



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 PM UTC

PDB ID : 2VF7 / pdb_00002vf7
Title : Crystal structure of UvrA2 from *Deinococcus radiodurans*
Authors : Timmins, J.; Gordon, E.; Caria, S.; Leonard, G.; Kuo, M.S.; Monchois, V.;
McSweeney, S.
Deposited on : 2007-10-31
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

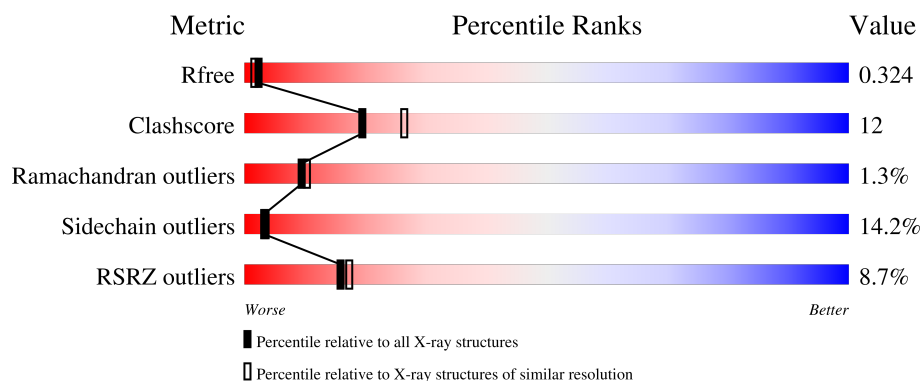
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
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	842	8% 70% 20% 6% .
1	B	842	9% 68% 23% 5% .
1	C	842	8% 66% 24% 6% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19508 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.

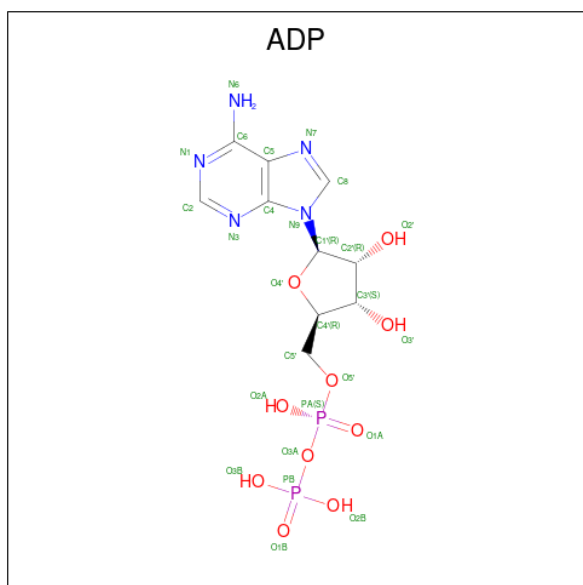
- Molecule 1 is a protein called EXCINUCLEASE ABC, SUBUNIT A..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	23	0
			6245	3918	1131	1177	19			
1	B	813	Total	C	N	O	S	0	26	0
			6240	3912	1134	1175	19			
1	C	814	Total	C	N	O	S	0	23	0
			6257	3930	1134	1174	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	GLN	engineered mutation	UNP Q9RYW8
B	746	ARG	GLN	engineered mutation	UNP Q9RYW8
C	746	ARG	GLN	engineered mutation	UNP Q9RYW8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

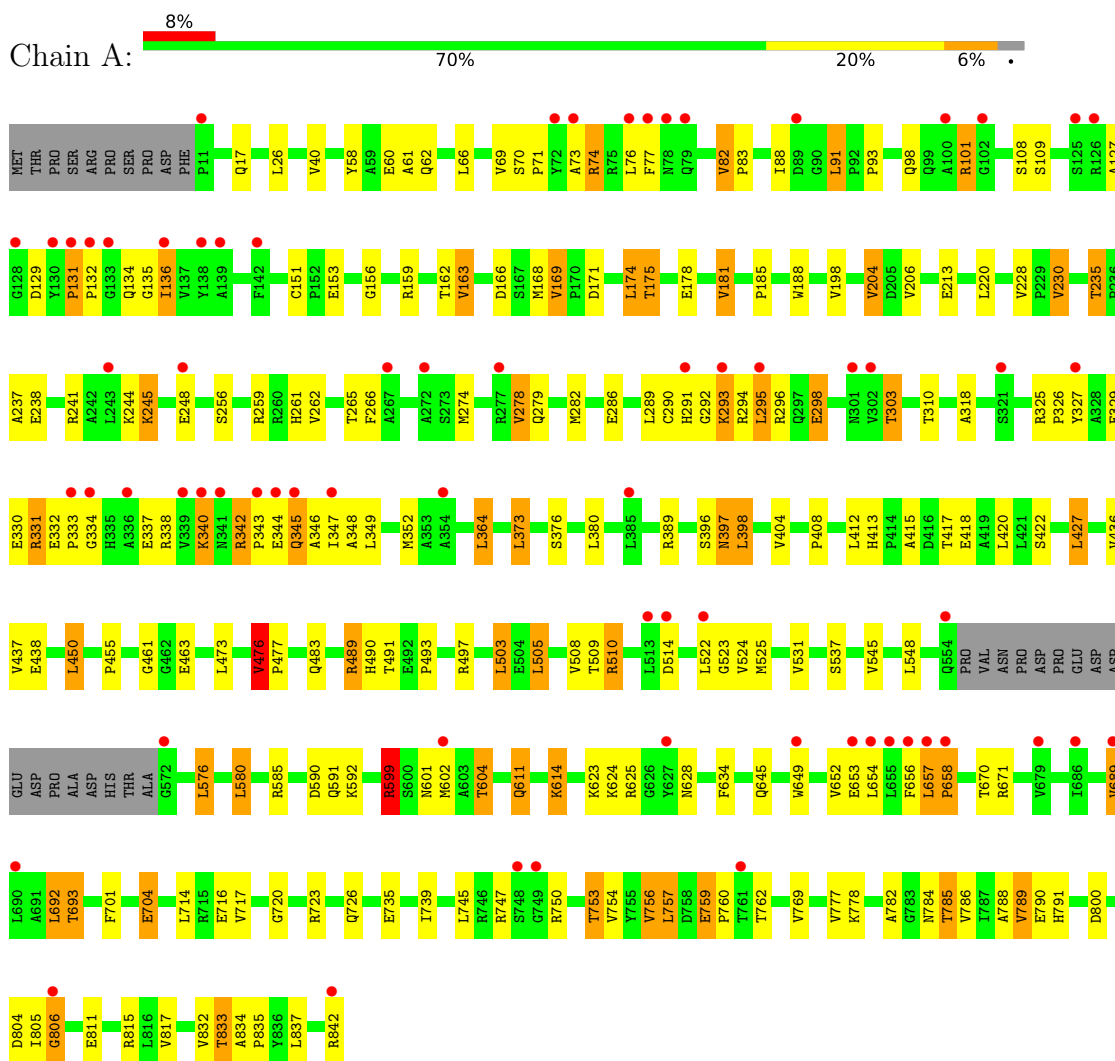
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	178	Total	O	0	0
			178	178		
5	B	232	Total	O	0	0
			232	232		
5	C	187	Total	O	0	0
			187	187		

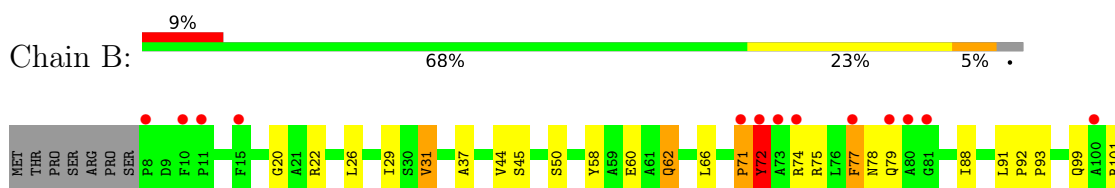
3 Residue-property plots

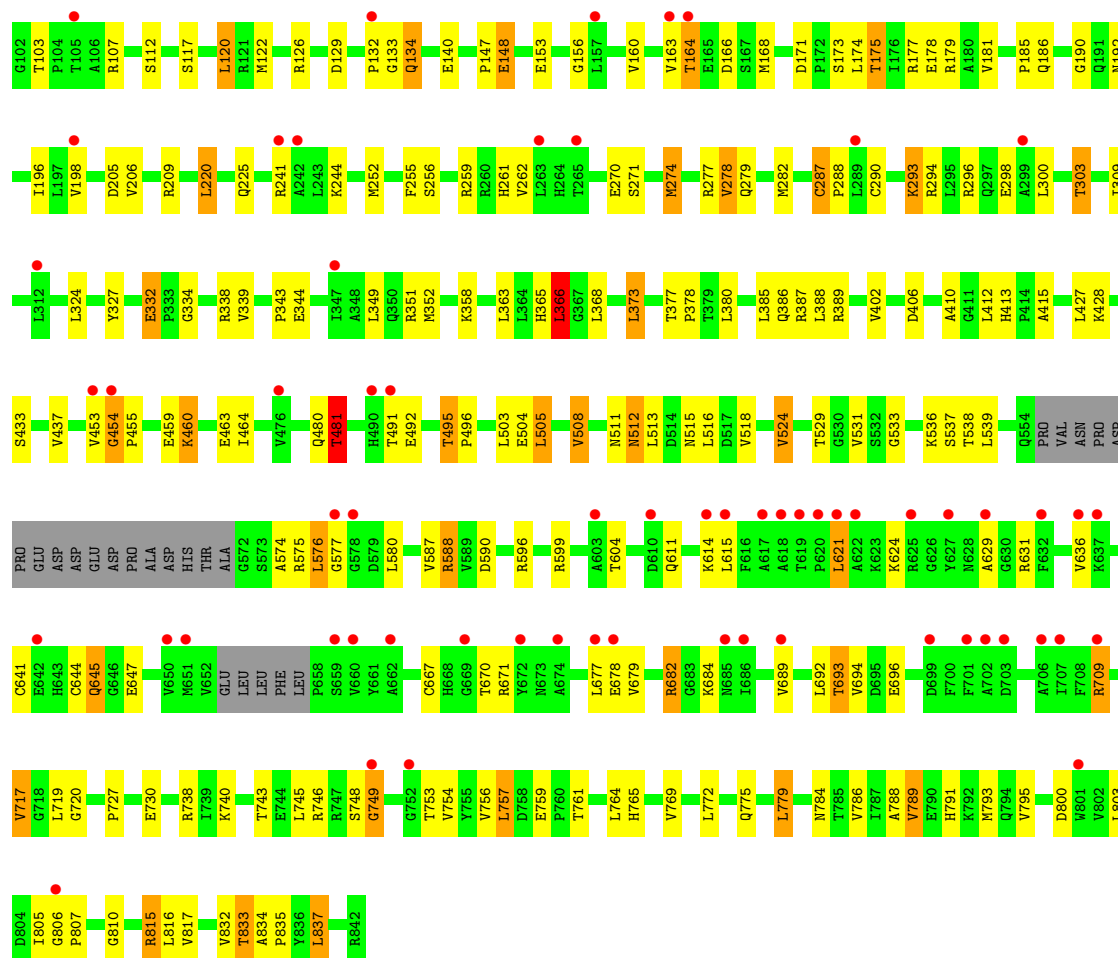
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EXCINUCLEASE ABC, SUBUNIT A.

