



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:20 AM UTC

PDB ID : 1HWI / pdb_00001hwi
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH FLUVASTATIN
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.30 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

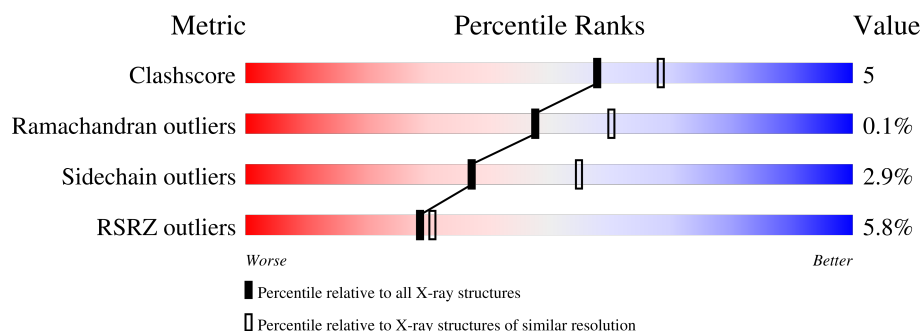
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	6% 72% 11% • 16%
1	B	467	7% 75% 10% • 15%
1	C	467	3% 69% 10% • 20%
1	D	467	3% 70% 9% • 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11798 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.

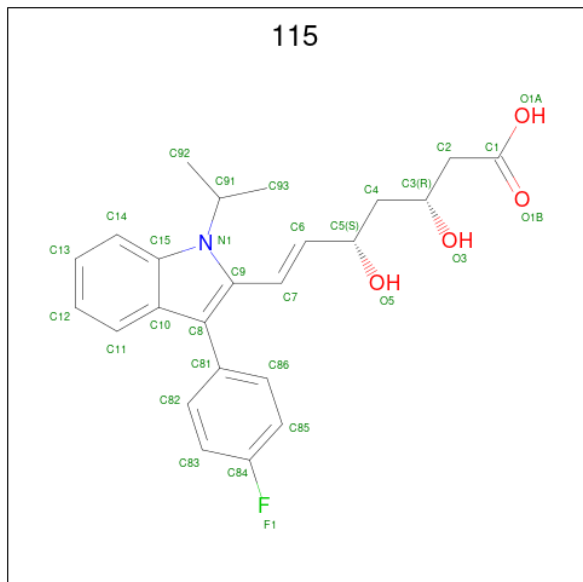
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			2913	1812	511	561	29			
1	B	399	Total	C	N	O	S	0	0	0
			2960	1844	519	568	29			
1	C	374	Total	C	N	O	S	0	0	0
			2763	1717	488	529	29			
1	D	374	Total	C	N	O	S	0	0	0
			2762	1715	488	530	29			

There are 20 discrepancies between the modelled and reference sequences:

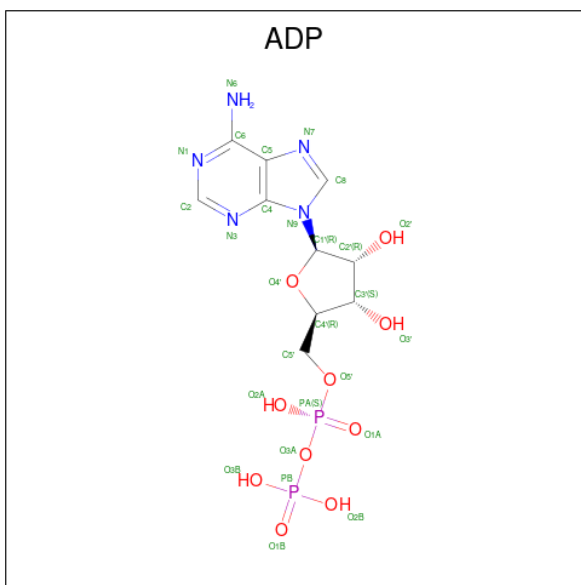
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	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,5S,6E)-7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1H-indol-2-yl]-3,5-dihydroxy hept-6-enoic acid (CCD ID: 115) (formula: $C_{24}H_{26}FNO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	24	1	1	4		
2	B	1	Total	C	F	N	O	0	0
			30	24	1	1	4		
2	C	1	Total	C	F	N	O	0	0
			30	24	1	1	4		
2	D	1	Total	C	F	N	O	0	0
			30	24	1	1	4		

- 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 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

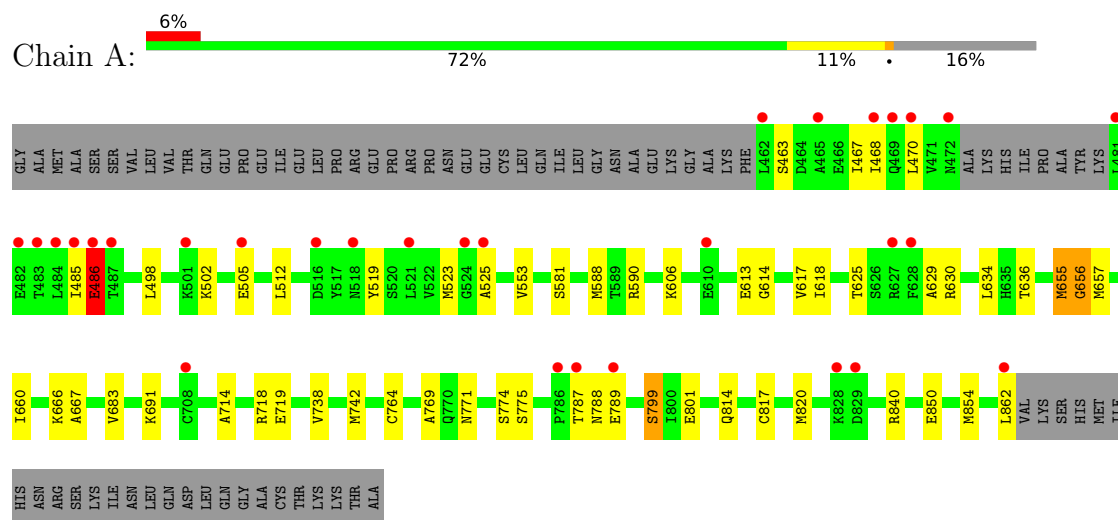
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0
4	B	54	Total O 54 54	0	0
4	C	44	Total O 44 44	0	0
4	D	51	Total O 51 51	0	0

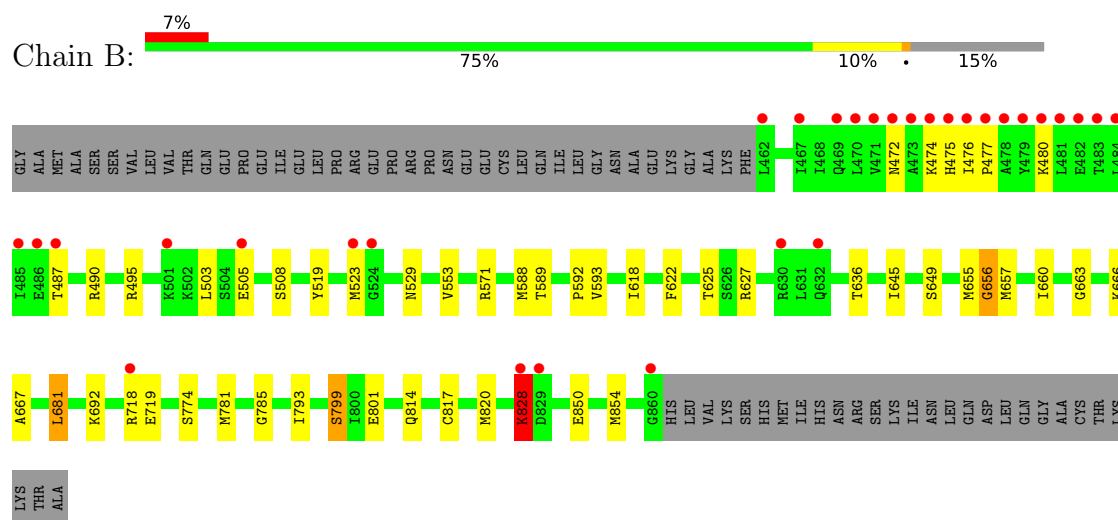
3 Residue-property plots [i](#)

