



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:51 AM UTC

PDB ID : 1HW8 / pdb_00001hw8
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	:	4-5-2 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

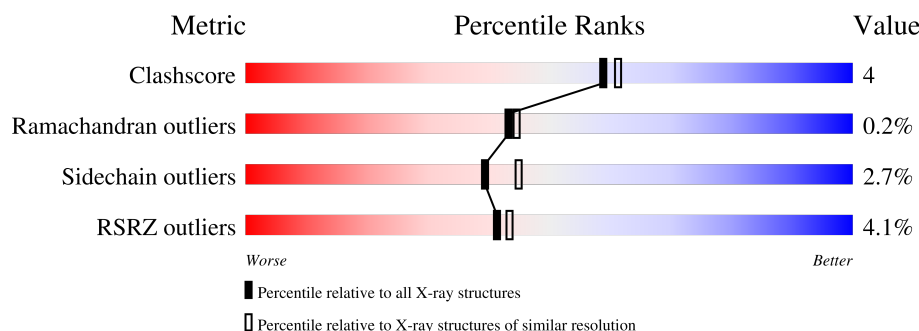
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	
1	B	467	
1	C	467	
1	D	467	

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.

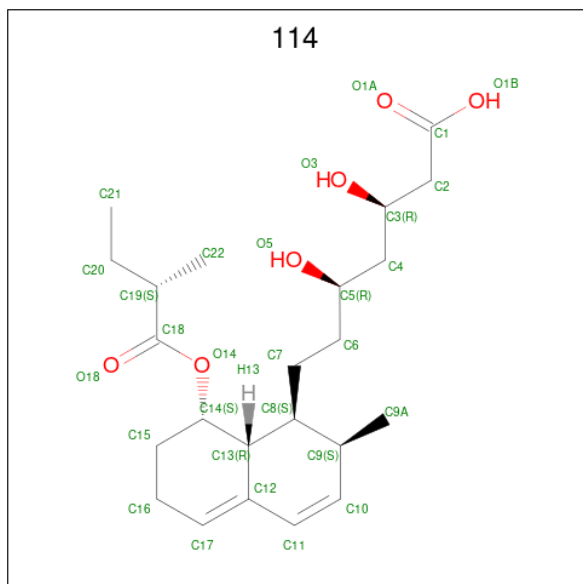
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3004	1867	527	580	30			
1	B	410	Total	C	N	O	S	0	0	0
			3055	1904	536	585	30			
1	C	373	Total	C	N	O	S	0	0	0
			2755	1711	487	528	29			
1	D	372	Total	C	N	O	S	0	0	0
			2751	1709	486	527	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 (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 (CCD ID: 114) (formula: $C_{23}H_{36}O_6$).



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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

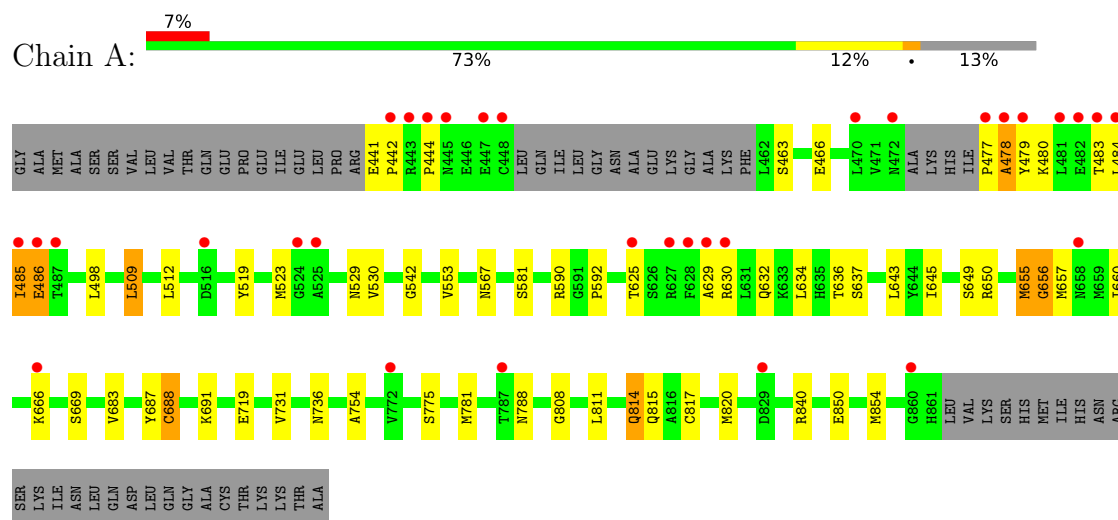
- Molecule 4 is water.

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		

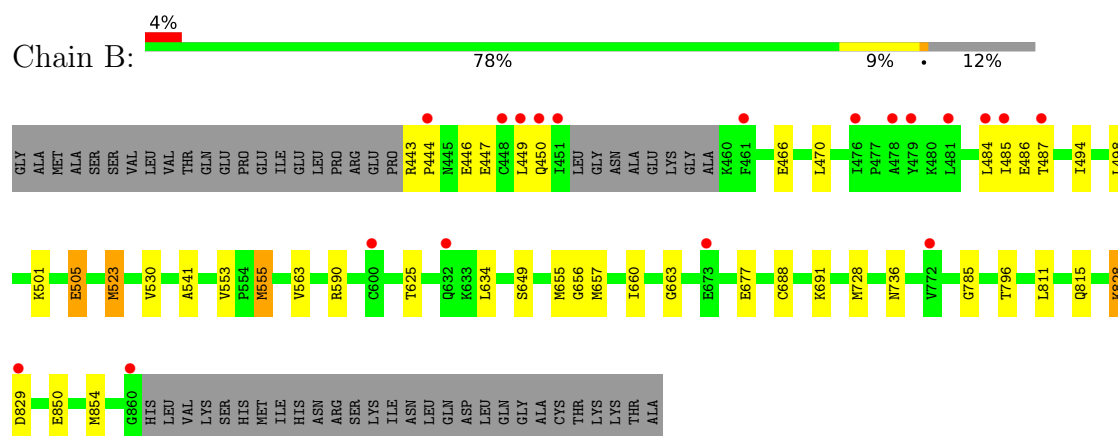
3 Residue-property plots

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.

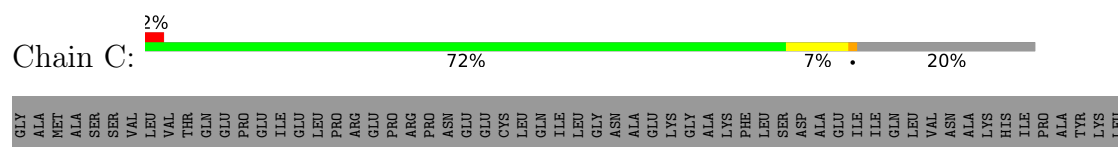
• Molecule 1: HMG-COA REDUCTASE

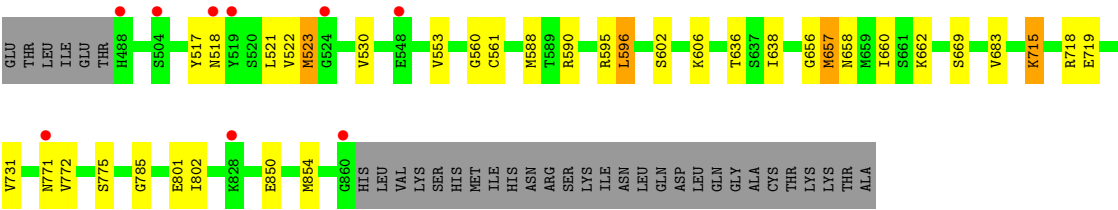


• Molecule 1: HMG-COA REDUCTASE

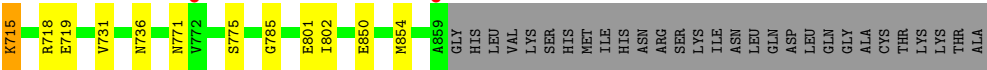
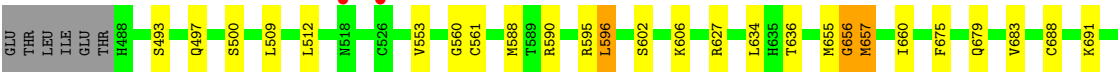
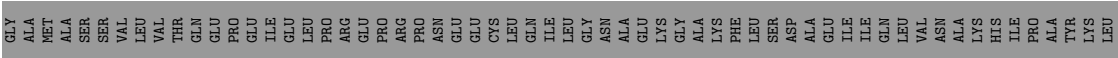


