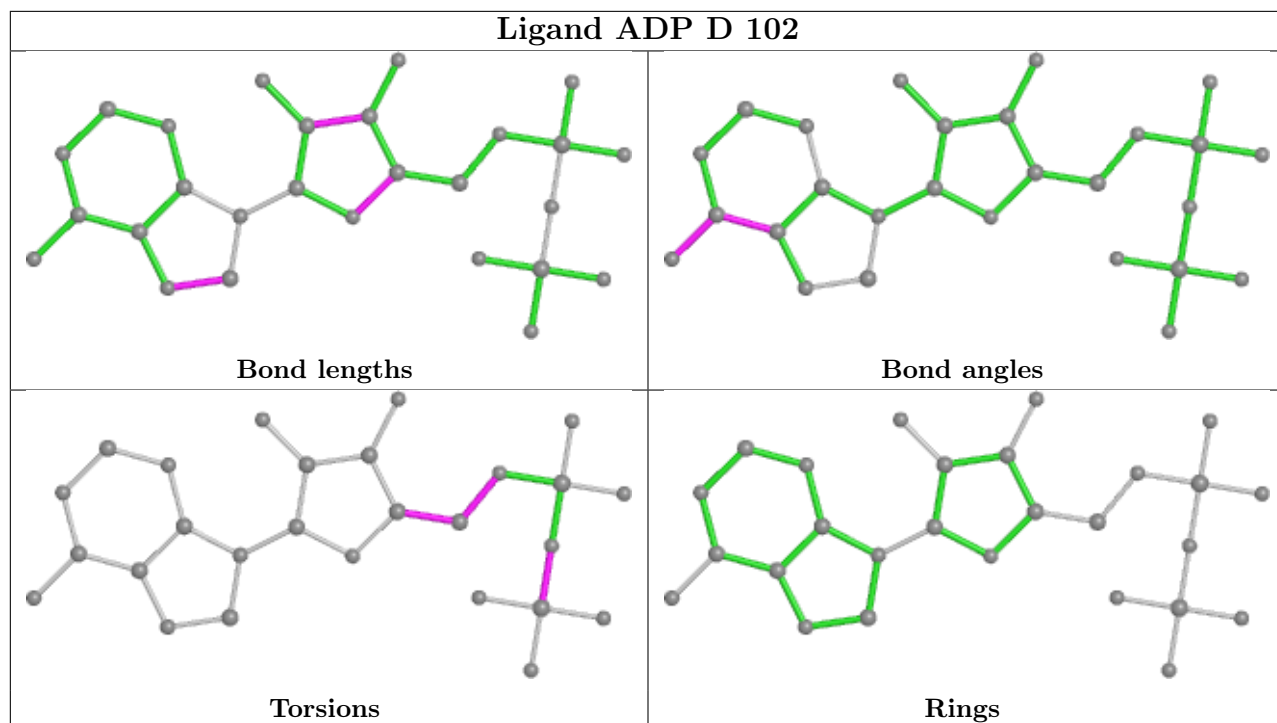
Mol	Chain	Res	Type	Atoms
3	D	102	ADP	C4'-C5'-O5'-PA
2	B	1	114	C22-C19-C20-C21
3	D	102	ADP	PA-O3A-PB-O1B
2	A	2	114	O1B-C1-C2-C3