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

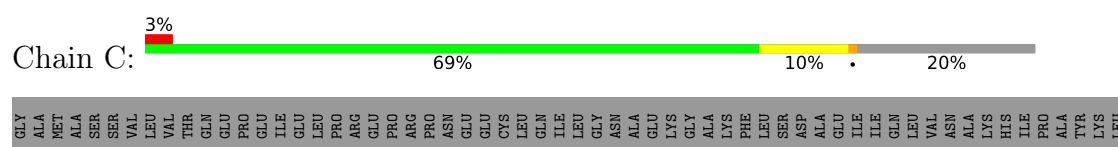
• Molecule 1: HMG-COA REDUCTASE

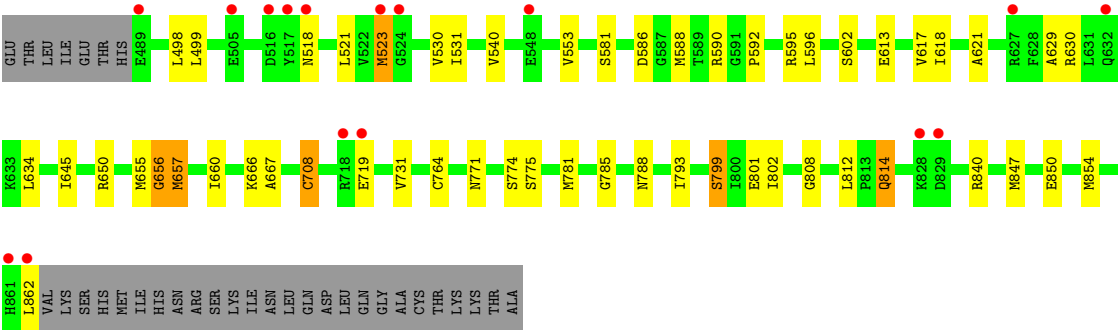


• Molecule 1: HMG-COA REDUCTASE

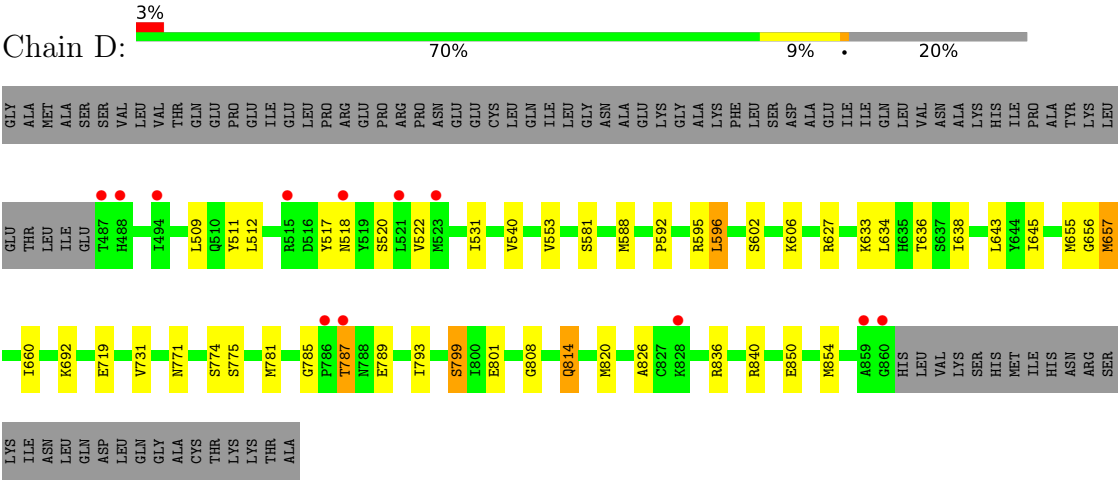


• Molecule 1: HMG-COA REDUCTASE





● 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	74.77Å 175.06Å 74.84Å 90.00° 118.25° 90.00°	Depositor
Resolution (Å)	43.77 – 2.30 43.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.77-2.30) 96.3 (43.77-2.30)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.214 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.024 for h,-k,-h-l 0.024 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11798	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: 115, 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	0.52	0/2952	0.94	8/3991 (0.2%)
1	B	0.56	0/3002	0.97	10/4060 (0.2%)
1	C	0.52	0/2802	0.95	8/3787 (0.2%)
1	D	0.55	0/2801	0.95	9/3786 (0.2%)
All	All	0.54	0/11557	0.95	35/15624 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	553	VAL	N-CA-C	9.99	117.85	107.76
1	A	553	VAL	N-CA-C	9.64	117.49	107.76
1	B	553	VAL	N-CA-C	9.34	117.19	107.76
1	D	553	VAL	N-CA-C	8.95	116.80	107.76
1	B	785	GLY	CA-C-N	8.32	128.81	119.32
1	B	785	GLY	C-N-CA	8.32	128.81	119.32
1	C	785	GLY	CA-C-N	7.91	128.33	119.32
1	C	785	GLY	C-N-CA	7.91	128.33	119.32
1	D	656	GLY	N-CA-C	7.52	124.69	114.92
1	B	656	GLY	N-CA-C	7.03	125.02	115.32
1	C	656	GLY	N-CA-C	6.98	124.96	115.32
1	A	505	GLU	CA-C-N	6.92	127.50	119.47
1	A	505	GLU	C-N-CA	6.92	127.50	119.47
1	A	656	GLY	N-CA-C	6.89	124.82	115.32
1	B	655	MET	N-CA-C	-6.13	104.60	111.28
1	D	719	GLU	N-CA-C	6.05	119.14	111.69
1	A	655	MET	N-CA-C	-5.89	104.86	111.28
1	B	505	GLU	CA-C-N	5.80	125.66	119.28
1	B	505	GLU	C-N-CA	5.80	125.66	119.28
1	B	719	GLU	N-CA-C	5.80	118.82	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	719	GLU	N-CA-C	5.76	118.77	111.69
1	A	719	GLU	N-CA-C	5.73	118.74	111.69
1	C	655	MET	N-CA-C	-5.72	105.14	111.71
1	C	764	CYS	N-CA-C	5.46	118.94	112.72
1	D	785	GLY	CA-C-N	5.45	126.66	119.84
1	D	785	GLY	C-N-CA	5.45	126.66	119.84
1	D	655	MET	N-CA-C	-5.41	105.39	111.28
1	A	764	CYS	N-CA-C	5.32	118.78	112.72
1	B	799	SER	N-CA-C	5.28	119.28	109.56
1	C	799	SER	N-CA-C	5.25	119.23	109.56
1	D	512	LEU	CA-C-N	5.25	125.19	119.78
1	D	512	LEU	C-N-CA	5.25	125.19	119.78
1	B	828	LYS	N-CA-C	5.09	117.22	111.11
1	A	799	SER	N-CA-C	5.08	118.90	109.56
1	D	799	SER	N-CA-C	5.02	118.80	109.56

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	2913	0	2947	24	0
1	B	2960	0	3000	30	0
1	C	2763	0	2795	29	0
1	D	2762	0	2791	24	0
2	A	30	0	25	1	0
2	B	30	0	25	1	0
2	C	30	0	25	1	0
2	D	30	0	25	0	0
3	B	54	0	24	1	0
3	D	27	0	12	2	0
4	A	50	0	0	0	0
4	B	54	0	0	0	0
4	C	44	0	0	1	0
4	D	51	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11798	0	11669	105	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 5.