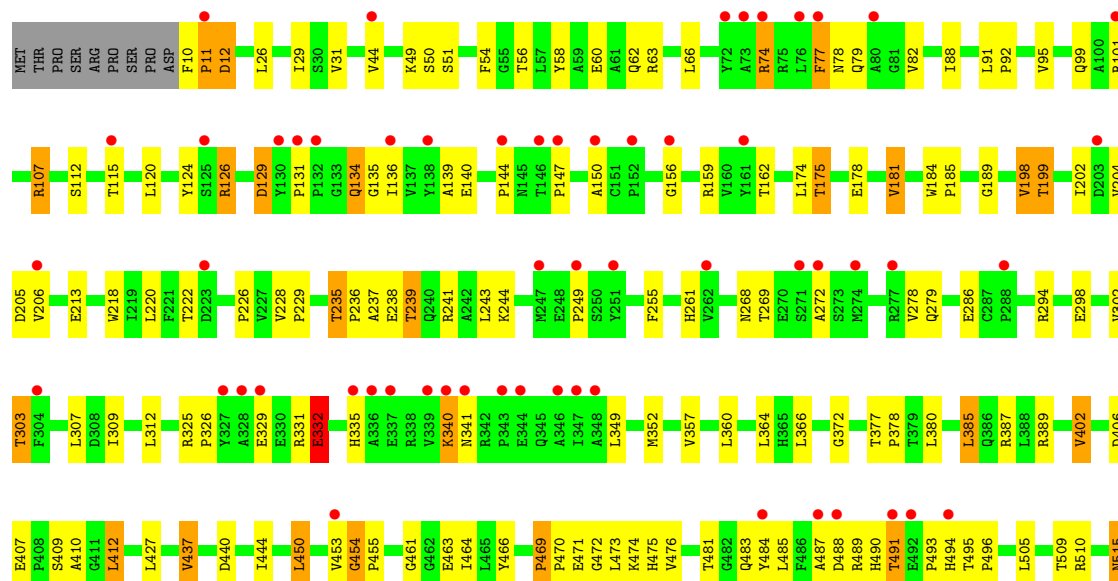


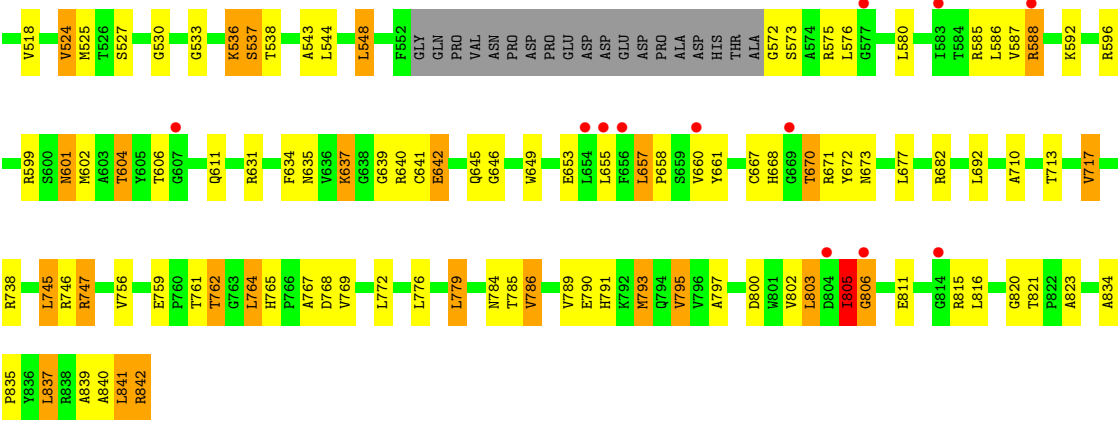
- Molecule 1: EXCINUCLEASE ABC, SUBUNIT A.





• Molecule 1: EXCINUCLEASE ABC, SUBUNIT A.





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.71Å 111.67Å 103.29Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.00-2.30) 95.0 (40.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.295 0.260 , 0.324	Depositor DCC
R_{free} test set	6448 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19508	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: ZN, ADP, MG

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	0.74	6/6375 (0.1%)	1.01	9/8662 (0.1%)
1	B	0.77	9/6376 (0.1%)	1.03	12/8661 (0.1%)
1	C	0.81	6/6395 (0.1%)	1.03	13/8689 (0.1%)
All	All	0.77	21/19146 (0.1%)	1.02	34/26012 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	GLN	C-N	22.74	1.68	1.33
1	B	682	ARG	C-N	13.32	1.50	1.33
1	B	72	TYR	CE1-CZ	10.08	1.62	1.38
1	B	682	ARG	NE-CZ	9.45	1.43	1.33
1	C	134	GLN	CD-NE2	-9.42	1.13	1.33
1	B	72	TYR	CG-CD1	9.41	1.59	1.39
1	A	330	GLU	CD-OE2	8.68	1.41	1.25
1	C	129	ASP	CG-OD2	7.50	1.39	1.25
1	A	657	LEU	CG-CD2	7.27	1.76	1.52
1	C	332	GLU	CD-OE1	6.06	1.36	1.25
1	A	657	LEU	CG-CD1	6.03	1.72	1.52
1	B	678	GLU	CD-OE2	6.00	1.36	1.25
1	A	344	GLU	CD-OE2	5.97	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	CD-OE1	5.96	1.36	1.25
1	C	340	LYS	CD-CE	5.77	1.69	1.52
1	A	476	VAL	CA-CB	5.69	1.59	1.54
1	B	72	TYR	CE2-CZ	5.65	1.51	1.38
1	B	682	ARG	CA-C	5.62	1.59	1.53
1	C	129	ASP	CG-OD1	5.51	1.35	1.25
1	B	678	GLU	CD-OE1	5.21	1.35	1.25
1	B	481	THR	CA-CB	5.15	1.61	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	ASN	N-CA-C	7.87	119.70	110.41
1	B	171	ASP	CA-C-N	7.84	127.48	119.56
1	B	171	ASP	C-N-CA	7.84	127.48	119.56
1	B	75	ARG	N-CA-C	-6.93	102.87	112.30
1	B	293	LYS	N-CA-C	-6.74	100.30	110.28
1	B	287	CYS	CA-C-N	6.43	126.66	119.32
1	B	287	CYS	C-N-CA	6.43	126.66	119.32
1	C	745	LEU	N-CA-C	6.43	118.09	111.14
1	B	153[A]	GLU	N-CA-C	6.15	119.25	111.69
1	C	372	GLY	N-CA-C	-6.04	104.48	112.82
1	B	682	ARG	O-C-N	6.04	130.99	123.32
1	A	230	VAL	N-CA-C	5.88	116.95	108.48
1	A	599	ARG	CB-CA-C	-5.78	101.20	110.79
1	C	134	GLN	O-C-N	5.70	131.09	122.94
1	A	476	VAL	CB-CA-C	5.67	116.47	111.08
1	A	295	LEU	N-CA-C	5.64	117.19	109.18
1	B	366	LEU	N-CA-C	-5.57	98.94	110.80
1	A	188	TRP	N-CA-C	5.56	118.06	111.33
1	A	228	VAL	N-CA-C	5.44	113.65	109.19
1	C	469	PRO	CA-C-N	5.42	125.76	119.47
1	C	469	PRO	C-N-CA	5.42	125.76	119.47
1	C	181	VAL	CB-CA-C	5.36	118.78	112.68
1	B	198	VAL	N-CA-CB	5.31	116.76	110.55
1	B	453	VAL	N-CA-C	5.28	115.91	108.36
1	C	402	VAL	CB-CA-C	-5.23	103.81	110.98
1	C	134	GLN	CG-CD-NE2	5.22	124.23	116.40
1	A	230	VAL	CB-CA-C	5.20	118.37	110.62
1	C	805	ILE	N-CA-C	5.19	116.06	108.53
1	C	484	TYR	N-CA-C	5.09	116.91	111.36
1	A	181	VAL	CB-CA-C	5.09	118.48	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	LEU	N-CA-C	-5.07	103.29	110.29
1	C	272	ALA	N-CA-C	-5.07	107.77	114.31
1	C	543	ALA	N-CA-C	5.03	116.45	111.07
1	B	72	TYR	CD1-CG-CD2	5.00	125.61	118.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	HIS	Peptide
1	B	682	ARG	Mainchain

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	6245	0	6115	134	0
1	B	6240	0	6100	145	0
1	C	6257	0	6158	153	0
2	A	54	0	24	1	0
2	B	54	0	24	1	0
2	C	54	0	24	6	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	C	1	0	0	0	0
5	A	178	0	0	12	0
5	B	232	0	0	19	0
5	C	187	0	0	23	0
All	All	19508	0	18445	434	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 12.