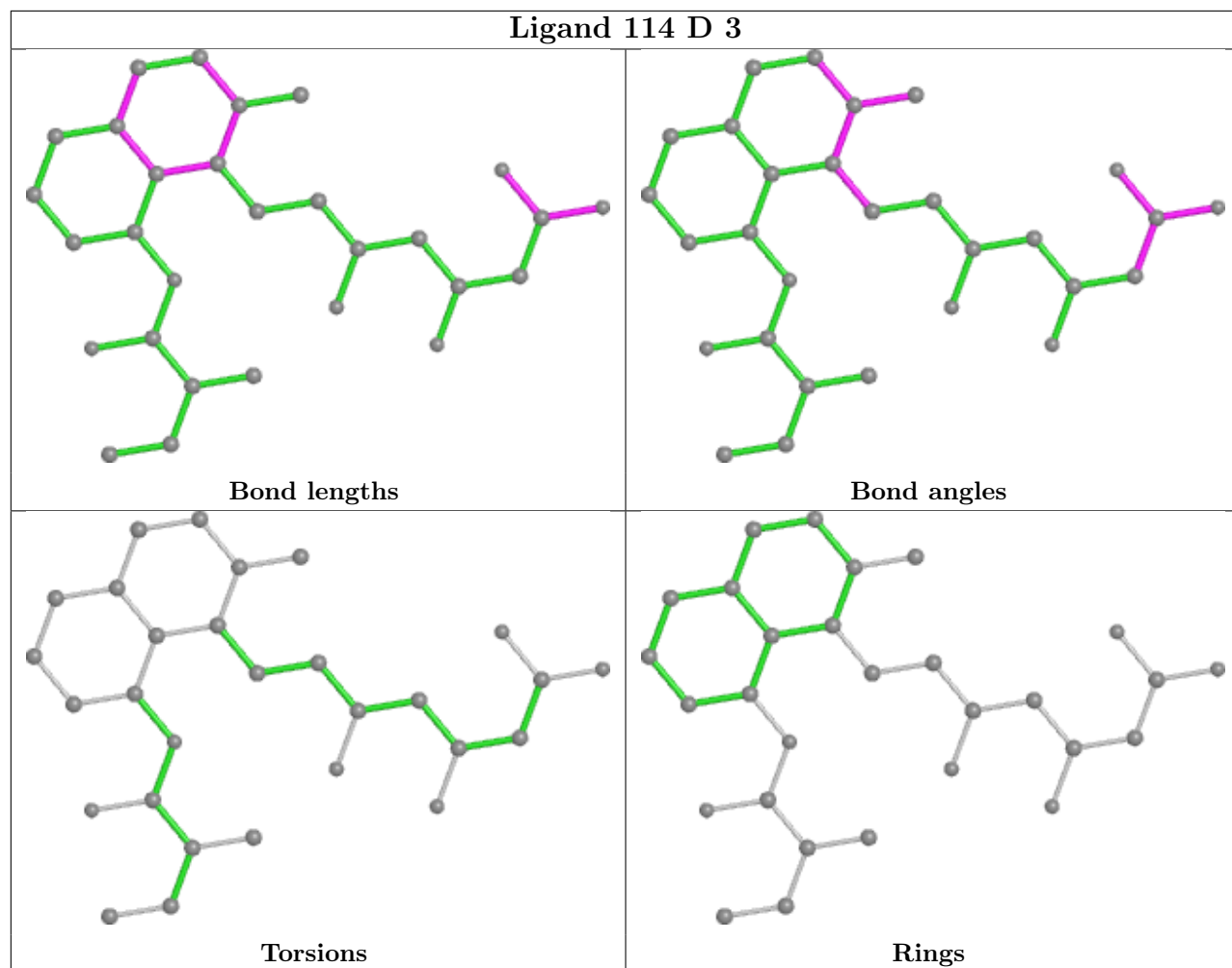
There are no ring outliers.