All (105) 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:HG21	1:B:663:GLY:HA2	1.57	0.87
1:B:625:THR:HG22	1:B:666:LYS:HD2	1.60	0.82
1:A:655:MET:SD	1:A:657:MET:HG2	2.25	0.77
1:C:708:CYS:SG	1:C:847:MET:SD	2.84	0.75
1:A:581:SER:OG	1:A:840:ARG:HD2	1.92	0.70
1:B:657:MET:HE3	1:B:657:MET:HA	1.74	0.68
1:A:656:GLY:O	1:A:660:ILE:HG12	1.98	0.64
1:D:657:MET:HE2	1:D:657:MET:HA	1.80	0.64
1:D:581:SER:OG	1:D:840:ARG:HD2	1.98	0.63
1:C:581:SER:OG	1:C:840:ARG:HD2	1.98	0.63
1:C:657:MET:HA	1:C:657:MET:HE2	1.81	0.63
1:D:826:ALA:HB1	3:D:103:ADP:HN61	1.64	0.62
1:D:588:MET:HE1	1:D:801:GLU:HG2	1.83	0.60
1:D:638:ILE:HG22	1:D:643:LEU:HD13	1.83	0.60
1:B:656:GLY:O	1:B:660:ILE:HG12	2.04	0.58
1:A:519:TYR:O	1:A:523:MET:HG2	2.03	0.58
1:B:622:PHE:O	1:B:625:THR:HG23	2.03	0.58
1:C:588:MET:HE1	1:C:801:GLU:HG2	1.85	0.57
1:A:787:THR:HB	1:A:789:GLU:HG2	1.86	0.57
1:B:495:ARG:HD2	1:B:529:ASN:HD22	1.70	0.56
1:A:485:ILE:HG22	1:A:486:GLU:N	2.22	0.55
1:C:596:LEU:HD13	1:C:602:SER:HA	1.90	0.54
1:B:649:SER:HB3	1:B:660:ILE:HD12	1.91	0.52
1:B:589:THR:O	1:B:657:MET:HE1	2.08	0.52
1:D:781:MET:HE2	1:D:793:ILE:HD12	1.92	0.52
1:C:523:MET:HE1	1:C:530:VAL:HG23	1.91	0.51
1:B:519:TYR:O	1:B:523:MET:HG2	2.11	0.50
1:C:781:MET:HE2	1:C:793:ILE:HD12	1.93	0.50
1:B:625:THR:HG21	1:B:663:GLY:CA	2.37	0.50
1:B:850:GLU:O	1:B:854:MET:HG2	2.12	0.50
1:C:708:CYS:SG	1:C:847:MET:CE	3.00	0.50
1:C:771:ASN:ND2	1:C:775:SER:OG	2.44	0.49
2:B:1:115:H21	2:B:1:115:H1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:GLY:O	1:C:660:ILE:HD13	2.12	0.49
1:D:771:ASN:ND2	1:D:775:SER:OG	2.45	0.49
1:A:817:CYS:HA	1:A:820:MET:HE3	1.92	0.49
1:B:477:PRO:HD2	1:B:480:LYS:HD2	1.93	0.49
1:A:618:ILE:HG23	1:A:667:ALA:HB1	1.95	0.49
1:A:463:SER:O	1:A:467:ILE:HG13	2.13	0.48
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.95	0.48
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.44	0.48
1:A:588:MET:HE1	1:A:801:GLU:HG2	1.95	0.48
1:A:771:ASN:ND2	1:A:775:SER:OG	2.47	0.47
1:D:836:ARG:NH1	4:D:1188:HOH:O	2.47	0.47
1:A:629:ALA:C	1:A:630:ARG:HD2	2.40	0.47
1:D:596:LEU:HD13	1:D:602:SER:HA	1.96	0.47
1:A:468:ILE:HG12	1:A:498:LEU:HD11	1.96	0.47
1:A:738:VAL:O	1:A:742:MET:HG2	2.15	0.47
1:C:531:ILE:HD13	1:D:540:VAL:CG2	2.46	0.46
1:C:613:GLU:O	1:C:617:VAL:HG23	2.16	0.46
1:D:517:TYR:HE2	1:D:522:VAL:HG21	1.80	0.46
1:B:487:THR:HG23	1:B:490:ARG:CB	2.46	0.46
1:A:590:ARG:HA	1:A:590:ARG:HD3	1.82	0.45
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.85	0.45
1:A:714:ALA:O	1:A:718:ARG:HG3	2.17	0.45
1:C:618:ILE:HG23	1:C:667:ALA:HB1	1.99	0.45
1:A:774:SER:HA	1:A:799:SER:O	2.17	0.45
1:D:787:THR:HB	1:D:789:GLU:CG	2.47	0.45
1:B:571:ARG:HG3	1:B:571:ARG:HH11	1.81	0.44
1:A:683:VAL:HG13	2:A:2:115:F1	2.06	0.44
1:C:499:LEU:HD21	1:D:820:MET:HE3	1.99	0.44
1:A:691:LYS:HE2	1:A:769:ALA:HB3	1.98	0.44
1:C:629:ALA:O	1:C:630:ARG:HD3	2.17	0.44
1:C:812:LEU:HD13	1:D:511:TYR:CE2	2.53	0.44
1:A:606:LYS:HG3	1:A:636:THR:OG1	2.18	0.44
1:B:593:VAL:HG13	1:B:681:LEU:HB3	1.98	0.44
1:C:808:GLY:O	1:C:814:GLN:HG3	2.18	0.44
1:D:774:SER:HA	1:D:799:SER:O	2.16	0.44
1:A:625:THR:CG2	1:A:666:LYS:HG3	2.49	0.43
1:B:781:MET:HE2	1:B:793:ILE:HD12	2.01	0.43
1:C:518:ASN:ND2	1:C:521:LEU:HD13	2.33	0.43
1:C:657:MET:HA	1:C:657:MET:CE	2.49	0.43
1:C:774:SER:HA	1:C:799:SER:O	2.18	0.43
1:C:540:VAL:CG2	1:D:531:ILE:HD13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:LYS:N	1:B:828:LYS:HD2	2.33	0.42
1:B:588:MET:HE1	1:B:801:GLU:HG2	2.00	0.42
1:D:636:THR:HB	1:D:643:LEU:HD11	2.01	0.42
1:D:692:LYS:HE2	1:D:692:LYS:HB2	1.90	0.42
1:D:850:GLU:O	1:D:854:MET:HG2	2.20	0.42
1:B:774:SER:HA	1:B:799:SER:O	2.19	0.42
1:C:586:ASP:HB3	1:C:650:ARG:HH12	1.85	0.42
1:B:571:ARG:HG3	1:B:571:ARG:NH1	2.35	0.42
1:B:627:ARG:HH22	3:B:102:ADP:PA	2.43	0.42
1:C:731:VAL:HG12	1:C:854:MET:HE1	2.02	0.41
1:D:592:PRO:HD2	1:D:645:ILE:O	2.20	0.41
2:C:4:115:H1	2:C:4:115:H21	2.01	0.41
1:A:850:GLU:O	1:A:854:MET:HG2	2.20	0.41
1:B:592:PRO:HD2	1:B:645:ILE:O	2.20	0.41
1:B:817:CYS:HA	1:B:820:MET:HE3	2.03	0.41
1:A:614:GLY:O	1:A:617:VAL:HG22	2.19	0.41
1:B:692:LYS:HE2	1:B:692:LYS:HB2	1.90	0.41
1:D:826:ALA:CB	3:D:103:ADP:HN61	2.31	0.41
1:C:850:GLU:O	1:C:854:MET:HG2	2.20	0.41
1:B:472:ASN:C	1:B:474:LYS:H	2.28	0.41
1:C:799:SER:HB2	4:C:1186:HOH:O	2.21	0.41
1:D:606:LYS:HG3	1:D:636:THR:OG1	2.21	0.41
1:A:485:ILE:CG2	1:A:486:GLU:N	2.83	0.41
1:B:503:LEU:HD13	1:B:508:SER:OG	2.21	0.41
1:C:592:PRO:HD2	1:C:645:ILE:O	2.20	0.41
1:D:731:VAL:HG12	1:D:854:MET:HE1	2.02	0.41
1:B:636:THR:HG22	1:B:645:ILE:HG23	2.03	0.41
1:D:808:GLY:O	1:D:814:GLN:HG3	2.21	0.41
1:B:475:HIS:HB2	1:B:476:ILE:HD12	2.03	0.40
1:C:621:ALA:O	1:C:666:LYS:HD3	2.21	0.40
1:B:618:ILE:HG23	1:B:667:ALA:HB1	2.03	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	389/467 (83%)	374 (96%)	13 (3%)	2 (0%)	24	31
1	B	397/467 (85%)	379 (96%)	18 (4%)	0	100	100
1	C	372/467 (80%)	359 (96%)	13 (4%)	0	100	100
1	D	372/467 (80%)	357 (96%)	15 (4%)	0	100	100
All	All	1530/1868 (82%)	1469 (96%)	59 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	A	525	ALA

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	313/375 (84%)	304 (97%)	9 (3%)	37	55
1	B	317/375 (84%)	313 (99%)	4 (1%)	61	77
1	C	295/375 (79%)	285 (97%)	10 (3%)	32	49
1	D	295/375 (79%)	283 (96%)	12 (4%)	27	41
All	All	1220/1500 (81%)	1185 (97%)	35 (3%)	37	55

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	LEU
1	A	486	GLU
1	A	502	LYS
1	A	512	LEU
1	A	613	GLU
1	A	634	LEU

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Mol	Chain	Res	Type
1	A	788	ASN
1	A	814	GLN
1	A	862	LEU
1	B	681	LEU
1	B	718	ARG
1	B	814	GLN
1	B	828	LYS
1	C	498	LEU
1	C	523	MET
1	C	595	ARG
1	C	634	LEU
1	C	657	MET
1	C	708	CYS
1	C	788	ASN
1	C	802	ILE
1	C	814	GLN
1	C	862	LEU
1	D	509	LEU
1	D	518	ASN
1	D	520	SER
1	D	595	ARG
1	D	596	LEU
1	D	627	ARG
1	D	633	LYS
1	D	634	LEU
1	D	657	MET
1	D	660	ILE
1	D	787	THR
1	D	814	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	472	ASN
1	A	488	HIS
1	A	497	GLN
1	A	510	GLN
1	A	635	HIS
1	A	648	GLN
1	A	771	ASN
1	A	788	ASN

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Mol	Chain	Res	Type
1	A	819	GLN
1	B	472	ASN
1	B	475	HIS
1	B	488	HIS
1	B	529	ASN
1	B	635	HIS
1	B	648	GLN
1	B	770	GLN
1	B	771	ASN
1	B	819	GLN
1	C	648	GLN
1	C	672	HIS
1	C	736	ASN
1	C	770	GLN
1	C	771	ASN
1	C	788	ASN
1	D	635	HIS
1	D	672	HIS
1	D	736	ASN
1	D	771	ASN
1	D	788	ASN
1	D	819	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	115	B	1	-	32,32,32	1.81	4 (12%)	40,45,45	1.64	4 (10%)
2	115	D	3	-	32,32,32	1.89	6 (18%)	40,45,45	1.64	5 (12%)
3	ADP	D	103	-	28,29,29	1.44	4 (14%)	43,45,45	0.87	1 (2%)
3	ADP	B	102	-	28,29,29	1.46	5 (17%)	43,45,45	0.72	0
2	115	C	4	-	32,32,32	1.85	6 (18%)	40,45,45	1.65	6 (15%)
2	115	A	2	-	32,32,32	1.87	4 (12%)	40,45,45	1.64	5 (12%)
3	ADP	B	101	-	28,29,29	1.41	4 (14%)	43,45,45	0.71	1 (2%)