• Molecule 1: HMG-COA REDUCTASE





● 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	73.83Å 173.00Å 75.18Å 90.00° 118.38° 90.00°	Depositor
Resolution (Å)	43.13 – 2.10 43.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (43.13-2.10) 89.2 (43.13-2.10)	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 0.189 , (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)	0.38 , 41.5	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	0.60	0/3046	0.99	9/4117 (0.2%)
1	B	0.65	1/3098 (0.0%)	0.98	10/4187 (0.2%)
1	C	0.62	0/2794	0.98	5/3776 (0.1%)
1	D	0.65	0/2790	1.01	13/3771 (0.3%)
All	All	0.63	1/11728 (0.0%)	0.99	37/15851 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-7.81	1.60	1.79

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	VAL	N-CA-C	8.96	116.81	107.76
1	D	553	VAL	N-CA-C	8.68	116.52	107.76
1	B	553	VAL	N-CA-C	8.66	116.51	107.76
1	C	553	VAL	N-CA-C	7.84	115.68	107.76
1	C	785	GLY	CA-C-N	7.51	127.05	119.24
1	C	785	GLY	C-N-CA	7.51	127.05	119.24
1	D	655	MET	N-CA-C	-7.46	103.15	111.28
1	A	656	GLY	N-CA-C	7.12	124.18	114.92
1	C	656	GLY	N-CA-C	7.08	124.12	114.92
1	D	656	GLY	N-CA-C	6.96	125.08	115.27
1	D	785	GLY	CA-C-N	6.95	126.47	119.24
1	D	785	GLY	C-N-CA	6.95	126.47	119.24
1	B	656	GLY	N-CA-C	6.36	124.10	115.32
1	A	509	LEU	N-CA-C	6.34	120.61	113.01
1	B	785	GLY	CA-C-N	6.23	126.43	119.32
1	B	785	GLY	C-N-CA	6.23	126.43	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	LEU	CA-C-N	6.15	126.11	119.78
1	D	512	LEU	C-N-CA	6.15	126.11	119.78
1	D	736	ASN	N-CA-C	5.97	118.74	111.82
1	A	736	ASN	N-CA-C	5.93	118.70	111.82
1	B	450	GLN	N-CA-C	-5.86	105.89	113.16
1	A	719	GLU	N-CA-C	5.82	117.70	111.36
1	B	655	MET	N-CA-C	-5.66	105.20	111.71
1	B	505	GLU	CA-C-N	5.64	126.01	119.47
1	B	505	GLU	C-N-CA	5.64	126.01	119.47
1	A	485	ILE	N-CA-C	5.61	116.17	110.05
1	D	657	MET	N-CA-C	5.52	116.98	111.07
1	D	675	PHE	CA-C-N	5.46	125.13	119.56
1	D	675	PHE	C-N-CA	5.46	125.13	119.56
1	B	736	ASN	N-CA-C	5.45	118.15	111.82
1	A	655	MET	N-CA-C	-5.41	105.38	111.28
1	D	691	LYS	N-CA-C	5.37	119.41	112.86
1	A	688	CYS	N-CA-C	5.32	116.77	110.97
1	D	719	GLU	N-CA-C	5.30	118.21	111.69
1	A	691	LYS	N-CA-C	5.26	119.28	112.86
1	C	719	GLU	N-CA-C	5.22	117.05	111.36
1	B	691	LYS	N-CA-C	5.08	119.42	113.23

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	3004	0	3026	40	0
1	B	3055	0	3094	24	0
1	C	2755	0	2784	26	0
1	D	2751	0	2781	15	0
2	A	29	0	35	2	0
2	B	29	0	35	0	0
2	C	29	0	35	2	0
2	D	29	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	103	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 (103) 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:C:523:MET:HE1	1:C:530:VAL:CG2	2.17	0.75
1:B:828:LYS:HD2	1:B:828:LYS:N	1.99	0.74
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.70	0.73
1:A:529:ASN:ND2	3:B:101:ADP:H2	1.88	0.72
1:C:523:MET:HA	1:C:523:MET:HE3	1.71	0.71
1:C:523:MET:HE2	4:C:1172:HOH:O	1.93	0.68
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:A:519:TYR:HB3	1:A:523:MET:HE3	1.77	0.65
1:C:523:MET:HE1	1:C:530:VAL:HG21	1.78	0.64
1:D:596:LEU:HD13	1:D:602:SER:HA	1.81	0.63
1:B:590:ARG:NH1	1:B:657:MET:HE1	2.14	0.63
1:D:595:ARG:HD2	1:D:679:GLN:OE1	1.98	0.63
1:A:781:MET:HE1	1:A:854:MET:HG3	1.79	0.63
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.80	0.62
1:C:518:ASN:HD21	1:C:521:LEU:HD13	1.64	0.60
1:B:590:ARG:HH12	1:B:657:MET:HE1	1.66	0.60
1:A:817:CYS:HA	1:A:820:MET:HE3	1.84	0.59
1:A:542:GLY:H	1:A:567:ASN:ND2	2.00	0.59
1:C:657:MET:HA	1:C:657:MET:HE2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:MET:HE1	1:B:530:VAL:HG23	1.86	0.56
1:B:523:MET:HE1	1:B:530:VAL:CG2	2.36	0.55
1:A:656:GLY:O	1:A:660:ILE:HG12	2.07	0.55
1:B:541:ALA:HB2	1:B:555:MET:HE2	1.89	0.55
1:C:850:GLU:O	1:C:854:MET:HG2	2.07	0.54
1:C:523:MET:HE1	1:C:530:VAL:HG23	1.89	0.53
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
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: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:A:781:MET:CE	1:A:854:MET:HG3	2.42	0.49
1:A:477:PRO:O	1:A:478:ALA:HB3	2.13	0.49
1:D:588:MET:HE1	1:D:801:GLU:HG2	1.95	0.49
1:B:447:GLU:C	1:B:449:LEU:H	2.20	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:A:629:ALA:C	1:A:630:ARG:HD2	2.39	0.48
1:B:485:ILE:HD13	1:B:494:ILE:HD12	1.94	0.47
1:B:677:GLU:H	1:B:677:GLU:CD	2.21	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:B:728:MET:HE3	1:B:854:MET:HB2	1.98	0.45
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:588:MET:HE1	1:C:801:GLU:HG2	1.99	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: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:C:560:GLY:O	1:C:561:CYS:HB2	2.18	0.43
1:C:590:ARG:HB2	1:C:660:ILE:HG22	2.00	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:A:590:ARG:CZ	1:A:657:MET:HE1	2.49	0.43
1:A:731:VAL:HG12	1:A:854:MET:HE1	2.00	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:D:656:GLY:HA2	3:D:102:ADP:O1B	2.21	0.41
1:B:657:MET:HB3	1:B:657:MET:HE3	1.77	0.41
1:B:625:THR:HG21	1:B:663:GLY:HA2	2.01	0.41
1:D:731:VAL:HG12	1:D:854:MET:HE1	2.03	0.41
1:C:731:VAL:HG12	1:C:854:MET:HE1	2.02	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