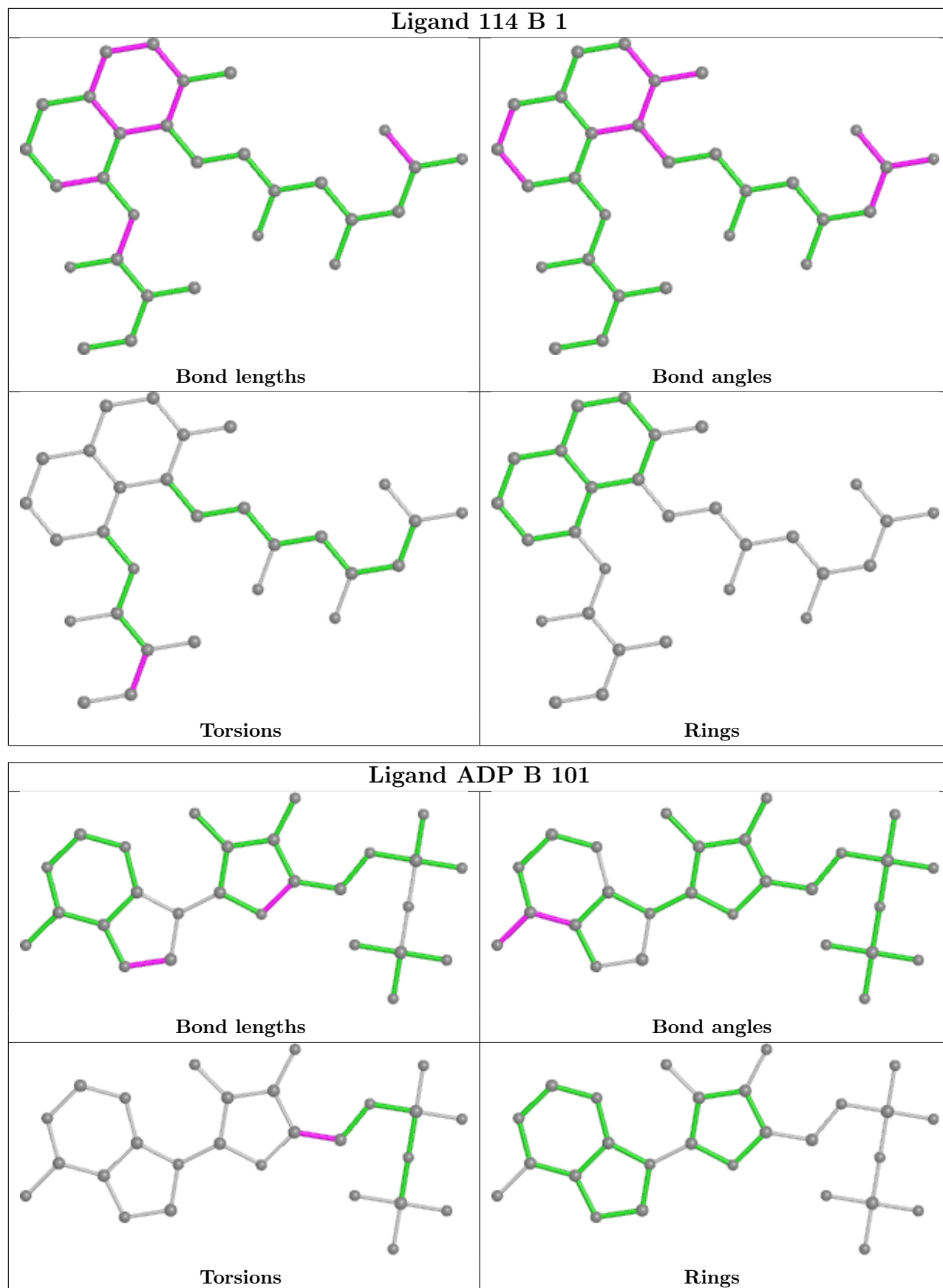
5 monomers are involved in 9 short contacts:

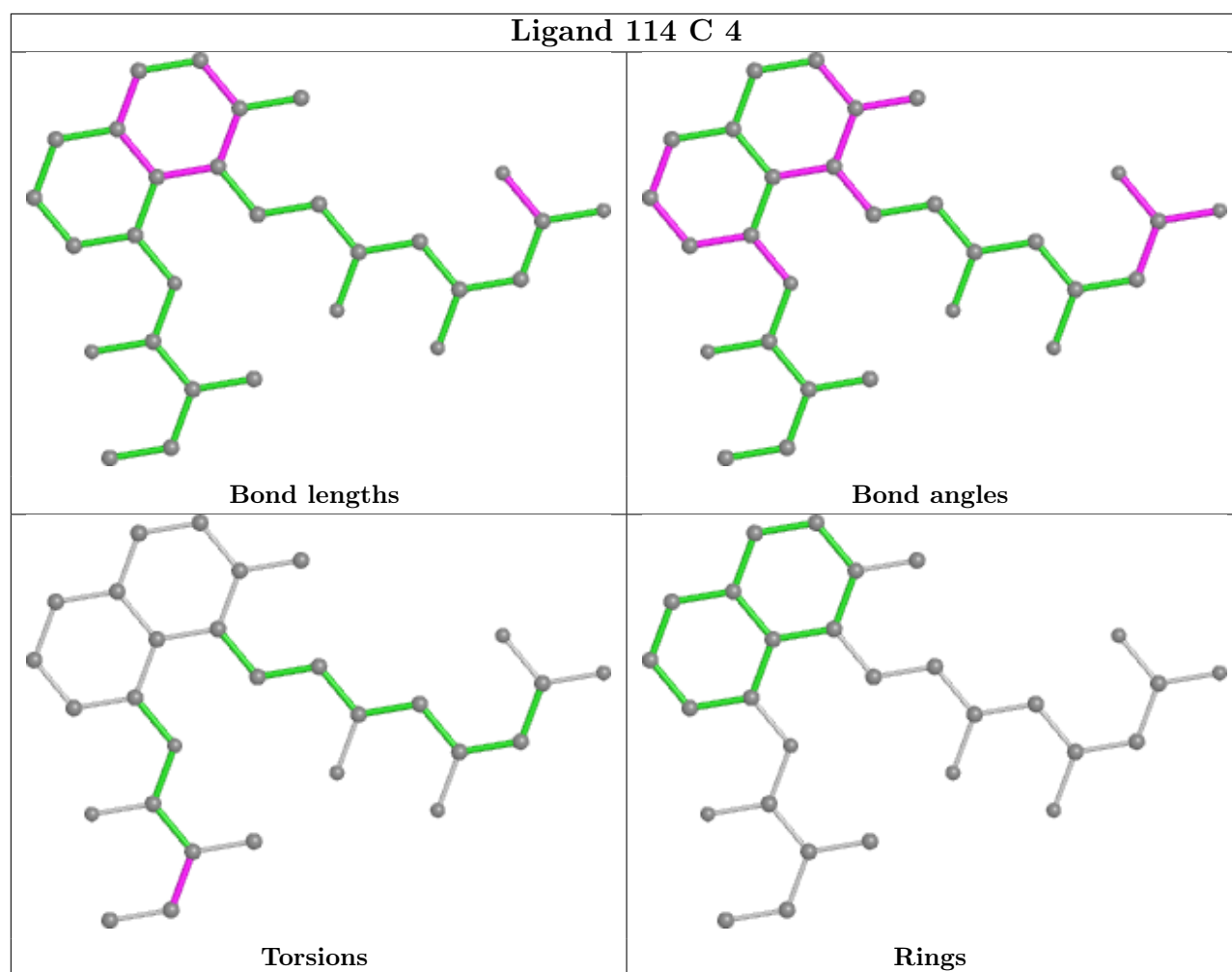
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	102	ADP	1	0
2	A	2	114	2	0
2	D	3	114	1	0
3	B	101	ADP	3	0
2	C	4	114	2	0