All (434) 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:A:657:LEU:CG	1:A:657:LEU:CD2	1.76	1.62
1:C:134:GLN:C	1:C:135:GLY:N	1.68	1.48
1:C:184:TRP:HB2	1:C:185:PRO:HD2	1.27	1.14
1:A:163:VAL:HG21	1:A:168:MET:HE3	1.32	1.11
1:C:657:LEU:HB3	1:C:658:PRO:HD2	1.39	1.04
2:C:902:ADP:H8	5:C:1116:HOH:O	1.48	0.95
1:C:747:ARG:H	1:C:747:ARG:HD2	1.31	0.95
1:C:107:ARG:HE	1:C:378:PRO:HG2	1.31	0.92
1:B:366:LEU:HG	5:B:1192:HOH:O	1.68	0.91
1:C:184:TRP:HB2	1:C:185:PRO:CD	2.01	0.90
1:C:588[A]:ARG:H	1:C:588[A]:ARG:HE	1.18	0.89
1:A:163:VAL:CG2	1:A:168:MET:HE3	2.04	0.88
1:B:377:THR:HA	1:B:380:LEU:HD13	1.56	0.87
1:A:175:THR:HG22	1:A:178:GLU:H	1.39	0.86
1:B:92:PRO:HG2	1:B:402:VAL:HG23	1.57	0.86
1:A:753:THR:HG23	1:A:784:ASN:ND2	1.92	0.84
1:B:524:VAL:HG13	1:B:800:ASP:HB2	1.59	0.84
1:C:765:HIS:HD2	1:C:767:ALA:H	1.26	0.83
1:C:198:VAL:HG23	1:C:239:THR:HG21	1.61	0.82
1:A:279:GLN:HA	1:A:282:MET:HE3	1.62	0.81
1:C:670:THR:HG21	1:C:677:LEU:HD11	1.62	0.81
1:A:649:TRP:HZ3	5:A:1051:HOH:O	1.63	0.80
1:C:175:THR:HG23	1:C:204:VAL:O	1.81	0.80
1:C:387:ARG:NH2	1:C:410:ALA:O	2.14	0.79
1:C:747:ARG:HD2	1:C:747:ARG:N	1.97	0.79
1:B:599:ARG:HG2	1:B:647:GLU:HG2	1.64	0.78
1:A:342:ARG:HG3	1:A:346:ALA:H	1.48	0.78
1:C:657:LEU:HB3	1:C:658:PRO:CD	2.13	0.78
1:B:761:THR:HA	1:B:764:LEU:HD22	1.64	0.77
1:C:790:GLU:HG2	1:C:795:VAL:HG22	1.67	0.77
1:B:133:GLY:HA2	1:C:797:ALA:O	1.82	0.77
1:A:537:SER:HB3	2:A:901:ADP:O2B	1.85	0.77
1:C:599:ARG:NH2	1:C:645:GLN:O	2.18	0.77
1:C:454:GLY:N	1:C:463:GLU:O	2.14	0.76
1:B:759:GLU:CG	1:B:791:HIS:HD2	2.00	0.74
1:B:290:CYS:SG	1:B:293:LYS:O	2.45	0.74
1:B:717:VAL:CG1	1:B:738:ARG:HB3	2.18	0.74
1:C:641:CYS:O	1:C:645:GLN:HA	1.86	0.73
1:A:657:LEU:CD2	1:A:657:LEU:CB	2.66	0.73
1:A:175:THR:HG21	5:A:1096:HOH:O	1.89	0.73
1:B:759:GLU:HG2	1:B:791:HIS:CD2	2.22	0.73
1:A:693:THR:HG23	1:A:720:GLY:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:THR:HG22	1:B:765:HIS:HE2	1.55	0.72
1:A:649:TRP:CZ3	5:A:1051:HOH:O	2.39	0.72
1:B:366:LEU:HD12	5:B:1091:HOH:O	1.88	0.72
1:C:834:ALA:HB3	1:C:835:PRO:HD3	1.72	0.71
1:A:168:MET:HE1	1:A:259:ARG:HA	1.73	0.71
1:A:248[A]:GLU:HG2	5:A:1170:HOH:O	1.91	0.71
1:B:386:GLN:HE22	1:B:406:ASP:H	1.39	0.70
1:A:602:MET:HE2	1:A:714:LEU:HD22	1.74	0.69
1:B:759:GLU:CG	1:B:791:HIS:CD2	2.75	0.69
1:C:573:SER:HB2	5:C:1071:HOH:O	1.92	0.69
2:C:902:ADP:C8	5:C:1116:HOH:O	2.32	0.69
1:B:156:GLY:O	1:B:294:ARG:HD2	1.93	0.69
1:C:440:ASP:O	1:C:444:ILE:HG12	1.92	0.69
1:A:524:VAL:HG13	1:A:800:ASP:HB2	1.75	0.68
1:A:340:LYS:HE3	1:A:340:LYS:H	1.59	0.68
1:B:365:HIS:C	1:B:366:LEU:O	2.34	0.68
1:A:735:GLU:O	1:A:739:ILE:HG13	1.93	0.68
1:C:453:VAL:O	1:C:454:GLY:O	2.11	0.67
1:A:274:MET:HG3	5:A:1153:HOH:O	1.92	0.67
1:B:511:ASN:HD22	1:B:538:THR:CG2	2.07	0.67
1:B:31:VAL:HG13	1:B:464:ILE:HD13	1.76	0.67
1:B:60:GLU:HG2	1:B:88:ILE:HD12	1.76	0.67
1:A:524:VAL:CG1	1:A:800:ASP:HB2	2.25	0.67
1:A:701:PHE:HD2	1:A:704:GLU:HG3	1.59	0.67
1:C:475:HIS:HB2	5:C:1132:HOH:O	1.95	0.67
1:A:175:THR:HG22	1:A:178:GLU:N	2.08	0.66
1:C:599:ARG:HE	1:C:635:ASN:HD22	1.43	0.66
1:B:122:MET:HG2	1:B:126[A]:ARG:HH12	1.60	0.66
1:B:262:VAL:CG1	1:B:282:MET:HE2	2.26	0.66
1:C:66:LEU:HB3	1:C:74:ARG:HG2	1.77	0.66
1:A:523:GLY:H	1:A:785:THR:HG22	1.61	0.65
1:C:134:GLN:CA	1:C:135:GLY:N	2.58	0.65
1:A:293:LYS:HD3	1:A:310:THR:HG21	1.78	0.65
1:B:717:VAL:HG13	1:B:738:ARG:HB3	1.76	0.65
1:B:621:LEU:HD12	1:B:679:VAL:HG22	1.78	0.64
1:B:179[A]:ARG:NH2	1:B:185:PRO:O	2.31	0.64
1:B:290:CYS:HB2	1:B:293:LYS:O	1.97	0.64
1:C:226:PRO:HD2	1:C:255:PHE:HB3	1.79	0.64
1:A:156:GLY:O	1:A:294:ARG:HD2	1.96	0.64
1:C:717:VAL:HG13	1:C:738:ARG:HB3	1.78	0.64
1:C:235:THR:HG22	1:C:238:GLU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:HB2	1:A:91:LEU:HD13	1.79	0.63
1:C:657:LEU:CB	1:C:658:PRO:HD2	2.24	0.63
1:A:455:PRO:HD2	1:A:461:GLY:HA2	1.81	0.63
1:C:841:LEU:O	1:C:842:ARG:C	2.40	0.63
1:B:693:THR:HG22	1:B:696:GLU:H	1.64	0.62
1:C:144:PRO:HG2	1:C:294:ARG:HH21	1.63	0.62
1:A:266:PHE:CD1	1:A:282:MET:HE1	2.35	0.62
1:C:129:ASP:HB2	1:C:303:THR:HG22	1.79	0.62
1:C:184:TRP:CB	1:C:185:PRO:HD2	2.18	0.62
1:A:652:VAL:C	1:A:654:LEU:H	2.07	0.61
1:C:29:ILE:HD13	1:C:464:ILE:HD11	1.83	0.61
1:B:262:VAL:HG13	1:B:282:MET:HE2	1.80	0.61
1:B:511:ASN:HD22	1:B:538:THR:HG21	1.66	0.61
1:B:717:VAL:HG12	1:B:719:LEU:HG	1.83	0.61
1:A:127:ALA:HB1	1:A:349:LEU:HD12	1.83	0.61
1:C:821:THR:HG22	1:C:823:ALA:H	1.66	0.61
1:C:44:VAL:CG1	5:C:1046:HOH:O	2.48	0.61
1:B:611:GLN:HA	1:B:614:LYS:HG2	1.83	0.60
1:B:20:GLY:O	1:B:22:ARG:NH1	2.34	0.60
1:C:811[A]:GLU:HG3	5:C:1124:HOH:O	2.00	0.60
1:A:759:GLU:OE2	1:A:790:GLU:OE2	2.19	0.60
1:B:71:PRO:HD2	1:B:72:TYR:CE1	2.36	0.60
1:B:576:LEU:HD13	1:B:580:LEU:HD11	1.82	0.60
1:C:806:GLY:N	1:C:815:ARG:O	2.33	0.60
1:B:62:GLN:O	1:B:66:LEU:HG	2.02	0.59
1:C:450:LEU:HD21	1:C:473:LEU:HD22	1.82	0.59
1:B:129:ASP:HB2	1:B:303:THR:HG22	1.84	0.59
1:B:175:THR:HG22	1:B:178[A]:GLU:HG2	1.84	0.59
1:C:115:THR:HB	5:C:1036:HOH:O	2.02	0.59
1:B:588:ARG:HH11	1:B:588:ARG:HB2	1.68	0.59
1:C:537:SER:HB2	2:C:901:ADP:O3B	2.03	0.59
1:A:657:LEU:O	1:A:658:PRO:C	2.46	0.59
1:C:218:TRP:HA	1:C:222:THR:HG23	1.85	0.59
1:B:50:SER:HB3	5:B:1030:HOH:O	2.02	0.59
1:A:93:PRO:HG2	1:B:93:PRO:HG2	1.84	0.58
1:B:175:THR:HG23	1:B:177:ARG:H	1.66	0.58
1:A:413:HIS:HD2	1:A:415:ALA:H	1.51	0.58
1:B:745:LEU:HD11	1:B:775:GLN:HE21	1.68	0.58
1:B:373:LEU:H	1:B:373:LEU:HD23	1.66	0.58
1:A:545:VAL:CG2	1:A:756:VAL:HG21	2.32	0.58
1:B:140:GLU:HG3	1:B:148:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:THR:HG21	5:A:1077:HOH:O	2.02	0.58
1:C:670:THR:O	1:C:671:ARG:HB2	2.04	0.58
1:C:842:ARG:HH11	1:C:842:ARG:HB3	1.67	0.58
1:C:60:GLU:HG2	1:C:88:ILE:HD12	1.85	0.58
1:B:611:GLN:O	1:B:615:LEU:HD23	2.03	0.57
1:B:508:VAL:HG12	1:B:516:LEU:O	2.04	0.57
1:A:175:THR:HG23	1:A:204:VAL:O	2.04	0.57
1:C:134:GLN:C	1:C:135:GLY:CA	2.72	0.57
5:B:1163:HOH:O	1:C:821:THR:HG23	2.05	0.57
1:B:689:VAL:O	1:B:692:LEU:HB2	2.05	0.57
1:B:74:ARG:O	1:B:74:ARG:HG3	2.05	0.56
1:B:209:ARG:NH1	5:B:1004:HOH:O	2.38	0.56
1:A:508:VAL:O	1:A:514:ASP:O	2.22	0.56
1:B:271:SER:HB3	1:B:274:MET:HB2	1.87	0.56
1:C:530:GLY:O	1:C:536:LYS:HE2	2.06	0.56
1:B:134:GLN:HE22	1:B:298:GLU:HB2	1.71	0.56
1:B:168:MET:HE3	1:B:220:LEU:HG	1.86	0.56
1:B:481:THR:HG22	1:B:765:HIS:NE2	2.19	0.56