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	398/467 (85%)	381 (96%)	14 (4%)	3 (1%)	16	12
1	B	406/467 (87%)	389 (96%)	17 (4%)	0	100	100
1	C	371/467 (79%)	359 (97%)	12 (3%)	0	100	100
1	D	370/467 (79%)	356 (96%)	14 (4%)	0	100	100
All	All	1545/1868 (83%)	1485 (96%)	57 (4%)	3 (0%)	43	44

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

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%)	315 (98%)	8 (2%)	42	48
1	B	328/375 (88%)	319 (97%)	9 (3%)	39	45
1	C	294/375 (78%)	287 (98%)	7 (2%)	43	49
1	D	294/375 (78%)	284 (97%)	10 (3%)	32	35
All	All	1239/1500 (83%)	1205 (97%)	34 (3%)	39	45

All (34) 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	688	CYS
1	A	788	ASN
1	A	814	GLN
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	688	CYS
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	715	LYS
1	C	802	ILE
1	D	500	SER
1	D	509	LEU
1	D	596	LEU
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	660	ILE
1	D	688	CYS
1	D	715	LYS
1	D	802	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	488	HIS
1	A	497	GLN
1	A	510	GLN
1	A	529	ASN

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Mol	Chain	Res	Type
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	B	472	ASN
1	B	488	HIS
1	B	510	GLN
1	B	635	HIS
1	B	672	HIS
1	B	819	GLN
1	C	736	ASN
1	C	819	GLN
1	D	488	HIS
1	D	635	HIS
1	D	642	ASN
1	D	648	GLN
1	D	672	HIS
1	D	736	ASN
1	D	788	ASN

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 oligosaccharides 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	-	28,29,29	1.70	5 (17%)	43,45,45	0.83	1 (2%)
2	114	B	1	-	30,30,30	1.84	9 (30%)	34,41,41	1.37	7 (20%)
2	114	D	3	-	30,30,30	1.89	7 (23%)	34,41,41	1.32	4 (11%)
2	114	A	2	-	30,30,30	1.88	9 (30%)	34,41,41	1.26	5 (14%)
3	ADP	B	101	-	28,29,29	1.41	4 (14%)	43,45,45	0.69	0
2	114	C	4	-	30,30,30	1.82	6 (20%)	34,41,41	1.42	7 (20%)

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	-	-	6/16/32/32	0/3/3/3
2	114	B	1	-	-	2/23/50/50	0/2/2/2
2	114	D	3	-	-	0/23/50/50	0/2/2/2
2	114	A	2	-	1/1/10/13	6/23/50/50	0/2/2/2
3	ADP	B	101	-	-	2/16/32/32	0/3/3/3
2	114	C	4	-	-	2/23/50/50	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	102	ADP	PA-O3A	5.43	1.65	1.59
2	A	2	114	O1A-C1	4.62	1.37	1.22
2	D	3	114	C9-C8	4.55	1.59	1.54
2	C	4	114	O1A-C1	4.45	1.36	1.22
2	B	1	114	C9-C8	4.30	1.58	1.54
2	D	3	114	O1A-C1	4.26	1.36	1.22
2	B	1	114	O1A-C1	4.18	1.35	1.22
2	D	3	114	C13-C12	4.14	1.57	1.52
2	C	4	114	C9-C8	4.07	1.58	1.54
2	A	2	114	C9-C8	3.89	1.58	1.54
2	C	4	114	C13-C12	3.83	1.57	1.52
3	B	101	ADP	PA-O3A	3.65	1.63	1.59
2	A	2	114	C13-C12	3.64	1.57	1.52
2	B	1	114	C13-C12	3.44	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	102	ADP	O4'-C4'	3.16	1.52	1.45
3	D	102	ADP	C8-N9	-3.02	1.32	1.37
2	C	4	114	C9-C10	2.93	1.55	1.50
3	B	101	ADP	C1'-N9	2.93	1.54	1.46
3	D	102	ADP	C1'-N9	2.73	1.53	1.46
3	B	101	ADP	C8-N9	-2.66	1.33	1.37
2	C	4	114	C13-C8	2.59	1.58	1.54
2	A	2	114	C9-C10	2.54	1.54	1.50
2	D	3	114	C9-C10	2.53	1.54	1.50
2	D	3	114	O1B-C1	-2.45	1.22	1.30
3	B	101	ADP	O4'-C4'	2.44	1.50	1.45
2	B	1	114	C13-C8	2.42	1.58	1.54
2	D	3	114	C11-C12	-2.41	1.36	1.43
2	A	2	114	C13-C8	2.33	1.58	1.54
2	B	1	114	C15-C14	2.24	1.56	1.52
2	B	1	114	O14-C18	2.19	1.39	1.34
2	A	2	114	O1B-C1	-2.17	1.23	1.30
2	C	4	114	C11-C12	-2.16	1.37	1.43
2	B	1	114	C11-C12	-2.15	1.37	1.43
2	A	2	114	C11-C12	-2.12	1.37	1.43
2	B	1	114	C11-C10	2.12	1.37	1.33
2	B	1	114	C9-C10	2.11	1.53	1.50
2	A	2	114	C15-C14	2.11	1.56	1.52
2	D	3	114	C13-C8	2.05	1.57	1.54
3	D	102	ADP	C2'-C3'	2.03	1.58	1.53
2	A	2	114	O14-C18	2.02	1.38	1.34

All (24) 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	-3.40	112.40	122.84
2	C	4	114	O1A-C1-C2	-3.27	112.80	122.84
2	C	4	114	O1B-C1-C2	3.27	124.16	114.00
2	A	2	114	O1A-C1-C2	-3.21	112.98	122.84
2	B	1	114	O1B-C1-C2	3.19	123.91	114.00
2	D	3	114	O1A-C1-C2	-3.18	113.09	122.84
2	A	2	114	O1B-C1-C2	3.15	123.79	114.00
2	D	3	114	O1B-C1-C2	3.00	123.33	114.00
2	C	4	114	C7-C8-C9	2.82	114.68	112.87
3	D	102	ADP	O4'-C1'-N9	2.71	113.30	108.09
2	C	4	114	C13-C8-C9	-2.69	109.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	114	C7-C8-C9	2.62	114.56	112.87
2	D	3	114	C9A-C9-C10	-2.60	106.33	110.73
2	A	2	114	C9A-C9-C10	-2.46	106.57	110.73
2	B	1	114	C7-C8-C13	2.44	115.82	112.50
2	A	2	114	C7-C8-C9	2.33	114.36	112.87
2	C	4	114	C9A-C9-C10	-2.32	106.81	110.73
2	B	1	114	C13-C8-C9	2.29	111.91	110.70
2	B	1	114	C15-C16-C17	2.19	115.46	111.91
2	A	2	114	C15-C16-C17	2.17	115.44	111.91
2	C	4	114	O14-C14-C15	2.15	112.90	108.42
2	B	1	114	C9A-C9-C10	-2.14	107.11	110.73
2	C	4	114	C15-C16-C17	2.14	115.38	111.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	114	C19

All (18) torsion outliers are listed below:

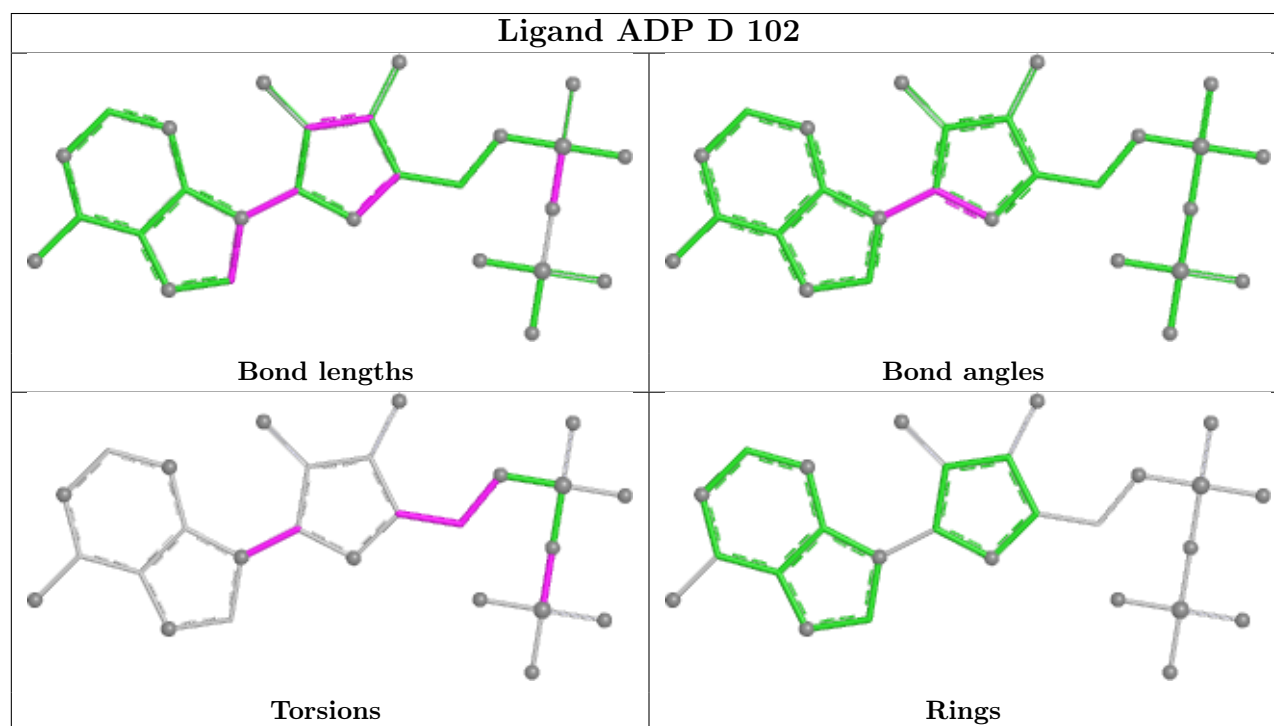
Mol	Chain	Res	Type	Atoms
2	C	4	114	C22-C19-C20-C21
3	B	101	ADP	O4'-C4'-C5'-O5'
3	D	102	ADP	PA-O3A-PB-O3B
3	B	101	ADP	C3'-C4'-C5'-O5'
3	D	102	ADP	C3'-C4'-C5'-O5'
2	A	2	114	C18-C19-C20-C21
2	C	4	114	C18-C19-C20-C21
2	A	2	114	C22-C19-C20-C21
3	D	102	ADP	O4'-C4'-C5'-O5'
2	B	1	114	C18-C19-C20-C21
2	A	2	114	O18-C18-C19-C20
2	A	2	114	O14-C18-C19-C20
3	D	102	ADP	C4'-C5'-O5'-PA
3	D	102	ADP	PA-O3A-PB-O1B
2	B	1	114	C22-C19-C20-C21
2	A	2	114	O1B-C1-C2-C3
3	D	102	ADP	O4'-C1'-N9-C8
2	A	2	114	O5-C5-C6-C7

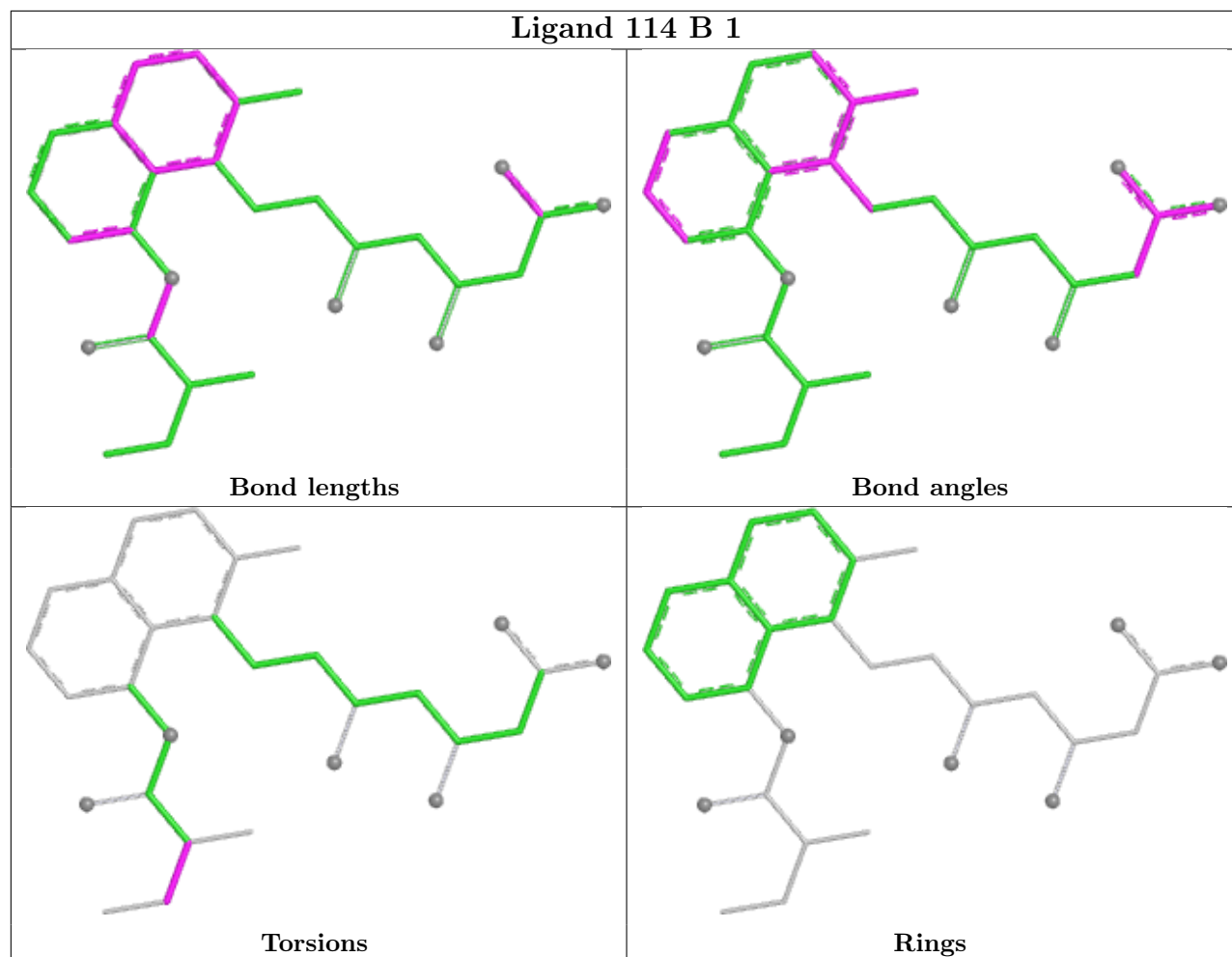
There are no ring outliers.