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









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/467 (86%)	0.13	32 (7%) 12 16	20, 34, 69, 99	0
1	B	410/467 (87%)	-0.07	9 (2%) 62 66	20, 33, 60, 88	0
1	C	373/467 (79%)	0.05	13 (3%) 44 50	20, 33, 54, 80	0
1	D	372/467 (79%)	-0.13	10 (2%) 54 60	21, 32, 50, 61	0
All	All	1559/1868 (83%)	-0.00	64 (4%) 37 43	20, 33, 57, 99	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	9.0
1	C	524	GLY	7.1
1	A	448	CYS	5.1
1	A	470	LEU	5.1
1	A	829	ASP	4.8
1	A	482	GLU	4.6
1	A	446	GLU	4.2
1	A	479	TYR	4.2
1	D	523	MET	3.9
1	B	448	CYS	3.7
1	A	447	GLU	3.6
1	A	445	ASN	3.5
1	D	746	ILE	3.5
1	A	478	ALA	3.3
1	D	524	GLY	3.3
1	B	449	LEU	3.3
1	A	628	PHE	3.2
1	A	485	ILE	3.2
1	C	523	MET	3.1
1	A	486	GLU	3.1
1	A	464	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	3.0
1	B	446	GLU	2.9
1	C	627	ARG	2.9
1	A	828	LYS	2.9
1	A	477	PRO	2.8
1	A	627	ARG	2.8
1	A	501	LYS	2.8
1	C	746	ILE	2.7
1	B	461	PHE	2.7
1	D	490	ARG	2.7
1	A	467	ILE	2.7
1	A	483	THR	2.7
1	A	480	LYS	2.6
1	A	524	GLY	2.5
1	A	516	ASP	2.5
1	D	718	ARG	2.5
1	C	749	TYR	2.4
1	C	829	ASP	2.4
1	A	772	VAL	2.3
1	C	695	ALA	2.3
1	D	516	ASP	2.2
1	B	694	ALA	2.2
1	A	630	ARG	2.2
1	B	451	ILE	2.2
1	C	628	PHE	2.2
1	B	476	ILE	2.1
1	D	488	HIS	2.1
1	D	749	TYR	2.1
1	B	829	ASP	2.1
1	C	694	ALA	2.1
1	C	548	GLU	2.1
1	A	498	LEU	2.1
1	C	516	ASP	2.1
1	A	748	GLY	2.1
1	A	463	SER	2.1
1	B	485	ILE	2.1
1	A	481	LEU	2.1
1	A	629	ALA	2.1
1	D	515	ARG	2.1
1	D	698	TRP	2.1
1	C	515	ARG	2.0
1	A	469	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	521	LEU	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](#)

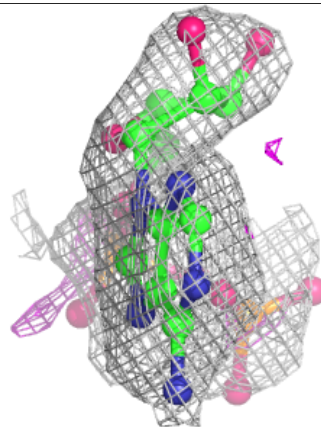
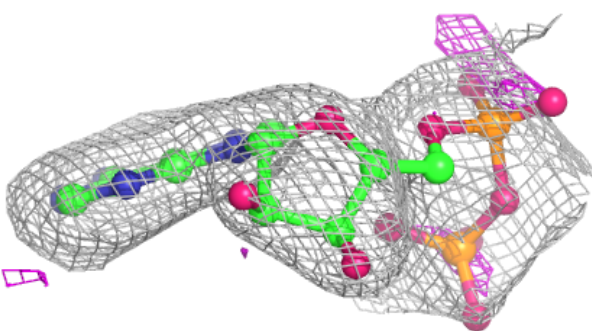
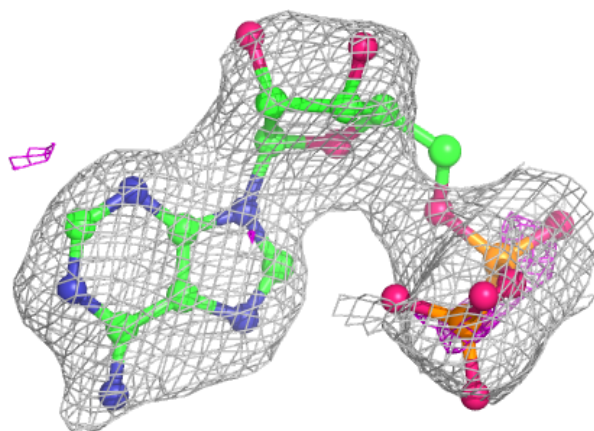
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	101	27/27	0.71	0.24	83,90,100,100	0
3	ADP	D	102	27/27	0.83	0.16	58,67,80,81	0
2	114	C	4	29/29	0.87	0.13	30,40,47,48	0
2	114	A	2	29/29	0.91	0.12	33,40,47,49	0
2	114	B	1	29/29	0.93	0.11	28,36,46,47	0
2	114	D	3	29/29	0.93	0.12	29,41,49,50	0