1:B:185:PRO:HG3	1:B:261:HIS:NE2	2.21	0.56
1:A:159:ARG:NH1	1:A:286:GLU:HG3	2.21	0.56
1:C:409:SER:O	1:C:412:LEU:HB2	2.06	0.56
1:C:495:THR:HG23	1:C:496:PRO:HD2	1.87	0.56
1:A:17:GLN:HB2	5:A:1105:HOH:O	2.05	0.55
1:A:325:ARG:N	1:A:326:PRO:HD2	2.21	0.55
1:A:524:VAL:HG13	1:A:800:ASP:CB	2.36	0.55
1:B:670:THR:HG21	1:B:677:LEU:HD11	1.88	0.55
1:A:759:GLU:O	1:A:762:THR:HG23	2.05	0.55
2:C:901:ADP:PA	5:C:1007:HOH:O	2.65	0.55
1:B:122:MET:HG2	1:B:126[A]:ARG:NH1	2.21	0.55
1:C:329:GLU:HG3	1:C:331:ARG:NH1	2.21	0.55
1:C:385:LEU:HD12	1:C:385:LEU:C	2.32	0.55
1:A:159:ARG:HH11	1:A:286:GLU:HG3	1.71	0.55
1:A:329:GLU:HB2	1:A:331:ARG:HD2	1.89	0.55
1:A:628:ASN:HB2	5:A:1128:HOH:O	2.07	0.54
1:B:759:GLU:HG3	1:B:791:HIS:HD2	1.72	0.54
1:A:129:ASP:HB2	1:A:303:THR:HG22	1.90	0.54
1:B:29:ILE:HD13	1:B:464:ILE:HD11	1.89	0.54
1:B:278:VAL:HG13	1:B:282:MET:CE	2.38	0.54
1:C:49:LYS:HG2	2:C:902:ADP:O1B	2.07	0.54
1:B:512:ASN:HD21	1:B:810:GLY:C	2.15	0.54
1:B:764:LEU:HD13	5:B:1124:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD22	5:A:1006:HOH:O	2.07	0.54
1:B:29:ILE:HB	1:B:464:ILE:HD12	1.89	0.54
1:C:765:HIS:CD2	1:C:767:ALA:H	2.17	0.54
1:C:218:TRP:CD1	1:C:222:THR:HG21	2.43	0.54
1:B:748:SER:O	1:B:749:GLY:C	2.50	0.53
1:A:483:GLN:HB3	1:A:489:ARG:HG3	1.89	0.53
1:C:745:LEU:N	1:C:747:ARG:HH21	2.07	0.53
1:A:348:ALA:O	1:A:352:MET:HG3	2.08	0.53
1:A:185:PRO:HG3	1:A:261:HIS:NE2	2.23	0.53
1:B:791:HIS:CE1	5:B:1031:HOH:O	2.60	0.53
1:B:290:CYS:CB	1:B:293:LYS:O	2.57	0.53
1:A:342:ARG:NE	1:A:346:ALA:HB3	2.24	0.53
1:A:805:ILE:O	1:A:806:GLY:O	2.26	0.53
1:A:576:LEU:HD12	1:A:580:LEU:HD11	1.90	0.53
1:A:716[A]:GLU:OE2	1:A:778:LYS:NZ	2.39	0.53
1:A:503:LEU:HB2	1:A:522:LEU:HD21	1.90	0.52
1:A:804:ASP:OD1	1:A:833:THR:CG2	2.57	0.52
1:A:806:GLY:N	1:A:815:ARG:O	2.30	0.52
1:C:509:THR:HB	1:C:515:ASN:H	1.75	0.52
1:C:175:THR:HG22	1:C:178:GLU:H	1.74	0.52
1:A:497:ARG:NH2	1:A:777:VAL:HG13	2.25	0.52
1:A:757:LEU:O	1:A:788:ALA:HA	2.09	0.52
1:B:480:GLN:NE2	5:B:1006:HOH:O	2.43	0.52
1:A:74:ARG:HH21	1:A:76:LEU:HD12	1.75	0.51
1:A:373:LEU:HD23	1:A:373:LEU:H	1.76	0.51
1:A:670:THR:O	1:A:671:ARG:HB2	2.09	0.51
1:C:54:PHE:HA	1:C:58:TYR:HB3	1.93	0.51
1:C:759:GLU:OE2	1:C:791:HIS:ND1	2.39	0.51
1:A:168:MET:HE1	1:A:259:ARG:CA	2.39	0.51
1:A:318:ALA:HA	1:A:364:LEU:HD11	1.93	0.51
1:B:173:SER:HB3	5:B:1004:HOH:O	2.09	0.51
1:B:717:VAL:HG11	1:B:738:ARG:HB3	1.90	0.51
1:C:185:PRO:HD3	1:C:261:HIS:CE1	2.46	0.51
1:A:604:THR:HG21	5:A:1114:HOH:O	2.10	0.51
1:C:790:GLU:OE2	1:C:795:VAL:HG21	2.11	0.51
1:B:117:SER:O	1:B:120:LEU:HD12	2.11	0.51
1:C:185:PRO:HG2	1:C:189:GLY:C	2.34	0.51
1:A:689:VAL:O	1:A:692:LEU:HB2	2.12	0.51
1:C:670:THR:HG22	1:C:672:TYR:H	1.76	0.51
1:B:511:ASN:HD22	1:B:538:THR:HG22	1.76	0.50
1:A:693:THR:CG2	1:A:720:GLY:O	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:NH2	1:B:410:ALA:O	2.45	0.50
1:C:802:VAL:N	1:C:820:GLY:O	2.43	0.50
1:A:599:ARG:NH2	1:A:645:GLN:O	2.38	0.50
1:A:753:THR:HG23	1:A:784:ASN:HD22	1.70	0.50
1:C:44:VAL:HG12	5:C:1046:HOH:O	2.10	0.50
1:C:92:PRO:HG2	1:C:402:VAL:CG2	2.42	0.50
1:B:455:PRO:HD2	1:B:460:LYS:O	2.11	0.49
1:B:508:VAL:CG1	1:B:516:LEU:O	2.61	0.49
1:B:793:MET:CE	1:B:837:LEU:HG	2.42	0.49
1:B:77:PHE:C	1:B:79:GLN:H	2.21	0.49
1:C:175:THR:HG21	5:C:1171:HOH:O	2.12	0.49
1:A:235:THR:HG22	1:A:238:GLU:HG2	1.94	0.49
1:A:413:HIS:CD2	1:A:415:ALA:H	2.28	0.49
1:B:120:LEU:HD13	1:B:309:ILE:HD11	1.95	0.49
1:A:131:PRO:HB3	1:A:132:PRO:HD2	1.94	0.49
1:A:585:ARG:HB2	1:A:753:THR:HB	1.95	0.49
1:C:491:THR:HG21	5:C:1070:HOH:O	2.12	0.49
1:B:495:THR:HG23	5:B:1117:HOH:O	2.13	0.48
1:B:694:VAL:HB	1:B:720:GLY:HA2	1.94	0.48
1:C:49:LYS:HE2	1:C:437:VAL:CG2	2.44	0.48
1:C:510:ARG:HB3	1:C:572:GLY:HA2	1.94	0.48
1:A:74:ARG:C	1:A:76:LEU:H	2.19	0.48
1:A:804:ASP:OD1	1:A:833:THR:HG21	2.12	0.48
1:B:413:HIS:HE1	1:B:833:THR:HB	1.77	0.48
1:C:793:MET:HG2	1:C:837:LEU:HA	1.94	0.48
1:B:164:THR:HG23	1:B:166:ASP:H	1.78	0.48
1:B:37:ALA:HA	1:B:428:LYS:HD2	1.96	0.48
1:A:523:GLY:H	1:A:785:THR:CG2	2.26	0.48
1:C:634:PHE:O	1:C:646:GLY:HA3	2.14	0.48
1:B:225:GLN:HG2	1:B:255:PHE:O	2.14	0.48
1:B:670:THR:O	1:B:671:ARG:HB2	2.13	0.48
1:B:834:ALA:HB3	1:B:835:PRO:HD3	1.96	0.48
1:C:518:VAL:HG13	1:C:803:LEU:HD21	1.96	0.48
1:C:77:PHE:HB2	1:C:655:LEU:HG	1.95	0.47
1:C:601:ASN:ND2	1:C:604:THR:H	2.12	0.47
1:A:74:ARG:NH2	1:A:77:PHE:HA	2.29	0.47
1:A:689:VAL:HA	1:A:692:LEU:HD22	1.96	0.47
1:C:406:ASP:HA	1:C:437:VAL:HG13	1.95	0.47
1:A:74:ARG:HH22	1:A:77:PHE:HA	1.79	0.47
1:A:413:HIS:CE1	1:A:833:THR:HG22	2.49	0.47
1:B:44:VAL:CG1	1:B:45:SER:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:LEU:O	1:B:788:ALA:HA	2.14	0.47
1:C:576:LEU:HD13	1:C:580:LEU:HD11	1.95	0.47
1:C:229:PRO:HB3	1:C:249:PRO:HG3	1.96	0.47
1:C:49:LYS:HE2	1:C:437:VAL:HG23	1.96	0.47
1:C:332:GLU:CD	1:C:335:HIS:HD2	2.22	0.47
1:B:327:TYR:HB3	1:B:349:LEU:HD22	1.96	0.47
1:C:759:GLU:OE1	1:C:761:THR:HG22	2.14	0.47
1:A:290:CYS:O	1:A:292:GLY:N	2.45	0.47
1:B:743:THR:HG21	5:B:1213:HOH:O	2.14	0.47
1:B:179[A]:ARG:NH2	1:B:190:GLY:HA3	2.29	0.47
1:C:518:VAL:HG22	1:C:816:LEU:HD12	1.96	0.47
1:B:327:TYR:CD2	1:B:332:GLU:HG2	2.50	0.47
1:B:529:THR:C	1:B:536:LYS:HD3	2.40	0.47
1:B:277:ARG:HD2	5:B:1216:HOH:O	2.14	0.47
1:B:590:ASP:OD2	1:B:590:ASP:N	2.43	0.47
1:C:150:ALA:HB1	1:C:156:GLY:CA	2.45	0.47
1:C:759:GLU:HB3	1:C:762:THR:HG22	1.97	0.47
1:C:199:THR:HG21	1:C:228:VAL:HB	1.97	0.46
1:B:179[A]:ARG:HH22	1:B:190:GLY:HA3	1.80	0.46
1:C:235:THR:HG23	1:C:237:ALA:H	1.81	0.46
1:A:611:GLN:O	1:A:614:LYS:HB3	2.16	0.46
1:B:163:VAL:HG21	1:B:259:ARG:HG3	1.96	0.46
1:B:727:PRO:HG2	1:B:730:GLU:HG3	1.98	0.46
1:C:139:ALA:O	1:C:140:GLU:HB2	2.13	0.46
1:C:525:MET:HG3	1:C:786:VAL:HG22	1.97	0.46
1:A:505:LEU:HD22	1:A:508:VAL:HG22	1.97	0.46
1:B:504:GLU:O	1:B:576:LEU:HA	2.16	0.46
1:C:450:LEU:HD12	1:C:450:LEU:C	2.40	0.46
1:A:171:ASP:HB3	1:A:174:LEU:HD22	1.98	0.46
1:B:775:GLN:O	1:B:779:LEU:HD22	2.16	0.46
1:C:466:TYR:OH	1:C:472:GLY:HA3	2.15	0.46
1:A:332:GLU:O	1:A:334:GLY:N	2.49	0.46
1:A:342:ARG:HE	1:A:346:ALA:HB3	1.81	0.46
1:B:413:HIS:HD2	1:B:415:ALA:CB	2.29	0.46
1:A:545:VAL:HG22	1:A:756:VAL:HG21	1.96	0.46
1:A:753:THR:CG2	1:A:784:ASN:ND2	2.70	0.46
1:B:492:GLU:HG2	5:B:1149:HOH:O	2.17	0.45
1:C:150:ALA:HB3	5:C:1010:HOH:O	2.15	0.45
1:B:278:VAL:HG13	1:B:282:MET:HE1	1.97	0.45
1:C:510:ARG:HG3	1:C:538:THR:HG23	1.99	0.45