5 monomers are involved in 9 short contacts:

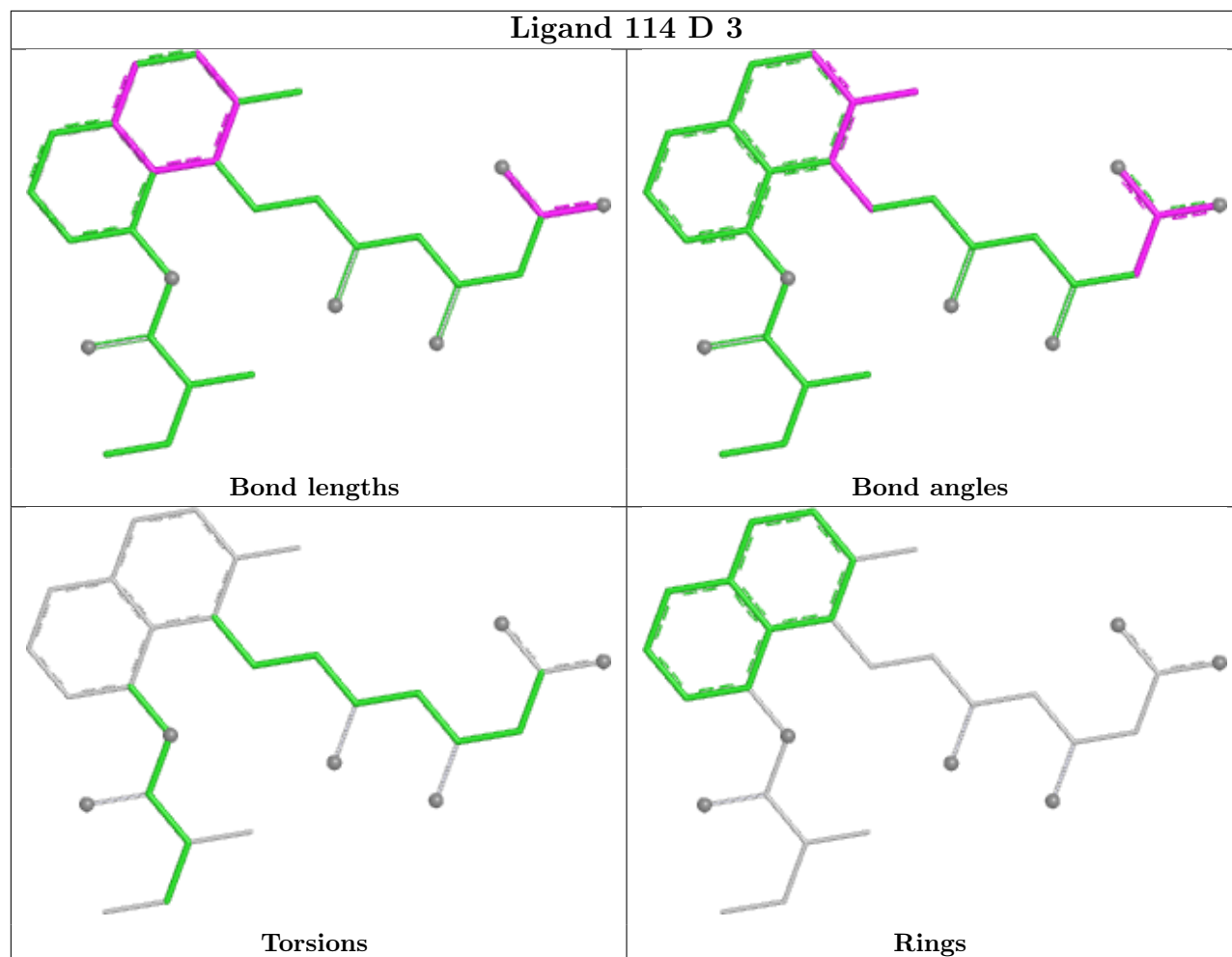
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	102	ADP	1	0
2	D	3	114	1	0
2	A	2	114	2	0
3	B	101	ADP	3	0
2	C	4	114	2	0

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.