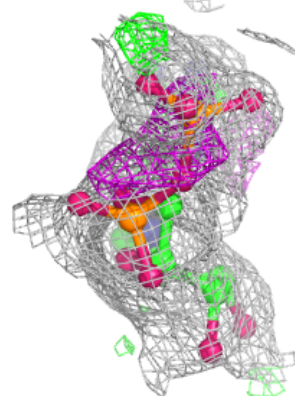
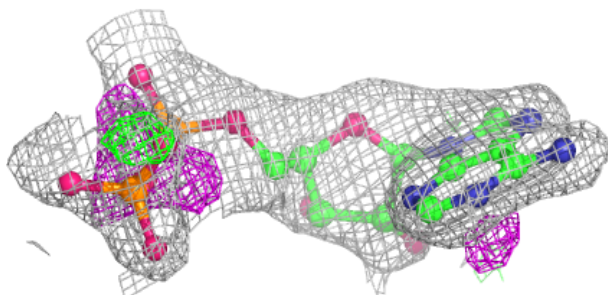
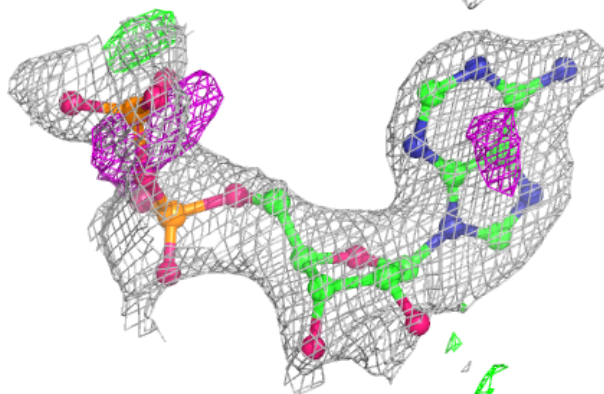
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

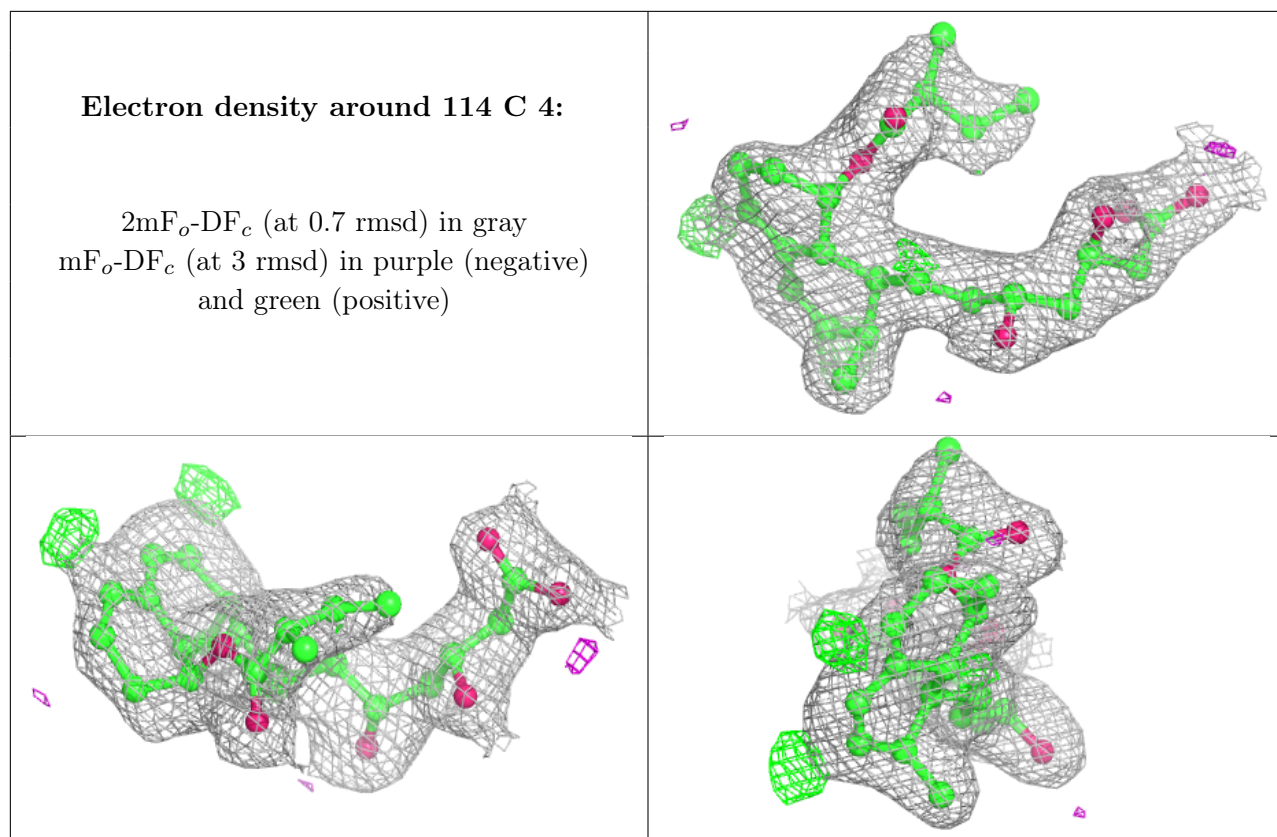
Electron density around ADP B 101:

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

**Electron density around ADP D 102:**

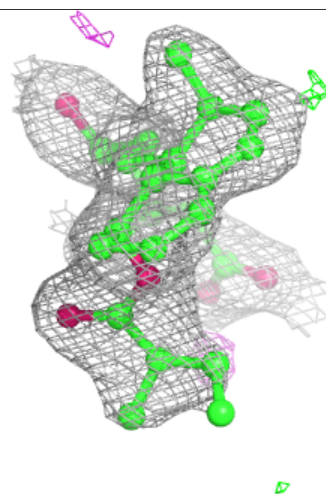
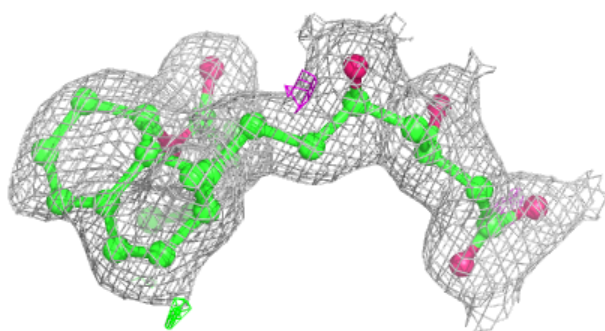
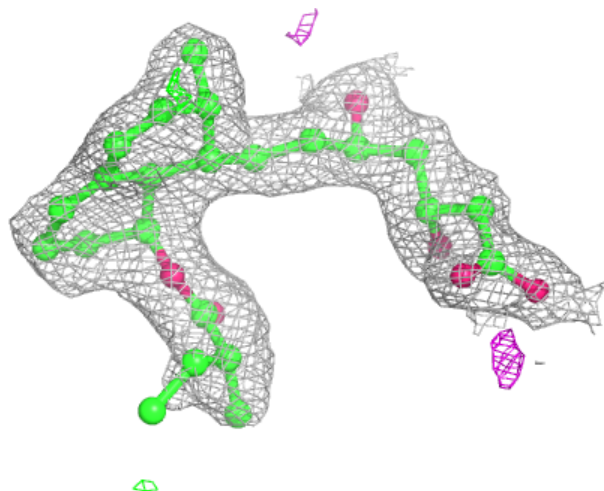
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