1:A:293:LYS:H	1:A:293:LYS:HG2	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PHE:O	1:C:79:GLN:N	2.49	0.45
1:C:776:LEU:O	1:C:779:LEU:HD22	2.17	0.45
1:C:779:LEU:C	1:C:779:LEU:HD23	2.41	0.45
1:C:126:ARG:HD3	1:C:352:MET:HE1	1.97	0.45
1:B:29:ILE:HD13	1:B:464:ILE:CD1	2.46	0.45
1:B:779:LEU:O	1:B:784:ASN:HB2	2.16	0.45
1:A:408:PRO:HB2	1:A:420:LEU:HD11	1.98	0.45
1:C:488:ASP:CG	1:C:488:ASP:O	2.59	0.45
1:B:177:ARG:NH1	1:B:205:ASP:OD1	2.50	0.45
1:C:325:ARG:HD2	5:C:1068:HOH:O	2.17	0.45
1:C:494:HIS:HB3	5:C:1165:HOH:O	2.15	0.45
1:B:377:THR:N	1:B:378:PRO:CD	2.80	0.45
1:C:471:GLU:O	1:C:474:LYS:HE3	2.17	0.45
1:C:481:THR:O	1:C:485:LEU:HD23	2.17	0.45
1:C:710:ALA:O	1:C:713:THR:OG1	2.34	0.45
1:B:339:VAL:O	1:B:343:PRO:HG3	2.17	0.44
1:B:539:LEU:HD22	1:B:805:ILE:HD11	1.99	0.44
1:C:77:PHE:C	1:C:79:GLN:H	2.24	0.44
1:A:757:LEU:HB3	1:A:760:PRO:HG3	1.99	0.44
1:B:279:GLN:HA	1:B:282:MET:HG2	2.00	0.44
1:B:759:GLU:HG3	1:B:791:HIS:CD2	2.51	0.44
1:C:779:LEU:O	1:C:784:ASN:HB2	2.16	0.44
1:C:481:THR:OG1	1:C:765:HIS:HE1	2.00	0.44
1:C:120:LEU:O	1:C:124:TYR:HD1	2.00	0.44
1:A:450:LEU:C	1:A:450:LEU:HD12	2.42	0.44
1:C:764:LEU:HG	1:C:768:ASP:HB3	1.99	0.44
1:A:265:THR:HB	1:A:278:VAL:HG21	1.99	0.44
1:A:408:PRO:HD2	1:A:438:GLU:OE1	2.18	0.44
1:A:599:ARG:NH2	1:A:634:PHE:O	2.49	0.44
1:B:413:HIS:CD2	1:B:415:ALA:H	2.36	0.44
1:C:184:TRP:CD1	5:C:1080:HOH:O	2.70	0.44
1:C:213:GLU:HG2	5:C:1143:HOH:O	2.17	0.44
1:C:667:CYS:O	1:C:668:HIS:HB2	2.16	0.44
1:B:454:GLY:N	1:B:463:GLU:O	2.32	0.44
1:C:360:LEU:O	1:C:364:LEU:HD23	2.17	0.44
1:C:51:SER:O	1:C:56:THR:HG23	2.18	0.43
1:C:131:PRO:HB2	1:C:134:GLN:HG3	1.99	0.43
1:A:237:ALA:O	1:A:241[A]:ARG:HG3	2.17	0.43
1:A:476:VAL:HA	1:A:477:PRO:HD3	1.67	0.43
1:B:148:GLU:H	1:B:148:GLU:HG2	1.51	0.43
1:A:58:TYR:HB2	1:A:404:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:H	1:A:657:LEU:HD23	1.83	0.43
1:A:135:GLY:O	1:A:136:ILE:HG13	2.18	0.43
1:A:274:MET:CG	5:A:1153:HOH:O	2.62	0.43
1:C:385:LEU:C	1:C:385:LEU:CD1	2.91	0.43
1:C:601:ASN:C	1:C:601:ASN:HD22	2.26	0.43
1:C:637:LYS:HB3	5:C:1161:HOH:O	2.18	0.43
1:B:92:PRO:HG2	1:B:402:VAL:CG2	2.37	0.43
1:B:533:GLY:O	2:B:901:ADP:H5'2	2.18	0.43
1:C:839:ALA:O	1:C:842:ARG:HG3	2.18	0.43
1:C:524:VAL:HG22	1:C:800:ASP:OD2	2.19	0.43
1:C:660:VAL:HG22	1:C:661:TYR:H	1.84	0.43
1:C:840:ALA:HA	5:C:1009:HOH:O	2.19	0.43
1:C:82:VAL:HG12	5:C:1038:HOH:O	2.18	0.43
1:C:159:ARG:NH2	1:C:286:GLU:HG3	2.34	0.43
1:A:156:GLY:HA2	1:A:294:ARG:O	2.19	0.42
1:B:505:LEU:HD22	1:B:574:ALA:HB1	2.01	0.42
1:B:709:ARG:HG3	1:B:746:ARG:CZ	2.49	0.42
1:C:115:THR:O	1:C:115:THR:HG22	2.19	0.42
1:A:40:VAL:HA	1:A:436:VAL:O	2.20	0.42
1:A:701:PHE:CD2	1:A:704:GLU:HG3	2.48	0.42
1:C:150:ALA:CB	5:C:1010:HOH:O	2.66	0.42
1:C:243:LEU:HD21	5:C:1083:HOH:O	2.19	0.42
1:C:533:GLY:HA2	2:C:901:ADP:O2A	2.20	0.42
1:A:396:SER:O	1:A:397:ASN:HB2	2.20	0.42
1:B:413:HIS:HD2	1:B:415:ALA:H	1.67	0.42
1:A:296:ARG:HB3	1:A:298:GLU:HG3	2.02	0.42
1:A:327:TYR:HD2	1:A:349:LEU:HD21	1.84	0.42
1:A:497:ARG:HH22	1:A:777:VAL:HG13	1.83	0.42
1:A:262:VAL:HG22	5:A:1019:HOH:O	2.18	0.42
1:A:548:LEU:HD11	1:A:754:VAL:HG11	2.02	0.42
1:B:58:TYR:CZ	1:B:62:GLN:HG3	2.54	0.42
1:B:689:VAL:HA	1:B:692:LEU:HD13	2.01	0.42
1:C:745:LEU:HD23	1:C:745:LEU:HA	1.92	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.91	0.42
1:A:657:LEU:CD2	1:A:657:LEU:HG	2.20	0.42
1:B:147:PRO:O	1:B:296:ARG:NH1	2.51	0.42
1:B:807:PRO:HD3	1:B:815[A]:ARG:HD3	2.02	0.42
1:C:670:THR:O	1:C:671:ARG:CB	2.68	0.42
1:A:60:GLU:HG2	1:A:88:ILE:HD12	2.01	0.42
1:A:151:CYS:SG	1:A:289:LEU:HD23	2.60	0.42
1:A:450:LEU:HD21	1:A:473:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:CD	1:B:344:GLU:O	2.63	0.42
1:C:495:THR:CG2	1:C:496:PRO:HD2	2.50	0.42
1:C:747:ARG:H	1:C:747:ARG:CD	2.16	0.42
1:A:66:LEU:HA	1:A:69:VAL:HG22	2.01	0.41
1:B:495:THR:HA	1:B:496:PRO:HD3	1.77	0.41
1:C:455:PRO:HD2	1:C:461:GLY:HA2	2.01	0.41
1:A:235:THR:HG22	1:A:238:GLU:CG	2.50	0.41
1:B:588:ARG:HB2	1:B:588:ARG:NH1	2.34	0.41
1:B:192:ASN:O	1:B:196:ILE:HG13	2.21	0.41
1:B:684:LYS:HE3	1:B:692:LEU:HD11	2.01	0.41
1:B:793:MET:HE3	1:B:837:LEU:HG	2.01	0.41
1:C:530:GLY:C	1:C:536:LYS:HE2	2.45	0.41
1:C:631:ARG:O	1:C:639:GLY:HA3	2.20	0.41
1:A:71:PRO:C	1:A:73:ALA:H	2.27	0.41
1:A:169:VAL:O	1:A:169:VAL:HG22	2.20	0.41
1:A:398:LEU:CD2	5:B:1142:HOH:O	2.68	0.41
1:B:252:MET:HB3	1:B:252:MET:HE3	1.83	0.41
1:C:611[A]:GLN:NE2	5:C:1018:HOH:O	2.53	0.41
1:C:805:ILE:O	1:C:806:GLY:O	2.38	0.41
1:C:483:GLN:HA	1:C:487:ALA:HB3	2.02	0.41
1:B:186:GLN:HG3	5:B:1017:HOH:O	2.20	0.41
1:A:509:THR:O	1:A:510:ARG:HB2	2.20	0.41
1:B:641:CYS:HB2	1:B:667:CYS:HB3	2.03	0.41
1:C:236:PRO:O	1:C:239:THR:HG22	2.20	0.41
1:C:640:ARG:NE	1:C:642:GLU:OE2	2.50	0.41
1:C:469:PRO:HA	1:C:470:PRO:HD3	1.91	0.41
1:C:544:LEU:O	1:C:548:LEU:HB2	2.20	0.41
1:A:723:ARG:HB2	1:A:726:GLN:HB2	2.03	0.41
1:A:834:ALA:HB3	1:A:835:PRO:CD	2.51	0.41
1:B:287:CYS:HA	1:B:288:PRO:HD3	1.82	0.41
1:B:368:LEU:HD13	1:B:388:LEU:HD23	2.03	0.41
1:B:387:ARG:NH1	5:B:1019:HOH:O	2.53	0.41
1:B:433:SER:HB3	5:B:1061:HOH:O	2.19	0.41
1:C:92:PRO:HG2	1:C:402:VAL:HG23	2.01	0.41
1:A:602:MET:HG3	1:A:739:ILE:HD13	2.03	0.41
1:A:750:ARG:C	1:A:782:ALA:O	2.63	0.41
1:B:241[A]:ARG:CZ	1:B:241[A]:ARG:HB2	2.50	0.41
1:B:413:HIS:CE1	1:B:833:THR:HB	2.56	0.41
1:C:50:SER:HB3	5:C:1126:HOH:O	2.21	0.41
1:C:62:GLN:O	1:C:66:LEU:HG	2.20	0.41
1:C:63:ARG:HD2	1:C:82:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:ASN:ND2	1:C:604:THR:HB	2.35	0.41
1:A:82:VAL:HG12	1:A:83:PRO:HD2	2.03	0.40
1:A:759:GLU:HG3	1:A:791:HIS:ND1	2.36	0.40
1:B:279:GLN:HA	1:B:282:MET:HE3	2.03	0.40
1:B:693:THR:HG23	1:B:720:GLY:O	2.21	0.40
1:B:334:GLY:O	1:B:338:ARG:HG3	2.21	0.40
1:C:510:ARG:HG3	1:C:538:THR:CG2	2.52	0.40
1:A:74:ARG:C	1:A:76:LEU:N	2.80	0.40
1:A:804:ASP:OD1	1:A:833:THR:HG23	2.21	0.40
1:B:644:CYS:C	1:B:645:GLN:HG2	2.46	0.40
1:B:815[B]:ARG:HD2	5:B:1044:HOH:O	2.21	0.40
1:C:11:PRO:HB2	1:C:12:ASP:H	1.58	0.40
1:C:325:ARG:N	1:C:326:PRO:CD	2.85	0.40
1:C:649:TRP:CD1	1:C:661:TYR:HB3	2.56	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	811/842 (96%)	748 (92%)	51 (6%)	12 (2%)	8	8
1	B	809/842 (96%)	748 (92%)	51 (6%)	10 (1%)	10	12
1	C	812/842 (96%)	756 (93%)	46 (6%)	10 (1%)	10	12
All	All	2432/2526 (96%)	2252 (93%)	148 (6%)	32 (1%)	9	10