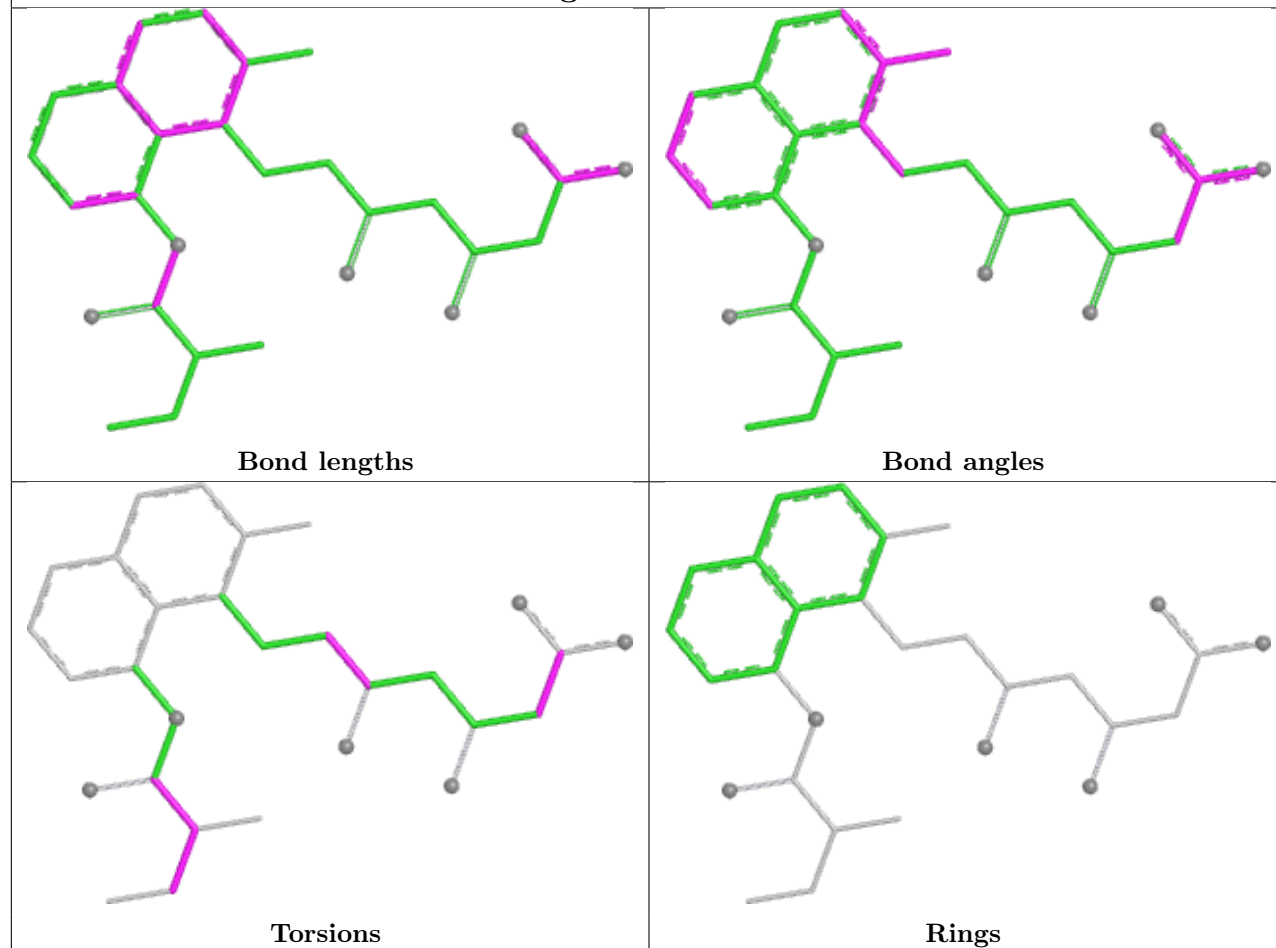




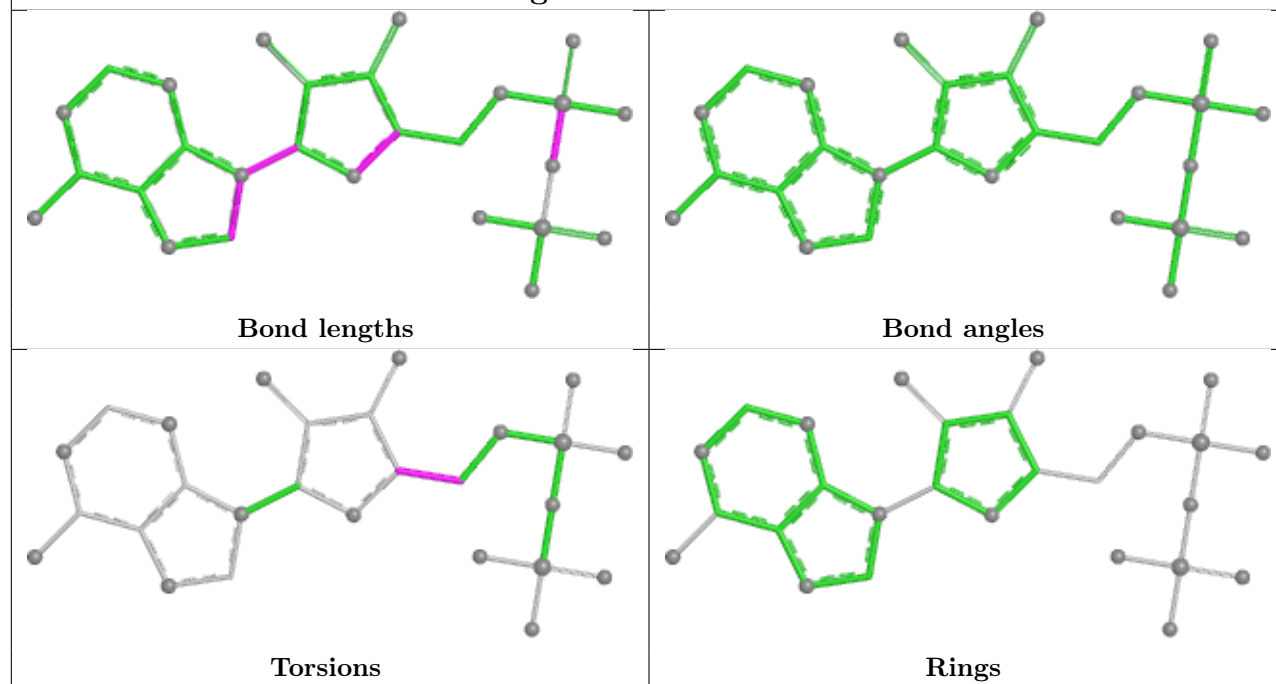
Ligand 114 D 3

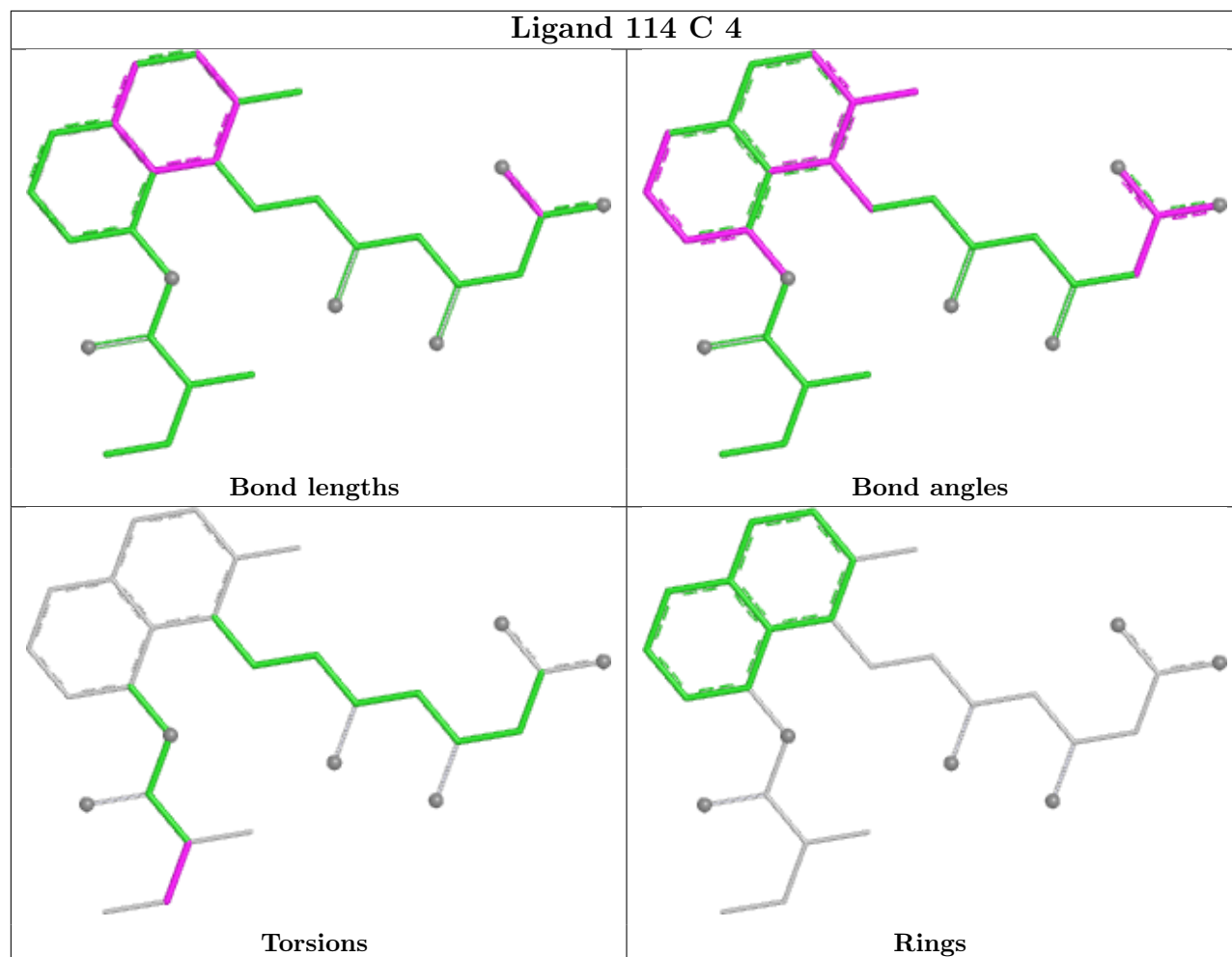


Ligand 114 A 2



Ligand ADP B 101





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%)	0.44	32 (7%) 18 20	20, 34, 69, 99	0
1	B	410/467 (87%)	0.32	19 (4%) 37 39	20, 33, 60, 88	0
1	C	373/467 (79%)	0.25	9 (2%) 59 62	20, 33, 54, 80	0
1	D	372/467 (79%)	0.17	4 (1%) 78 80	21, 32, 50, 61	0
All	All	1559/1868 (83%)	0.30	64 (4%) 41 43	20, 33, 57, 99	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	LEU	6.6
1	A	477	PRO	6.1
1	A	484	LEU	4.6
1	B	451	ILE	4.6
1	C	524	GLY	4.3
1	B	444	PRO	4.3
1	D	859	ALA	4.2
1	A	478	ALA	4.2
1	A	442	PRO	3.9
1	A	448	CYS	3.8
1	C	860	GLY	3.7
1	A	479	TYR	3.6
1	B	829	ASP	3.5
1	B	448	CYS	3.2
1	A	525	ALA	3.2
1	B	632	GLN	3.2
1	A	483	THR	3.1
1	C	548	GLU	3.0
1	C	518	ASN	3.0
1	B	485	ILE	2.9
1	B	450	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	461	PHE	2.8
1	A	444	PRO	2.8
1	C	488	HIS	2.7
1	A	482	GLU	2.7
1	A	443	ARG	2.7
1	B	479	TYR	2.7
1	A	447	GLU	2.7
1	A	481	LEU	2.6
1	A	829	ASP	2.6
1	A	629	ALA	2.6
1	B	772	VAL	2.5
1	A	860	GLY	2.5
1	D	526	CYS	2.5
1	A	516	ASP	2.5
1	A	445	ASN	2.5
1	A	485	ILE	2.4
1	A	486	GLU	2.4
1	B	476	ILE	2.4
1	A	472	ASN	2.4
1	B	484	LEU	2.3
1	A	630	ARG	2.3
1	B	487	THR	2.3
1	A	627	ARG	2.3
1	B	860	GLY	2.3
1	A	787	THR	2.3
1	C	771	ASN	2.3
1	B	600	CYS	2.3
1	D	772	VAL	2.2
1	A	524	GLY	2.2
1	A	487	THR	2.2
1	C	519	TYR	2.2
1	A	666	LYS	2.2
1	A	625	THR	2.2
1	A	658	ASN	2.1
1	C	828	LYS	2.1
1	D	518	ASN	2.1
1	B	478	ALA	2.1
1	C	504	SER	2.1
1	A	470	LEU	2.0
1	B	481	LEU	2.0
1	A	628	PHE	2.0
1	A	772	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	673	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