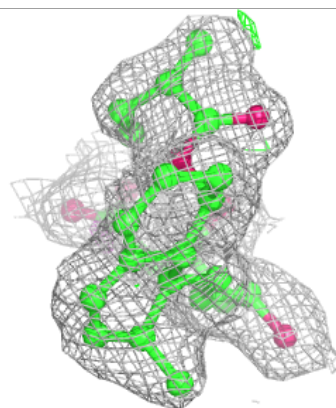
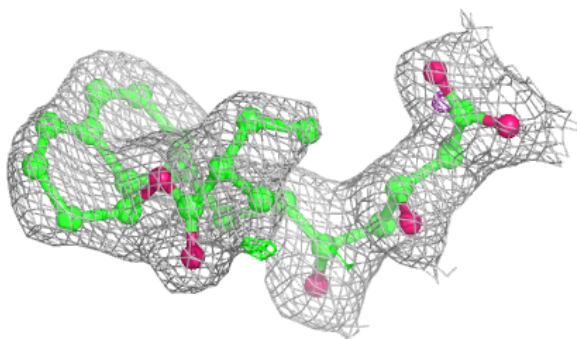
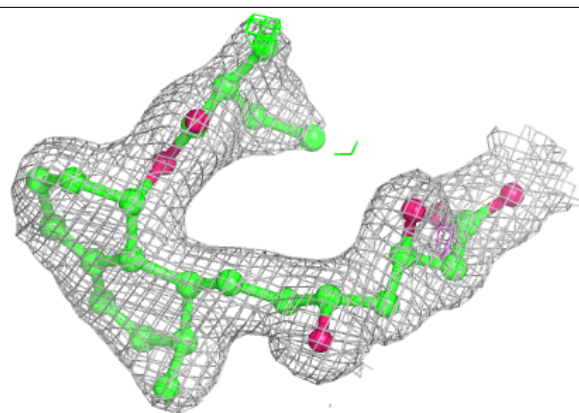
Electron density around 114 A 2:

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

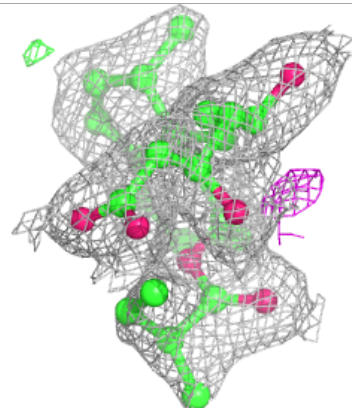
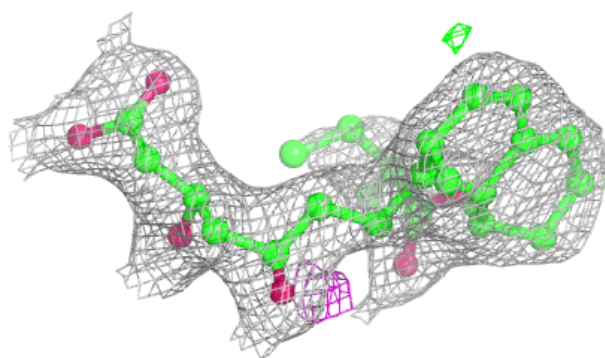
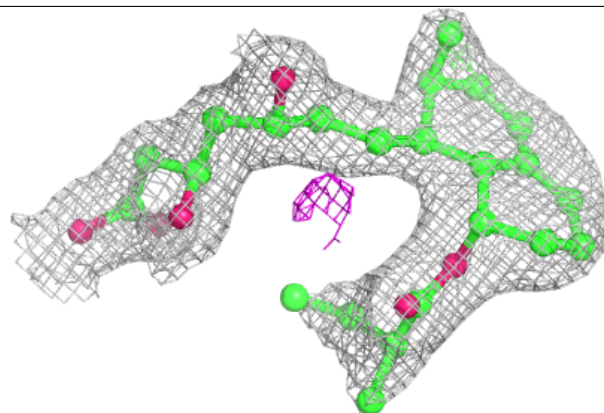


Electron density around 114 B 1:

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

**Electron density around 114 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.