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	345	GLN
1	A	806	GLY

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Mol	Chain	Res	Type
1	B	72	TYR
1	B	749	GLY
1	C	78	ASN
1	C	454	GLY
1	A	343	PRO
1	B	71	PRO
1	B	78	ASN
1	B	366	LEU
1	B	454	GLY
1	B	629	ALA
1	B	806	GLY
1	C	11	PRO
1	C	806	GLY
1	A	333	PRO
1	A	510	ARG
1	A	658	PRO
1	C	77	PHE
1	A	131	PRO
1	A	291	HIS
1	A	759	GLU
1	C	493	PRO
1	A	653	GLU
1	C	489	ARG
1	C	657	LEU
1	C	673	ASN
1	C	147	PRO
1	A	493	PRO
1	B	132	PRO
1	B	577	GLY

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	658/683 (96%)	560 (85%)	98 (15%)	3	3
1	B	657/683 (96%)	571 (87%)	86 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	659/683 (96%)	562 (85%)	97 (15%)	3	3
All	All	1974/2049 (96%)	1693 (86%)	281 (14%)	3	3

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	62	GLN
1	A	70	SER
1	A	74	ARG
1	A	82	VAL
1	A	91	LEU
1	A	98	GLN
1	A	101	ARG
1	A	108	SER
1	A	109	SER
1	A	134	GLN
1	A	136	ILE
1	A	153	GLU
1	A	162	THR
1	A	163	VAL
1	A	166	ASP
1	A	169	VAL
1	A	174	LEU
1	A	175	THR
1	A	181	VAL
1	A	198	VAL
1	A	204	VAL
1	A	206	VAL
1	A	213[A]	GLU
1	A	220	LEU
1	A	230	VAL
1	A	235	THR
1	A	244[A]	LYS
1	A	245	LYS
1	A	256	SER
1	A	278	VAL
1	A	293	LYS
1	A	295	LEU
1	A	298	GLU
1	A	303	THR
1	A	331	ARG

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Mol	Chain	Res	Type
1	A	337	GLU
1	A	338	ARG
1	A	340	LYS
1	A	342	ARG
1	A	345	GLN
1	A	347	ILE
1	A	364	LEU
1	A	373	LEU
1	A	376	SER
1	A	380	LEU
1	A	389	ARG
1	A	397	ASN
1	A	398	LEU
1	A	412	LEU
1	A	417	THR
1	A	418	GLU
1	A	422	SER
1	A	427	LEU
1	A	437	VAL
1	A	450	LEU
1	A	463	GLU
1	A	476	VAL
1	A	489	ARG
1	A	491	THR
1	A	503	LEU
1	A	505	LEU
1	A	525	MET
1	A	531	VAL
1	A	576	LEU
1	A	580	LEU
1	A	590[A]	ASP
1	A	591[A]	GLN
1	A	592	LYS
1	A	599	ARG
1	A	601	ASN
1	A	604	THR
1	A	611	GLN
1	A	614	LYS
1	A	623	LYS
1	A	624	LYS
1	A	625	ARG
1	A	656	PHE

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Mol	Chain	Res	Type
1	A	689	VAL
1	A	692	LEU
1	A	693	THR
1	A	704	GLU
1	A	717	VAL
1	A	745	LEU
1	A	747	ARG
1	A	753	THR
1	A	756	VAL
1	A	757	LEU
1	A	769	VAL
1	A	785	THR
1	A	786	VAL
1	A	789	VAL
1	A	811[A]	GLU
1	A	817	VAL
1	A	832	VAL
1	A	833	THR
1	A	837	LEU
1	A	842	ARG
1	B	26	LEU
1	B	31	VAL
1	B	62	GLN
1	B	72	TYR
1	B	77	PHE
1	B	91	LEU
1	B	99[A]	GLN
1	B	101	ARG
1	B	103	THR
1	B	107	ARG
1	B	112	SER
1	B	120	LEU
1	B	134	GLN
1	B	148	GLU
1	B	160	VAL
1	B	164	THR
1	B	174	LEU
1	B	175	THR
1	B	181	VAL
1	B	206	VAL
1	B	220	LEU
1	B	244	LYS

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Mol	Chain	Res	Type
1	B	256	SER
1	B	274	MET
1	B	278	VAL
1	B	300	LEU
1	B	303	THR
1	B	324	LEU
1	B	332	GLU
1	B	351	ARG
1	B	358	LYS
1	B	363	LEU
1	B	373	LEU
1	B	385	LEU
1	B	389	ARG
1	B	412	LEU
1	B	427	LEU
1	B	437	VAL
1	B	459[A]	GLU
1	B	460	LYS
1	B	481	THR
1	B	491	THR
1	B	495	THR
1	B	503	LEU
1	B	505	LEU
1	B	508	VAL
1	B	512	ASN
1	B	513	LEU
1	B	515	ASN
1	B	518	VAL
1	B	524	VAL
1	B	531	VAL
1	B	537	SER
1	B	575	ARG
1	B	576	LEU
1	B	587	VAL
1	B	588	ARG
1	B	596	ARG
1	B	604	THR
1	B	621	LEU
1	B	624	LYS
1	B	631	ARG
1	B	636	VAL
1	B	645	GLN

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Mol	Chain	Res	Type
1	B	693	THR
1	B	709	ARG
1	B	717	VAL
1	B	740	LYS
1	B	753	THR
1	B	754	VAL
1	B	756	VAL
1	B	757	LEU
1	B	769	VAL
1	B	772	LEU
1	B	779	LEU
1	B	786	VAL
1	B	789	VAL
1	B	795	VAL
1	B	803	LEU
1	B	815[A]	ARG
1	B	815[B]	ARG
1	B	816	LEU
1	B	817	VAL
1	B	832	VAL
1	B	833	THR
1	B	837	LEU
1	C	10	PHE
1	C	12	ASP
1	C	26	LEU
1	C	31	VAL
1	C	74	ARG
1	C	91	LEU
1	C	95	VAL
1	C	99	GLN
1	C	101	ARG
1	C	107	ARG
1	C	112	SER
1	C	126	ARG
1	C	136	ILE
1	C	162	THR
1	C	174	LEU
1	C	175	THR
1	C	181	VAL
1	C	198	VAL
1	C	199	THR
1	C	202	ILE

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Mol	Chain	Res	Type
1	C	205	ASP
1	C	206	VAL
1	C	220	LEU
1	C	235	THR
1	C	239	THR
1	C	241	ARG
1	C	244	LYS
1	C	269	THR
1	C	278	VAL
1	C	279	GLN
1	C	298	GLU
1	C	302	VAL
1	C	303	THR
1	C	307	LEU
1	C	309	ILE
1	C	312	LEU
1	C	332	GLU
1	C	340	LYS
1	C	341	ASN
1	C	349	LEU
1	C	357	VAL
1	C	366	LEU
1	C	377	THR
1	C	380	LEU
1	C	385	LEU
1	C	389	ARG
1	C	407	GLU
1	C	412	LEU
1	C	427	LEU
1	C	437	VAL
1	C	450	LEU
1	C	476	VAL
1	C	490	HIS
1	C	491	THR
1	C	505	LEU
1	C	515	ASN
1	C	524	VAL
1	C	527	SER
1	C	536	LYS
1	C	537	SER
1	C	548	LEU
1	C	575	ARG