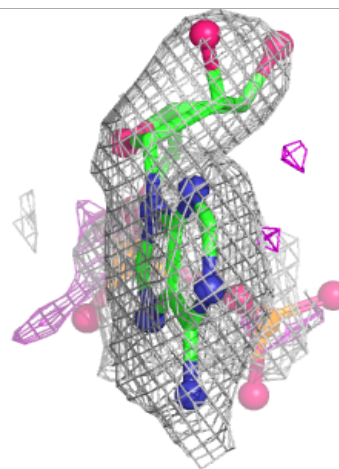
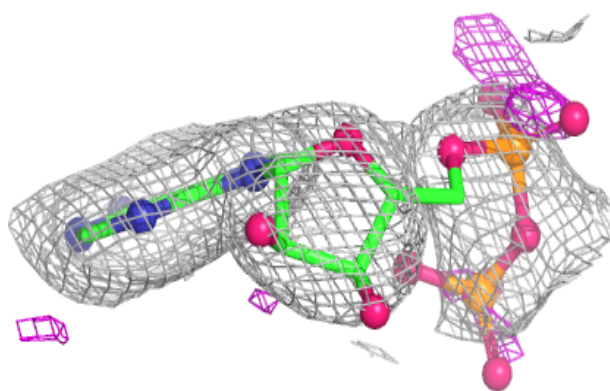
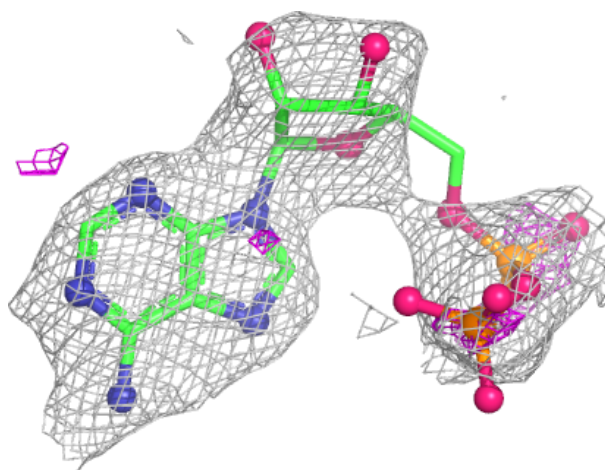
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.77	0.17	83,90,100,100	0
3	ADP	D	102	27/27	0.80	0.17	58,67,80,81	0
2	114	C	4	29/29	0.90	0.11	30,40,47,48	0
2	114	B	1	29/29	0.92	0.09	28,36,46,47	0
2	114	A	2	29/29	0.92	0.10	33,40,47,49	0
2	114	D	3	29/29	0.93	0.09	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.

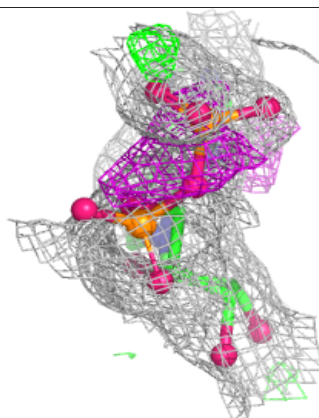
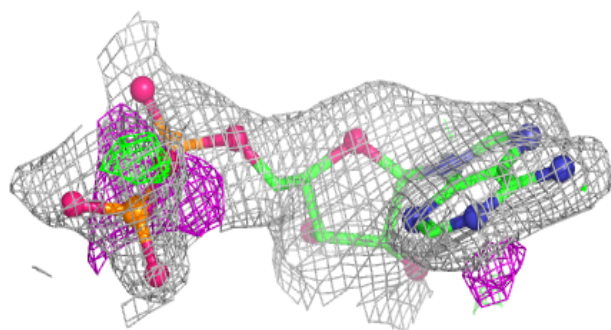
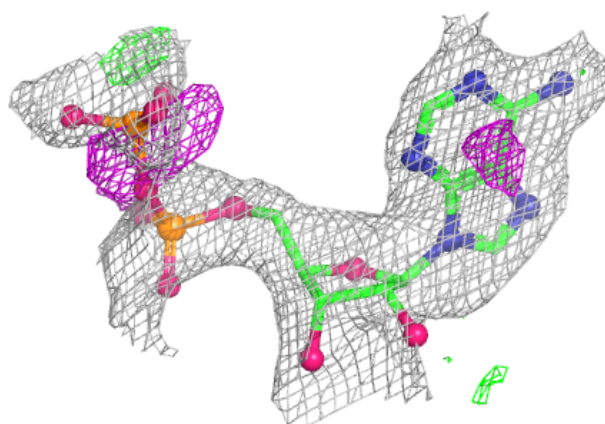
Electron density around ADP B 101:

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

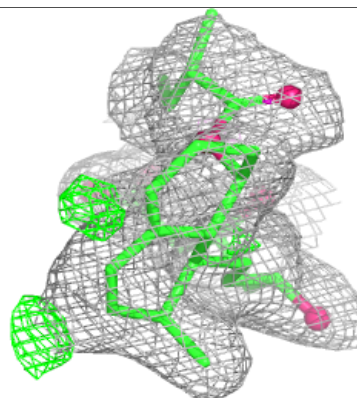
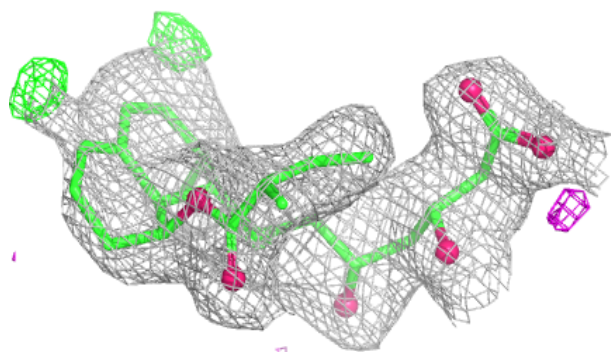
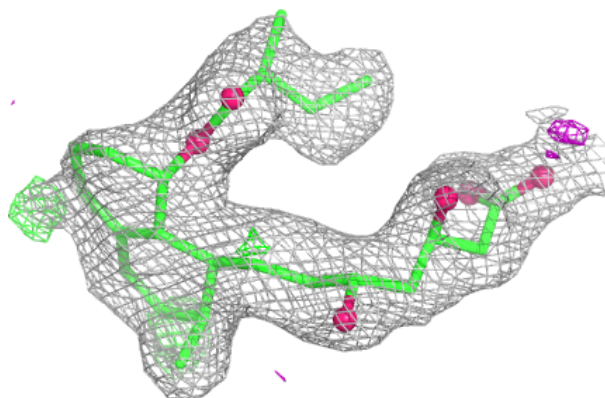


Electron density around ADP D 102:

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

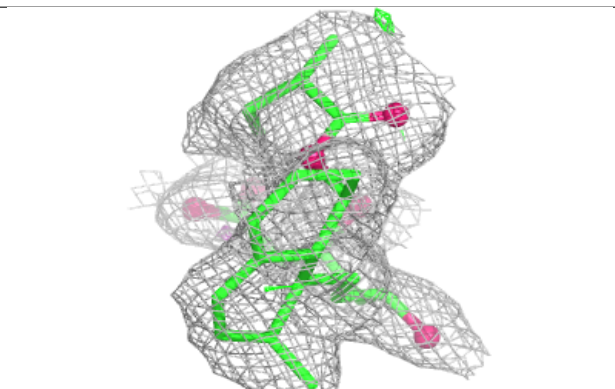
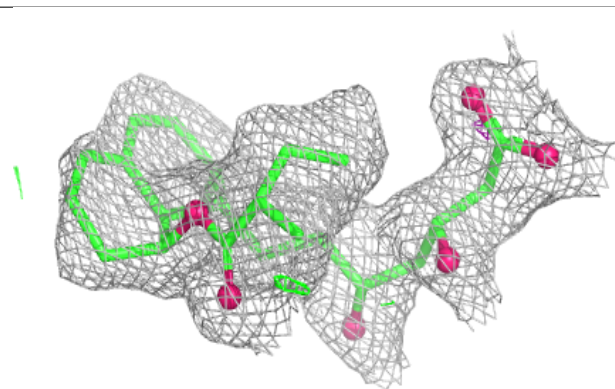
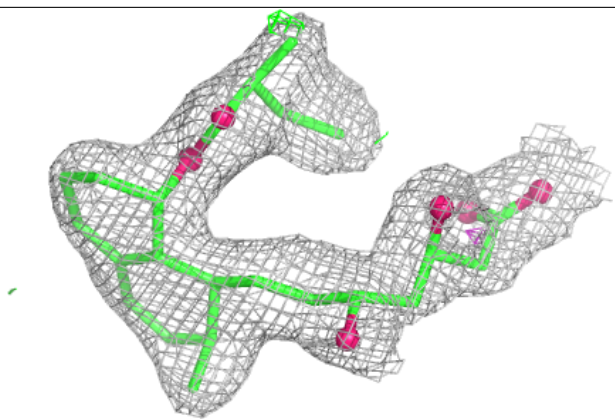
**Electron density around 114 C 4:**

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



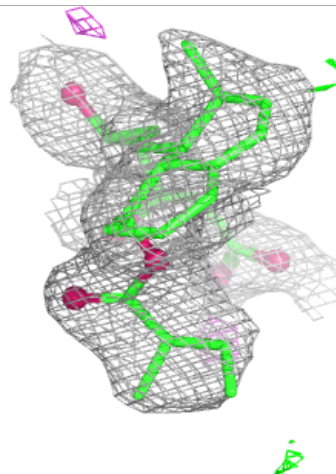
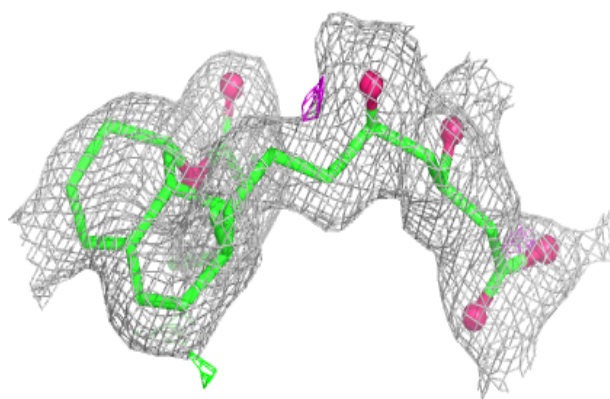
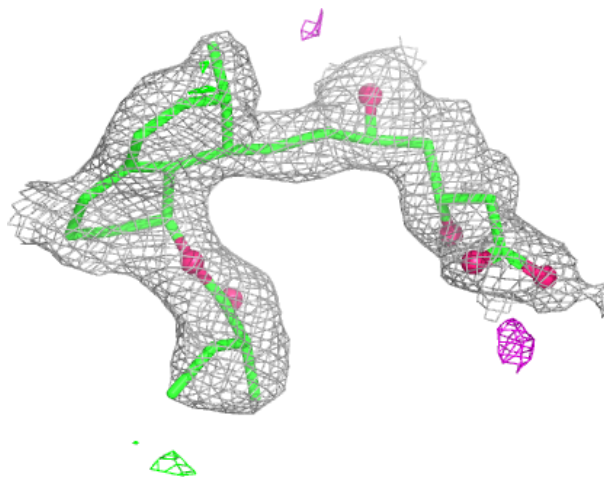
Electron density around 114 B 1:

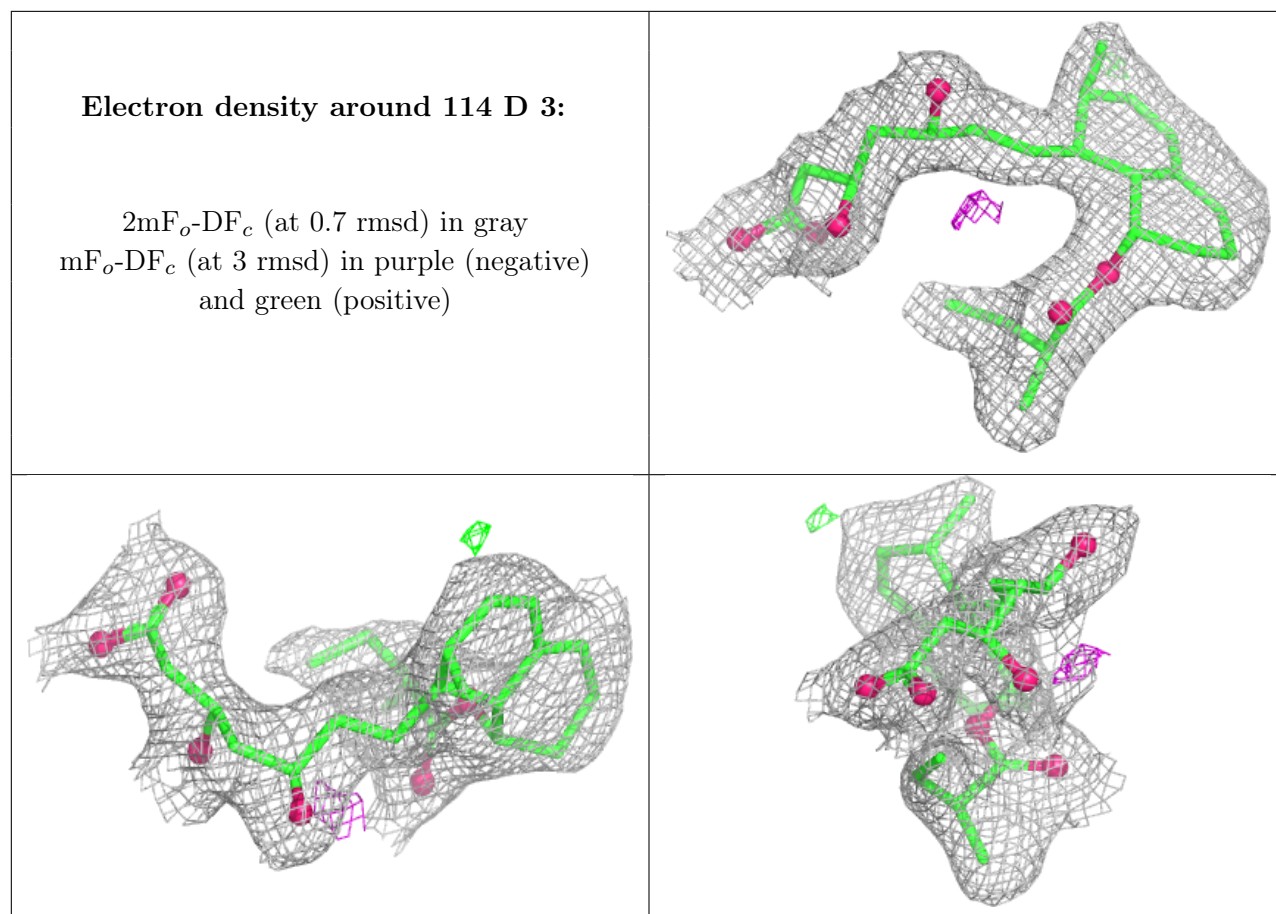
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 114 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.