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	115	B	1	-	-	1/21/21/21	0/3/3/3
2	115	D	3	-	-	2/21/21/21	0/3/3/3
3	ADP	D	103	-	-	6/16/32/32	0/3/3/3
3	ADP	B	102	-	-	5/16/32/32	0/3/3/3
2	115	C	4	-	-	2/21/21/21	0/3/3/3
2	115	A	2	-	-	2/21/21/21	0/3/3/3
3	ADP	B	101	-	-	4/16/32/32	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	115	C15-N1	-6.25	1.29	1.40
2	B	1	115	C15-N1	-6.01	1.29	1.40
2	A	2	115	C15-N1	-5.80	1.30	1.40
2	C	4	115	C15-N1	-5.70	1.30	1.40
2	C	4	115	C7-C9	-4.23	1.35	1.44
3	B	101	ADP	PA-O3A	4.11	1.63	1.59
2	A	2	115	C91-N1	3.84	1.54	1.48
3	B	102	ADP	PA-O3A	3.73	1.63	1.59
3	D	103	ADP	PA-O3A	3.69	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	115	C7-C9	-3.61	1.37	1.44
2	A	2	115	C7-C9	-3.56	1.37	1.44
2	D	3	115	C9-N1	3.49	1.47	1.39
2	C	4	115	C91-N1	3.41	1.53	1.48
2	D	3	115	C7-C9	-3.37	1.37	1.44
2	B	1	115	C9-N1	3.31	1.46	1.39
2	C	4	115	C9-N1	3.24	1.46	1.39
2	D	3	115	C91-N1	3.16	1.53	1.48
2	A	2	115	C9-N1	3.08	1.46	1.39
3	D	103	ADP	C1'-N9	2.87	1.54	1.46
3	B	102	ADP	C1'-N9	2.84	1.54	1.46
3	D	103	ADP	O4'-C4'	2.76	1.51	1.45
3	B	102	ADP	O4'-C4'	2.71	1.51	1.45
2	B	1	115	C91-N1	2.70	1.52	1.48
3	B	102	ADP	C8-N9	-2.65	1.33	1.37
3	B	101	ADP	C1'-N9	2.59	1.53	1.46
3	B	101	ADP	C8-N9	-2.52	1.33	1.37
3	D	103	ADP	C8-N9	-2.36	1.33	1.37
3	B	101	ADP	O4'-C4'	2.30	1.50	1.45
2	D	3	115	C83-C84	2.26	1.41	1.37
2	D	3	115	C81-C8	2.18	1.53	1.49
2	C	4	115	C83-C84	2.13	1.41	1.37
2	C	4	115	C10-C15	-2.13	1.38	1.41
3	B	102	ADP	C2'-C3'	2.13	1.59	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	115	C10-C8-C9	-6.13	101.19	106.59
2	D	3	115	C10-C8-C9	-6.13	101.19	106.59
2	A	2	115	C10-C8-C9	-5.88	101.41	106.59
2	C	4	115	C10-C8-C9	-5.69	101.58	106.59
2	A	2	115	C8-C9-N1	5.01	112.11	109.38
2	B	1	115	C8-C9-N1	4.72	111.95	109.38
2	C	4	115	C8-C9-N1	4.58	111.88	109.38
2	D	3	115	C8-C9-N1	4.57	111.87	109.38
2	B	1	115	C81-C8-C9	2.78	130.78	127.23
2	C	4	115	C81-C8-C9	2.72	130.70	127.23
2	A	2	115	C81-C8-C9	2.38	130.27	127.23
3	D	103	ADP	O4'-C1'-N9	2.36	112.62	108.09
2	C	4	115	C11-C10-C15	2.26	121.85	119.24
2	D	3	115	C10-C8-C81	2.22	128.94	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	115	C11-C10-C15	2.21	121.79	119.24
2	B	1	115	C14-C15-C10	-2.16	119.54	121.95
2	A	2	115	C14-C15-C10	-2.15	119.55	121.95
3	B	101	ADP	C4-N9-C8	2.11	107.95	105.74
2	C	4	115	C14-C15-C10	-2.08	119.63	121.95
2	D	3	115	C81-C8-C9	2.07	129.87	127.23
2	D	3	115	C85-C84-C83	-2.05	120.11	122.80
2	C	4	115	C15-N1-C9	-2.02	107.00	108.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	101	ADP	PA-O3A-PB-O2B
3	D	103	ADP	PA-O3A-PB-O3B
3	D	103	ADP	C3'-C4'-C5'-O5'
3	D	103	ADP	O4'-C4'-C5'-O5'
3	D	103	ADP	PA-O3A-PB-O1B
3	D	103	ADP	C4'-C5'-O5'-PA
3	B	101	ADP	C3'-C4'-C5'-O5'
3	B	102	ADP	PA-O3A-PB-O1B
3	B	101	ADP	O4'-C4'-C5'-O5'
3	B	102	ADP	O4'-C4'-C5'-O5'
3	B	102	ADP	C4'-C5'-O5'-PA
2	D	3	115	C6-C7-C9-C8
3	B	101	ADP	PA-O3A-PB-O3B
3	B	102	ADP	PA-O3A-PB-O2B
3	B	102	ADP	PA-O3A-PB-O3B
2	D	3	115	O1A-C1-C2-C3
2	B	1	115	C92-C91-N1-C9
3	D	103	ADP	O4'-C1'-N9-C8
2	A	2	115	O1A-C1-C2-C3
2	C	4	115	C92-C91-N1-C9
2	A	2	115	C6-C7-C9-C8
2	C	4	115	C6-C7-C9-C8

There are no ring outliers.

5 monomers are involved in 6 short contacts:

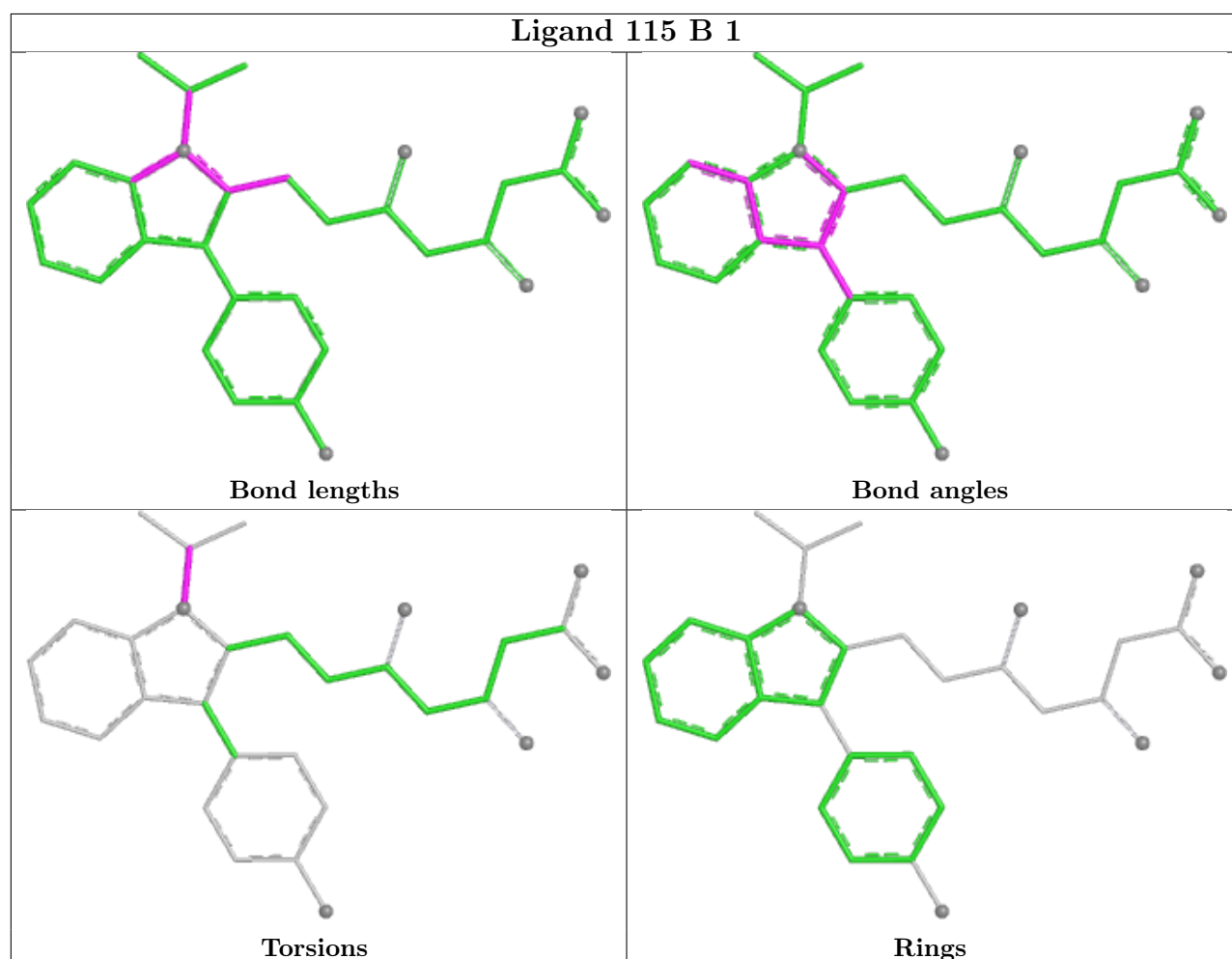
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	115	1	0

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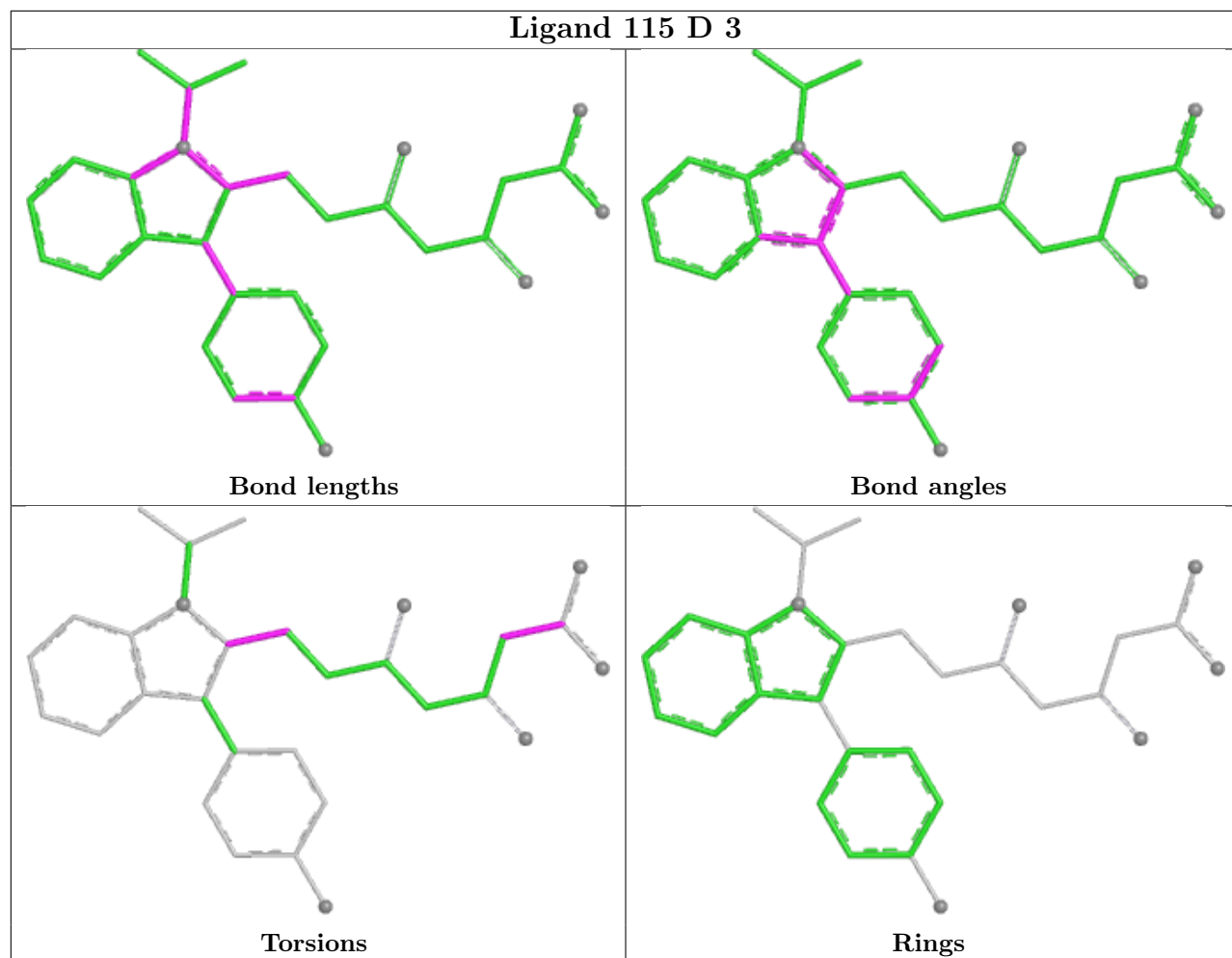
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	103	ADP	2	0
3	B	102	ADP	1	0
2	C	4	115	1	0
2	A	2	115	1	0