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Mol	Chain	Res	Type
1	C	585	ARG
1	C	586	LEU
1	C	587	VAL
1	C	588[A]	ARG
1	C	588[B]	ARG
1	C	592	LYS
1	C	596[A]	ARG
1	C	601	ASN
1	C	602[A]	MET
1	C	604	THR
1	C	637	LYS
1	C	642	GLU
1	C	653	GLU
1	C	670	THR
1	C	682	ARG
1	C	692	LEU
1	C	717	VAL
1	C	746	ARG
1	C	747	ARG
1	C	756	VAL
1	C	762	THR
1	C	764	LEU
1	C	769	VAL
1	C	772	LEU
1	C	779	LEU
1	C	785	THR
1	C	786	VAL
1	C	789	VAL
1	C	793	MET
1	C	795	VAL
1	C	803	LEU
1	C	805	ILE
1	C	837	LEU
1	C	841	LEU
1	C	842	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	99	GLN
1	A	134	GLN

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	397	ASN
1	A	413	HIS
1	A	432	ASN
1	A	542	GLN
1	A	582	GLN
1	A	591[A]	GLN
1	A	601	ASN
1	A	784	ASN
1	A	827	GLN
1	B	62	GLN
1	B	79	GLN
1	B	134	GLN
1	B	192	ASN
1	B	291	HIS
1	B	297	GLN
1	B	335	HIS
1	B	386	GLN
1	B	393	GLN
1	B	413	HIS
1	B	511	ASN
1	B	512	ASN
1	B	551	HIS
1	B	582	GLN
1	B	645	GLN
1	B	773[A]	GLN
1	B	775	GLN
1	B	784	ASN
1	B	794	GLN
1	C	62	GLN
1	C	78	ASN
1	C	99	GLN
1	C	134	GLN
1	C	335	HIS
1	C	393	GLN
1	C	494	HIS
1	C	582	GLN
1	C	591	GLN
1	C	601	ASN
1	C	611[A]	GLN
1	C	628	ASN
1	C	635	ASN

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Mol	Chain	Res	Type
1	C	643	HIS
1	C	673	ASN
1	C	765	HIS
1	C	775	GLN
1	C	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](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	C	902	4	28,29,29	1.52	5 (17%)	43,45,45	1.73	8 (18%)
2	ADP	B	902	-	28,29,29	1.45	3 (10%)	43,45,45	1.73	10 (23%)
2	ADP	B	901	-	28,29,29	1.49	4 (14%)	43,45,45	1.80	10 (23%)
2	ADP	C	901	-	28,29,29	1.44	4 (14%)	43,45,45	1.95	10 (23%)
2	ADP	A	902	-	28,29,29	1.37	4 (14%)	43,45,45	1.66	6 (13%)
2	ADP	A	901	-	28,29,29	1.51	5 (17%)	43,45,45	1.81	8 (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
2	ADP	C	902	4	-	3/16/32/32	0/3/3/3
2	ADP	B	902	-	-	0/16/32/32	0/3/3/3
2	ADP	B	901	-	-	0/16/32/32	0/3/3/3
2	ADP	C	901	-	-	3/16/32/32	0/3/3/3
2	ADP	A	902	-	-	1/16/32/32	0/3/3/3
2	ADP	A	901	-	-	6/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	ADP	C5-C4	5.51	1.48	1.39
2	B	901	ADP	C5-C4	4.98	1.48	1.39
2	B	902	ADP	C5-C4	4.92	1.47	1.39
2	A	901	ADP	C5-C4	4.90	1.47	1.39
2	C	901	ADP	C5-C4	4.68	1.47	1.39
2	A	902	ADP	C5-C4	4.65	1.47	1.39
2	A	901	ADP	C5-C6	2.88	1.49	1.41
2	B	902	ADP	C5-C6	2.86	1.49	1.41
2	B	901	ADP	C5-N7	-2.58	1.34	1.39
2	C	901	ADP	C5-C6	2.55	1.48	1.41
2	A	901	ADP	PA-O3A	2.52	1.62	1.59
2	C	902	ADP	C5-N7	-2.51	1.34	1.39
2	A	902	ADP	C5-C6	2.42	1.47	1.41
2	B	902	ADP	C8-N7	2.37	1.36	1.31
2	B	901	ADP	C5-C6	2.36	1.47	1.41
2	C	902	ADP	C5-C6	2.34	1.47	1.41
2	C	902	ADP	C4-N9	-2.33	1.32	1.37
2	C	901	ADP	C5-N7	-2.31	1.34	1.39
2	C	901	ADP	PA-O3A	2.26	1.61	1.59
2	A	902	ADP	C4-N9	-2.16	1.33	1.37
2	A	902	ADP	C5-N7	-2.14	1.35	1.39
2	A	901	ADP	C8-N7	2.13	1.35	1.31
2	B	901	ADP	C8-N7	2.11	1.35	1.31
2	A	901	ADP	C4-N9	-2.08	1.33	1.37
2	C	902	ADP	C8-N7	2.06	1.35	1.31

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	C5-C4-N3	-5.77	118.77	126.72
2	C	901	ADP	C5-C4-N3	-5.63	118.97	126.72
2	A	901	ADP	C5-C4-N3	-5.53	119.10	126.72
2	A	902	ADP	C5-C4-N3	-5.36	119.34	126.72
2	C	901	ADP	N3-C4-N9	5.15	135.92	127.17
2	B	901	ADP	N3-C4-N9	5.05	135.75	127.17
2	B	902	ADP	C5-C4-N3	-5.05	119.77	126.72
2	C	902	ADP	C5-C4-N3	-5.01	119.82	126.72
2	A	902	ADP	N3-C4-N9	4.83	135.38	127.17
2	A	901	ADP	N3-C4-N9	4.76	135.26	127.17
2	C	902	ADP	N3-C4-N9	4.49	134.81	127.17
2	B	902	ADP	N3-C4-N9	4.13	134.19	127.17
2	C	901	ADP	N3-C2-N1	-3.88	122.71	128.58
2	A	902	ADP	N3-C2-N1	-3.87	122.72	128.58
2	C	901	ADP	C2-N3-C4	3.79	121.09	111.83
2	A	901	ADP	C2-N3-C4	3.78	121.05	111.83
2	A	901	ADP	N3-C2-N1	-3.73	122.94	128.58
2	B	901	ADP	C2-N3-C4	3.54	120.47	111.83
2	A	902	ADP	C2-N3-C4	3.54	120.47	111.83
2	B	902	ADP	C2-N3-C4	3.47	120.31	111.83
2	B	901	ADP	N3-C2-N1	-3.43	123.39	128.58
2	B	902	ADP	N3-C2-N1	-3.30	123.59	128.58
2	C	902	ADP	C2-N3-C4	3.24	119.74	111.83
2	C	901	ADP	C4-N9-C8	3.23	109.13	105.74
2	C	902	ADP	N3-C2-N1	-3.12	123.86	128.58
2	B	902	ADP	C4-C5-N7	-3.12	107.02	110.58
2	B	902	ADP	C4-N9-C8	2.86	108.74	105.74
2	A	901	ADP	C4-N9-C8	2.85	108.73	105.74
2	C	902	ADP	O4'-C1'-N9	2.77	113.40	108.09
2	C	902	ADP	C2'-C1'-N9	2.72	120.06	113.30
2	C	901	ADP	C2'-C1'-N9	-2.66	106.70	113.30
2	A	901	ADP	C4-C5-N7	-2.64	107.56	110.58
2	A	902	ADP	C2-N1-C6	2.59	122.99	118.73
2	B	901	ADP	C4-C5-N7	-2.57	107.65	110.58
2	B	901	ADP	C4-N9-C8	2.52	108.38	105.74
2	C	901	ADP	C4-C5-N7	-2.49	107.73	110.58
2	A	902	ADP	C4-N9-C8	2.49	108.35	105.74
2	B	901	ADP	N6-C6-N1	2.46	123.87	118.38
2	B	902	ADP	C5-N7-C8	2.45	107.31	103.45
2	B	902	ADP	C6-C5-N7	2.25	136.43	132.09
2	B	901	ADP	C2-N1-C6	2.20	122.35	118.73
2	B	902	ADP	N9-C8-N7	-2.15	110.89	113.94
2	C	901	ADP	C5-N7-C8	2.11	106.77	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	ADP	O4'-C1'-N9	2.08	112.08	108.09
2	B	901	ADP	C5-N7-C8	2.07	106.70	103.45
2	B	901	ADP	O3B-PB-O2B	2.05	115.48	107.80
2	C	902	ADP	N6-C6-N1	2.04	122.92	118.38
2	C	901	ADP	C2-N1-C6	2.03	122.07	118.73
2	C	902	ADP	O4'-C1'-C2'	-2.03	102.27	106.62
2	A	901	ADP	C5'-C4'-C3'	-2.02	107.93	115.21
2	A	901	ADP	C2-N1-C6	2.01	122.03	118.73
2	C	901	ADP	O5'-C5'-C4'	2.01	115.82	108.99

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADP	PA-O3A-PB-O2B
2	A	901	ADP	PA-O3A-PB-O3B
2	A	901	ADP	C5'-O5'-PA-O1A
2	A	901	ADP	O4'-C4'-C5'-O5'
2	A	901	ADP	C3'-C4'-C5'-O5'
2	C	902	ADP	C5'-O5'-PA-O2A
2	C	902	ADP	C5'-O5'-PA-O3A
2	C	901	ADP	O4'-C4'-C5'-O5'
2	C	901	ADP	C3'-C4'-C5'-O5'
2	A	901	ADP	C5'-O5'-PA-O3A
2	C	902	ADP	C5'-O5'-PA-O1A
2	C	901	ADP	C4'-C5'-O5'-PA
2	A	902	ADP	PB-O3A-PA-O2A