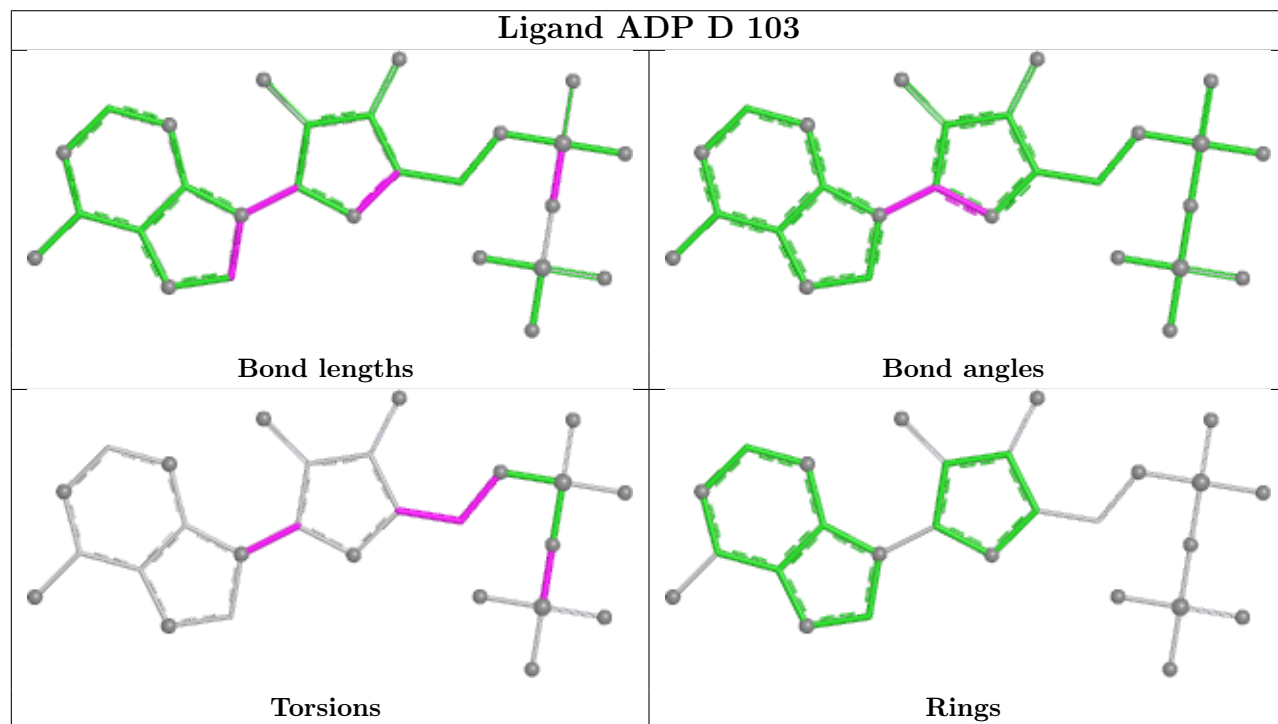
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

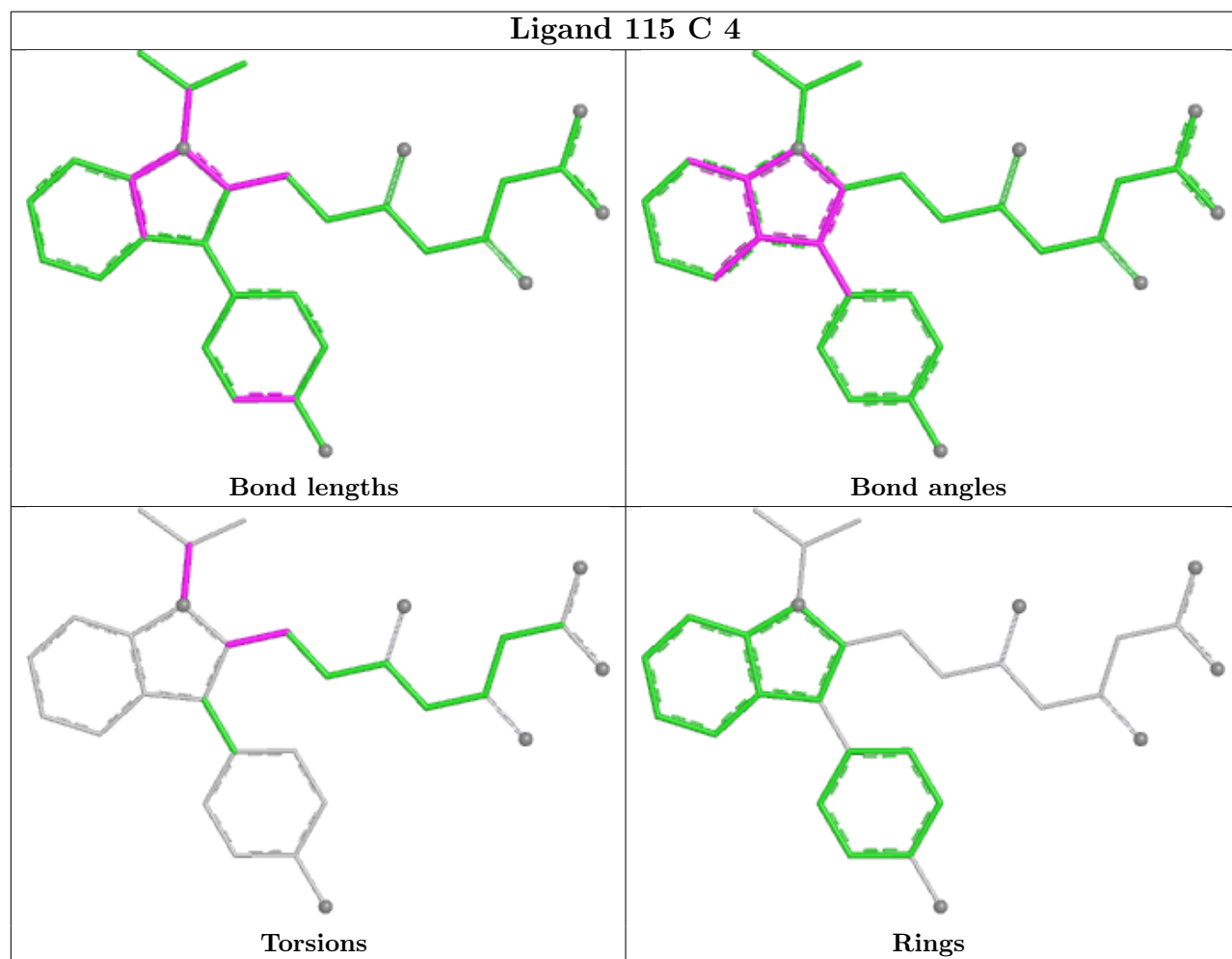
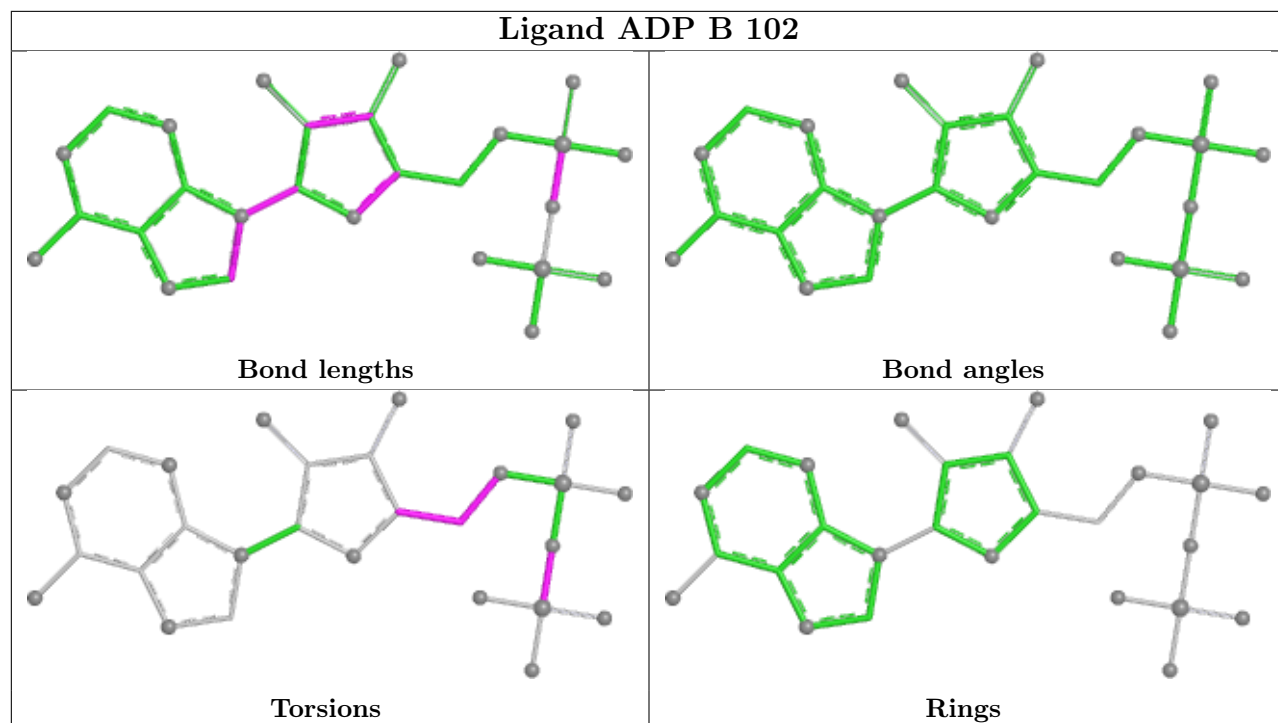


Ligand 115 D 3

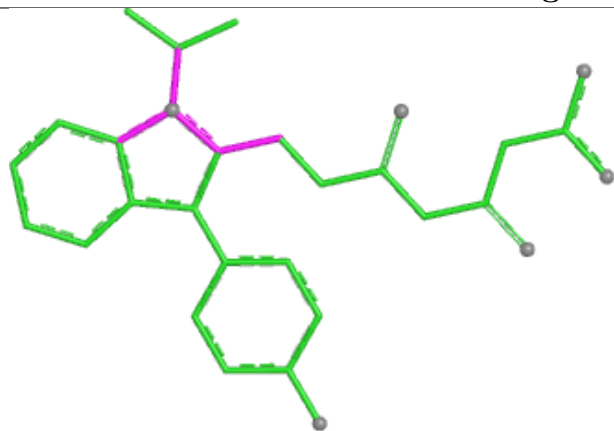


Ligand ADP D 103

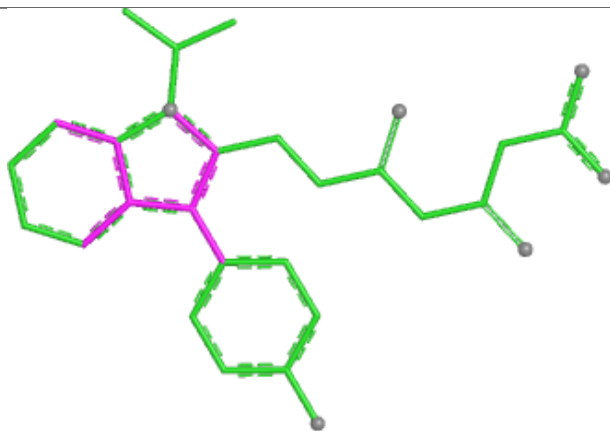




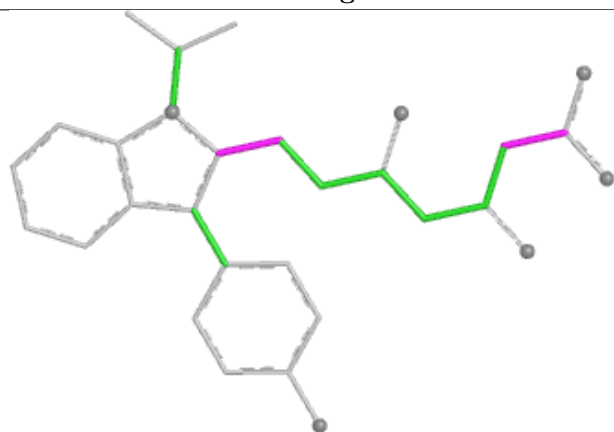
Ligand 115 A 2



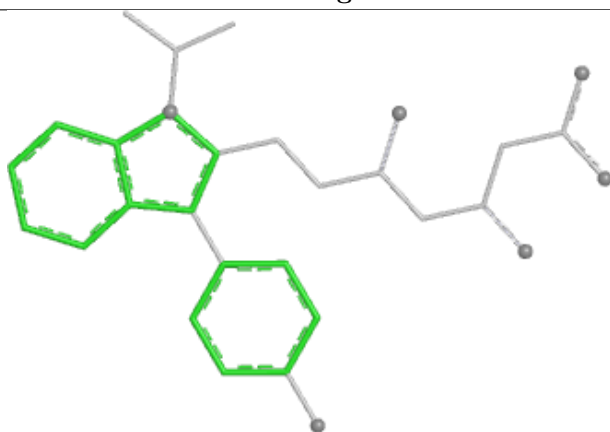
Bond lengths



Bond angles

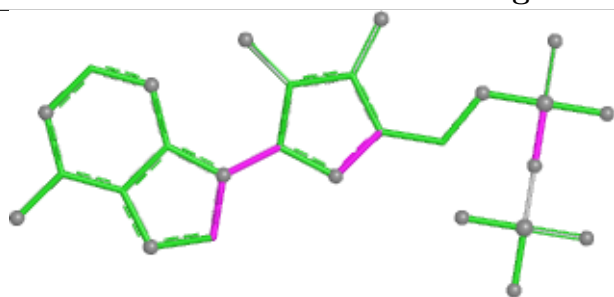


Torsions

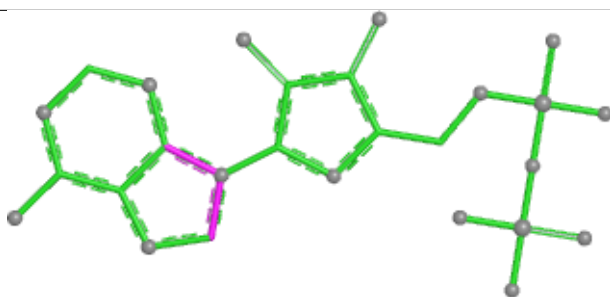


Rings

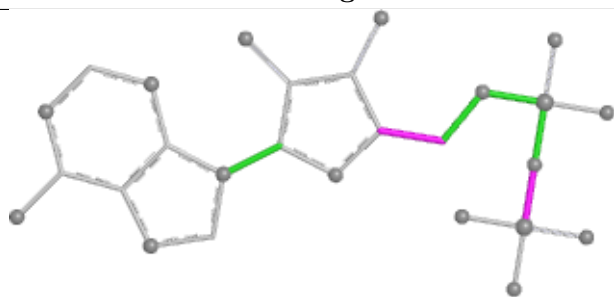
Ligand ADP B 101



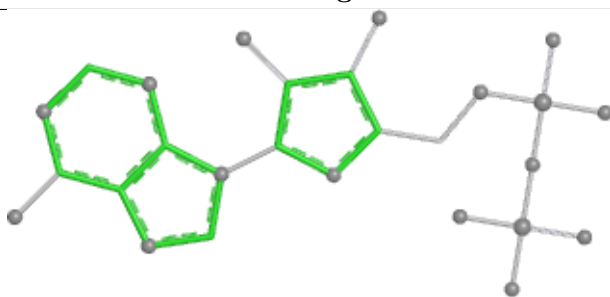
Bond lengths



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	393/467 (84%)	0.41	30 (7%) 20 21	10, 24, 56, 94	0
1	B	399/467 (85%)	0.37	31 (7%) 19 21	9, 23, 57, 97	0
1	C	374/467 (80%)	0.29	16 (4%) 40 41	10, 25, 49, 71	0
1	D	374/467 (80%)	0.18	12 (3%) 50 52	10, 22, 48, 72	0
All	All	1540/1868 (82%)	0.32	89 (5%) 29 31	9, 24, 53, 97	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	471	VAL	5.7
1	B	462	LEU	5.3
1	A	484	LEU	5.3
1	B	474	LYS	5.1
1	B	484	LEU	5.1
1	B	473	ALA	5.0
1	A	481	LEU	5.0
1	A	485	ILE	4.7
1	C	862	LEU	4.7
1	D	487	THR	4.6
1	A	487	THR	4.5
1	B	475	HIS	4.4
1	B	485	ILE	4.3
1	B	476	ILE	4.3
1	D	523	MET	4.2
1	B	487	THR	4.2
1	A	462	LEU	4.0
1	A	525	ALA	4.0
1	A	483	THR	3.9
1	B	478	ALA	3.9
1	B	477	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	787	THR	3.7
1	A	470	LEU	3.7
1	B	469	GLN	3.7
1	D	786	PRO	3.7
1	C	828	LYS	3.6
1	D	518	ASN	3.5
1	B	486	GLU	3.5
1	B	483	THR	3.5
1	B	470	LEU	3.5
1	B	472	ASN	3.4
1	B	479	TYR	3.4
1	B	482	GLU	3.3
1	A	524	GLY	3.3
1	B	630	ARG	3.3
1	A	789	GLU	3.3
1	C	516	ASP	3.3
1	B	828	LYS	3.3
1	A	786	PRO	3.1
1	D	488	HIS	3.1
1	D	860	GLY	3.0
1	A	516	ASP	2.9
1	C	489	GLU	2.9
1	C	523	MET	2.9
1	C	627	ARG	2.9
1	B	524	GLY	2.8
1	C	861	HIS	2.8
1	A	862	LEU	2.8
1	A	468	ILE	2.8
1	C	524	GLY	2.7
1	A	829	ASP	2.7
1	A	787	THR	2.6
1	A	469	GLN	2.5
1	A	486	GLU	2.5
1	B	467	ILE	2.5
1	B	829	ASP	2.5
1	D	859	ALA	2.5
1	B	480	LYS	2.5
1	A	472	ASN	2.5
1	D	515	ARG	2.4
1	B	860	GLY	2.4
1	A	627	ARG	2.4
1	A	482	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	610	GLU	2.4
1	C	548	GLU	2.3
1	C	719	GLU	2.3
1	A	465	ALA	2.3
1	B	501	LYS	2.3
1	D	494	ILE	2.3
1	A	521	LEU	2.3
1	B	481	LEU	2.3
1	D	828	LYS	2.3
1	C	517	TYR	2.3
1	A	505	GLU	2.3
1	A	501	LYS	2.3
1	C	829	ASP	2.2
1	C	718	ARG	2.2
1	D	521	LEU	2.2
1	C	505	GLU	2.2
1	B	505	GLU	2.2
1	C	518	ASN	2.1
1	B	632	GLN	2.1
1	A	828	LYS	2.1
1	C	632	GLN	2.1
1	A	708	CYS	2.0
1	A	518	ASN	2.0
1	B	718	ARG	2.0
1	A	628	PHE	2.0
1	B	523	MET	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](#)

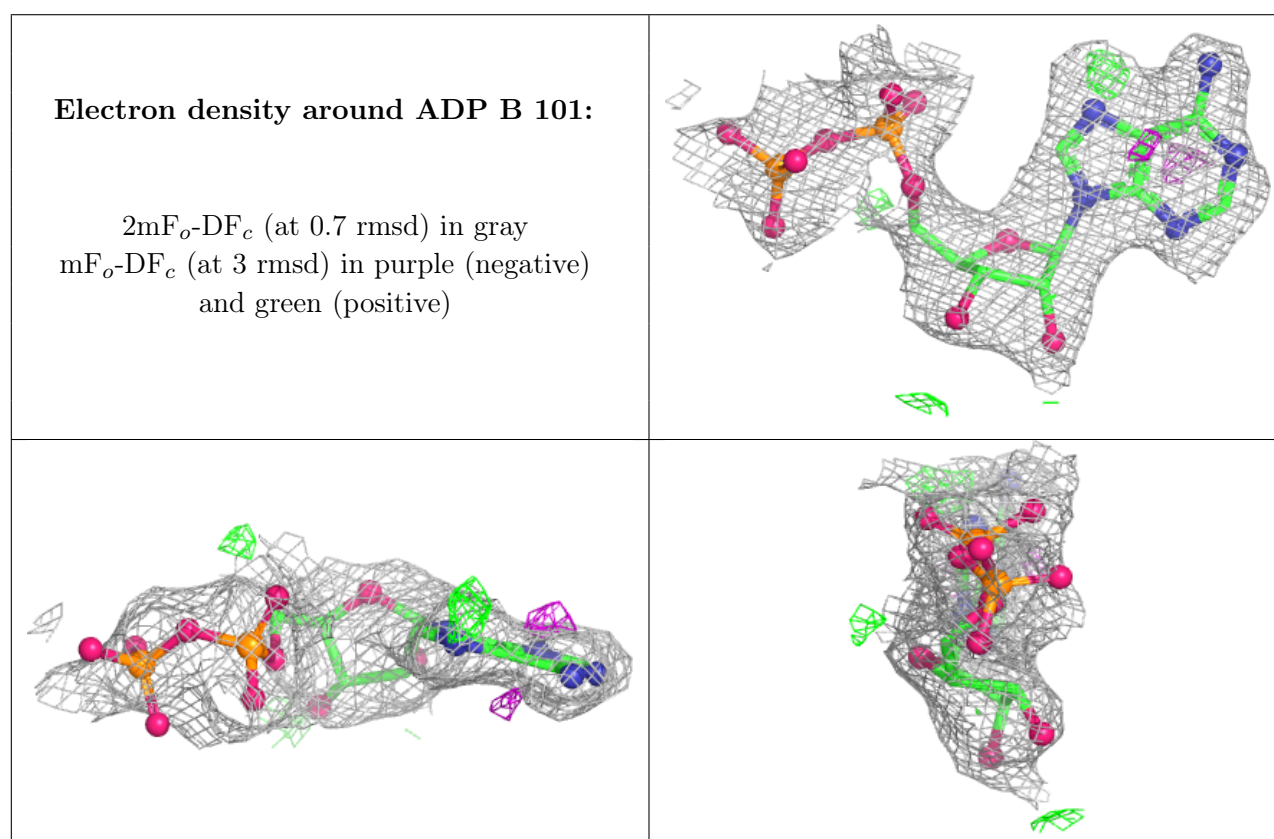
There are no oligosaccharides in this entry.

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.

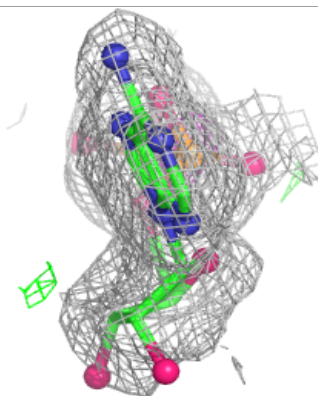
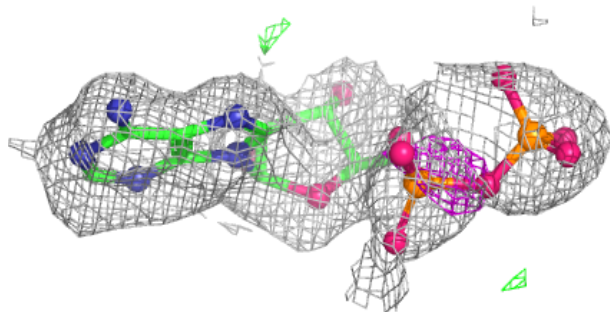
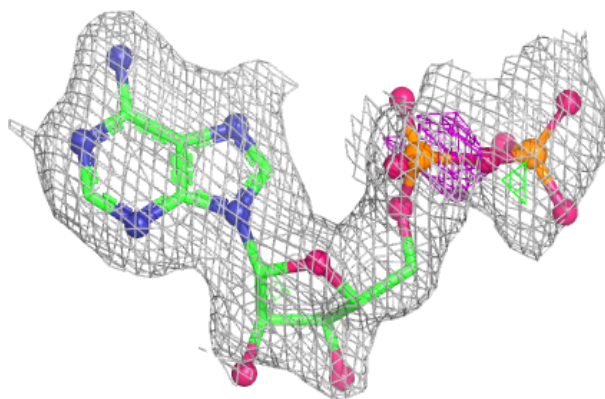
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	101	27/27	0.72	0.15	45,61,94,95	0
3	ADP	B	102	27/27	0.82	0.15	31,58,76,76	0
3	ADP	D	103	27/27	0.84	0.14	33,48,71,73	0
2	115	C	4	30/30	0.91	0.10	18,24,34,43	0
2	115	D	3	30/30	0.92	0.09	19,25,33,37	0
2	115	A	2	30/30	0.93	0.09	18,24,31,34	0
2	115	B	1	30/30	0.95	0.08	14,22,34,43	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.

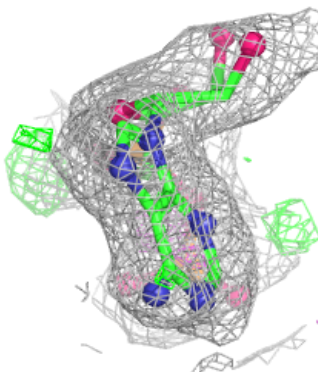
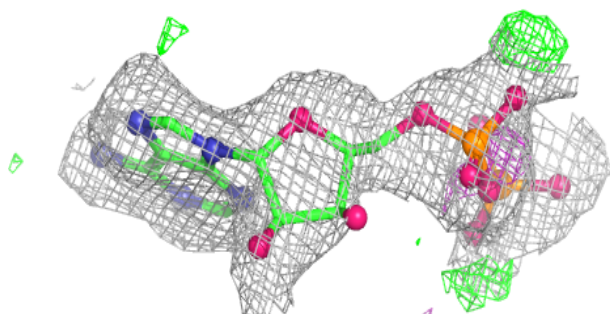
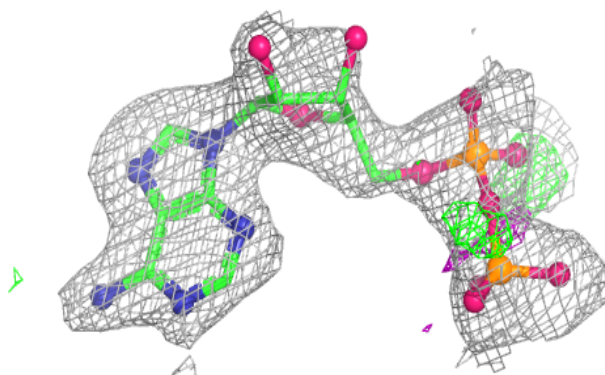


Electron density around ADP B 102:

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

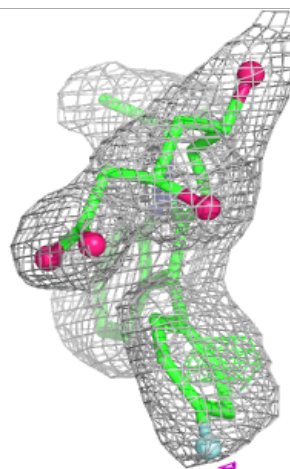
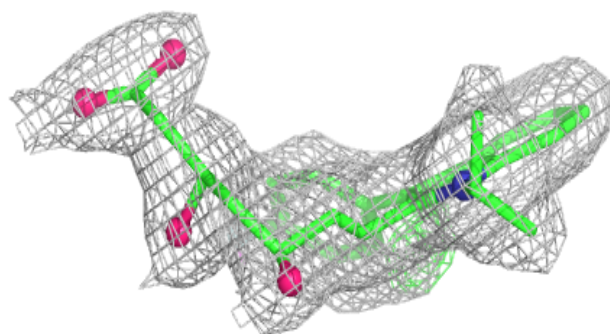
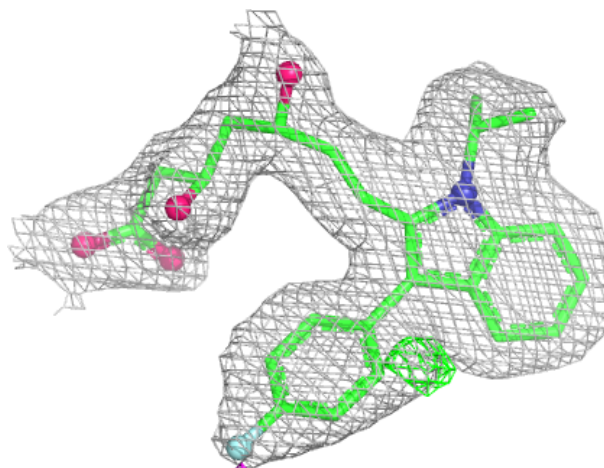
**Electron density around ADP D 103:**

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



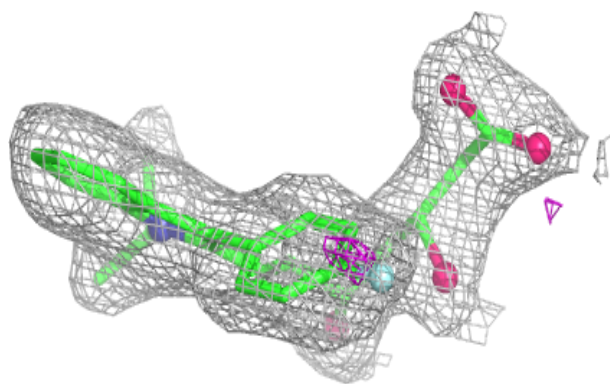
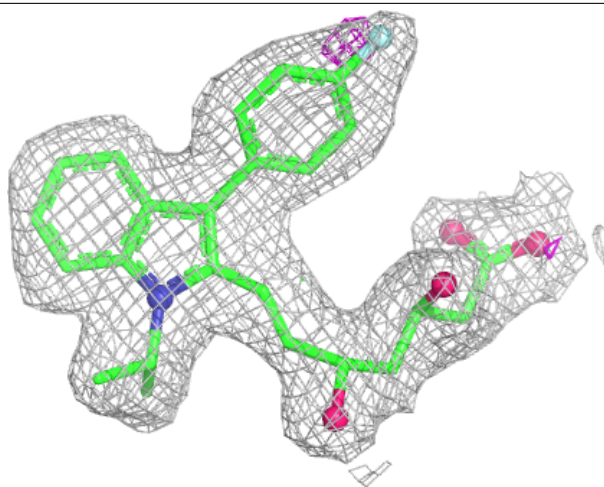
Electron density around 115 C 4:

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



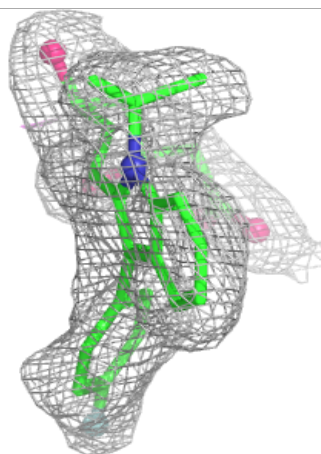
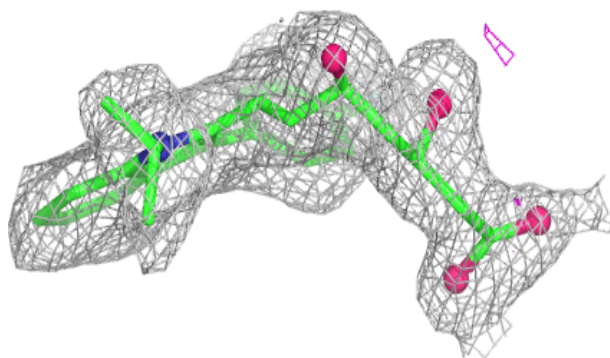
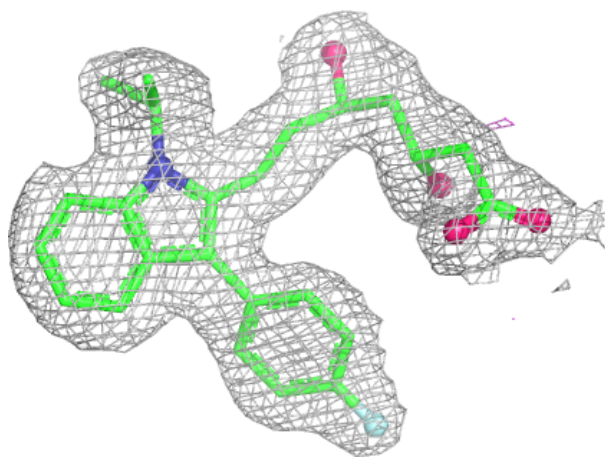
Electron density around 115 D 3:

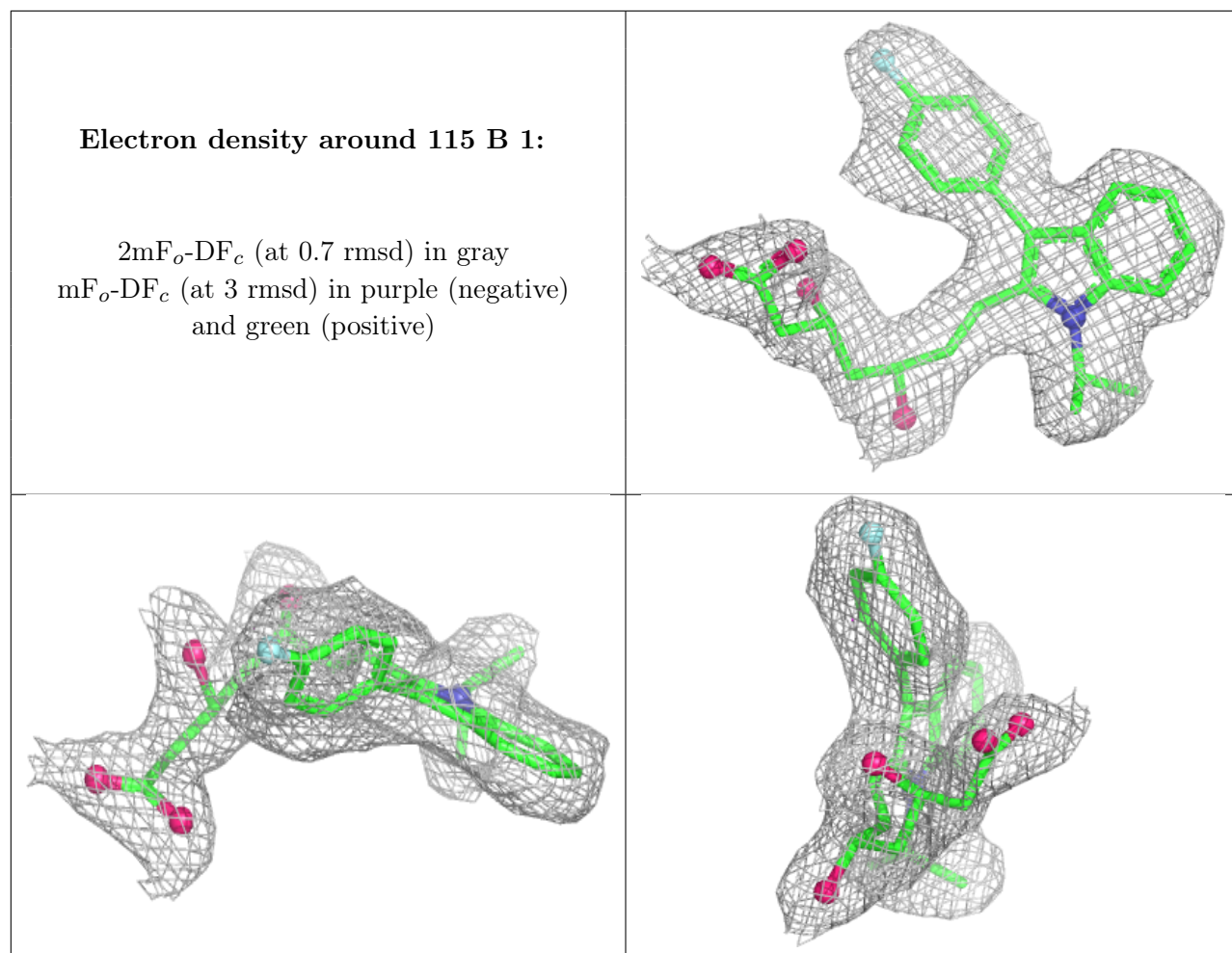
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 115 Å 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 ⓘ

There are no such residues in this entry.