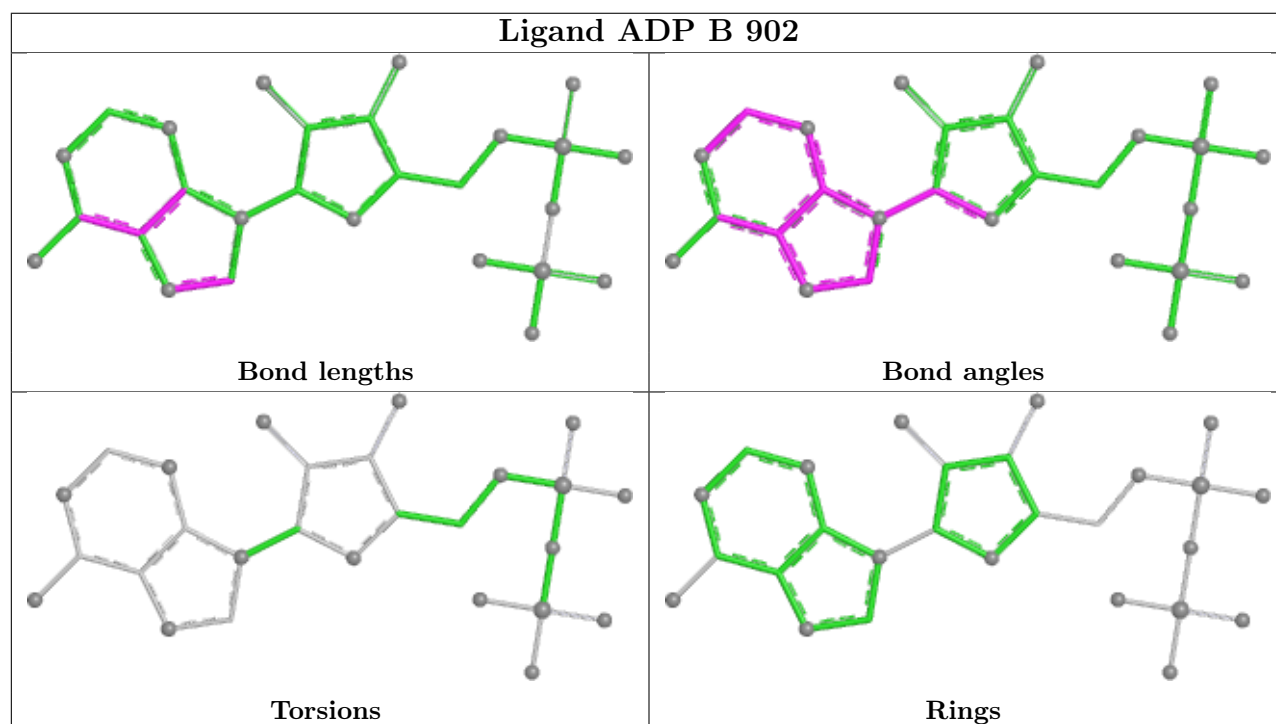
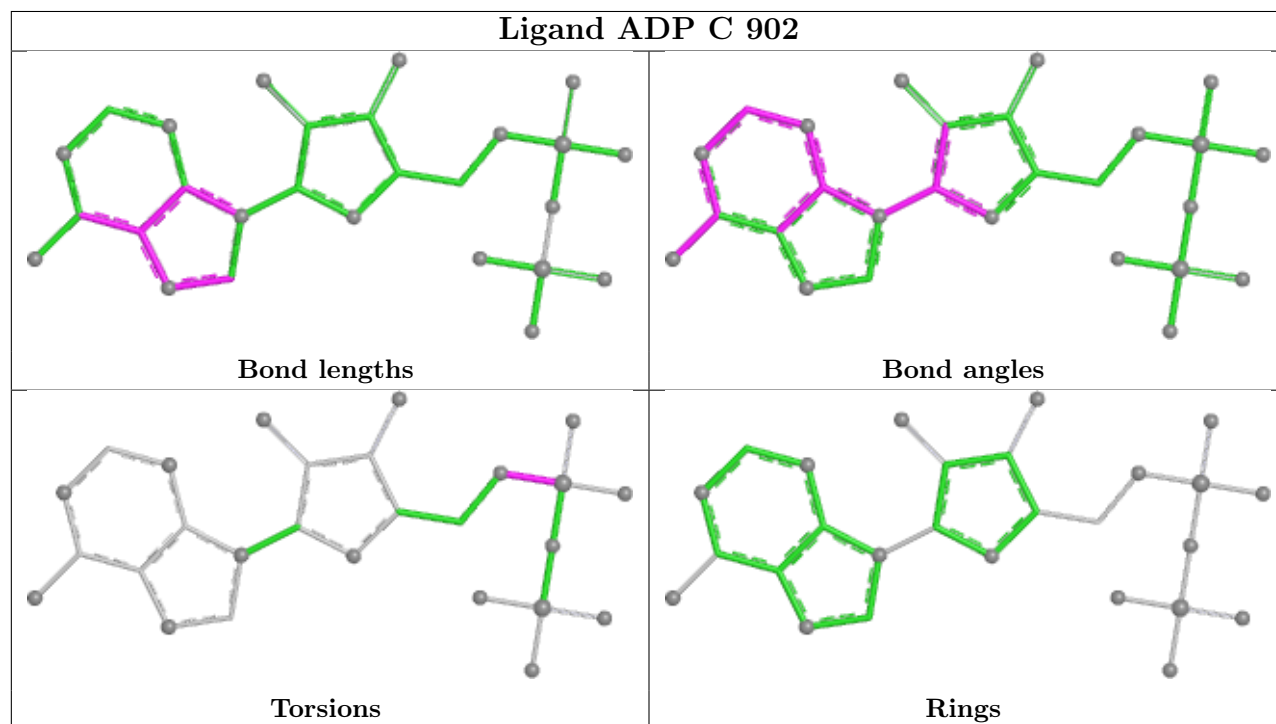
There are no ring outliers.

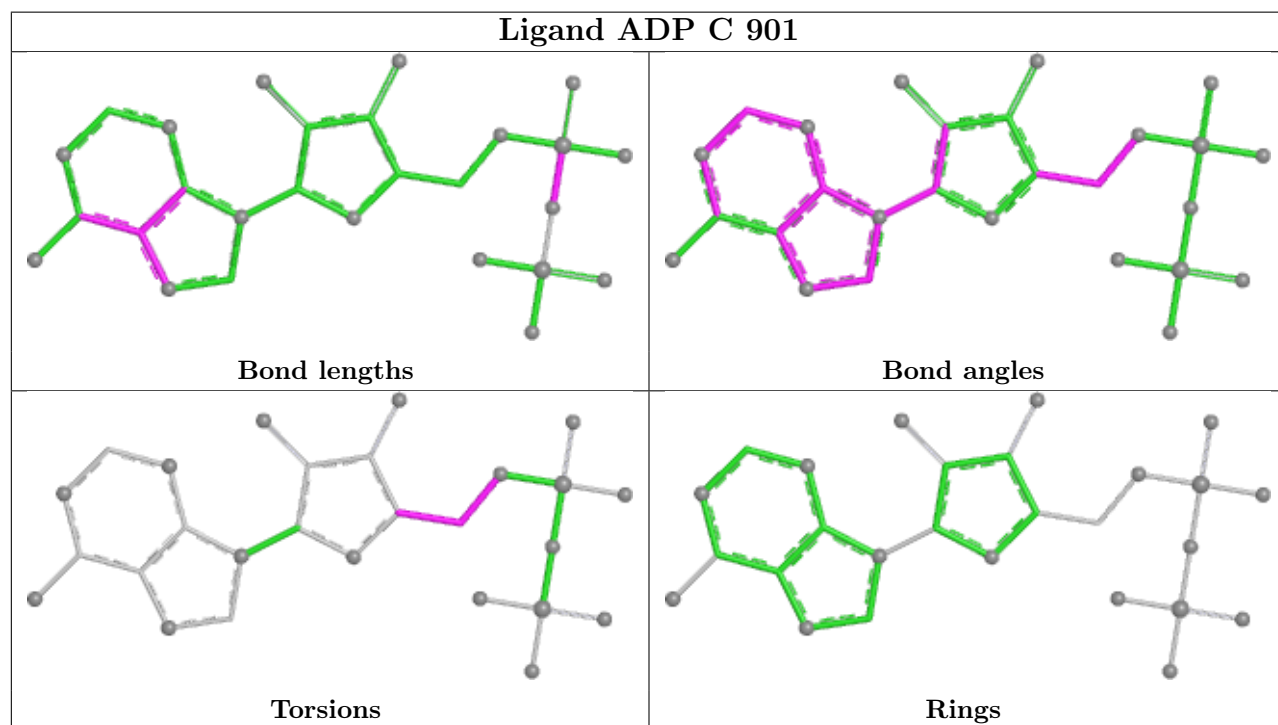
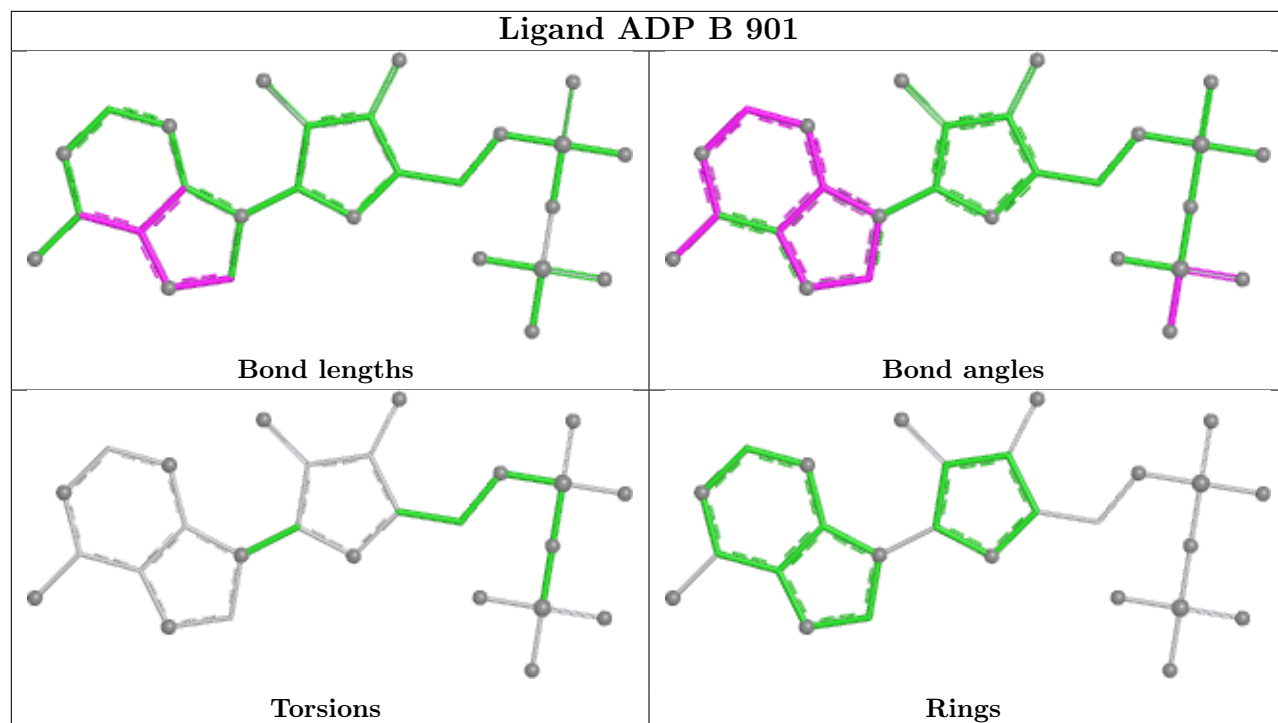
4 monomers are involved in 8 short contacts:

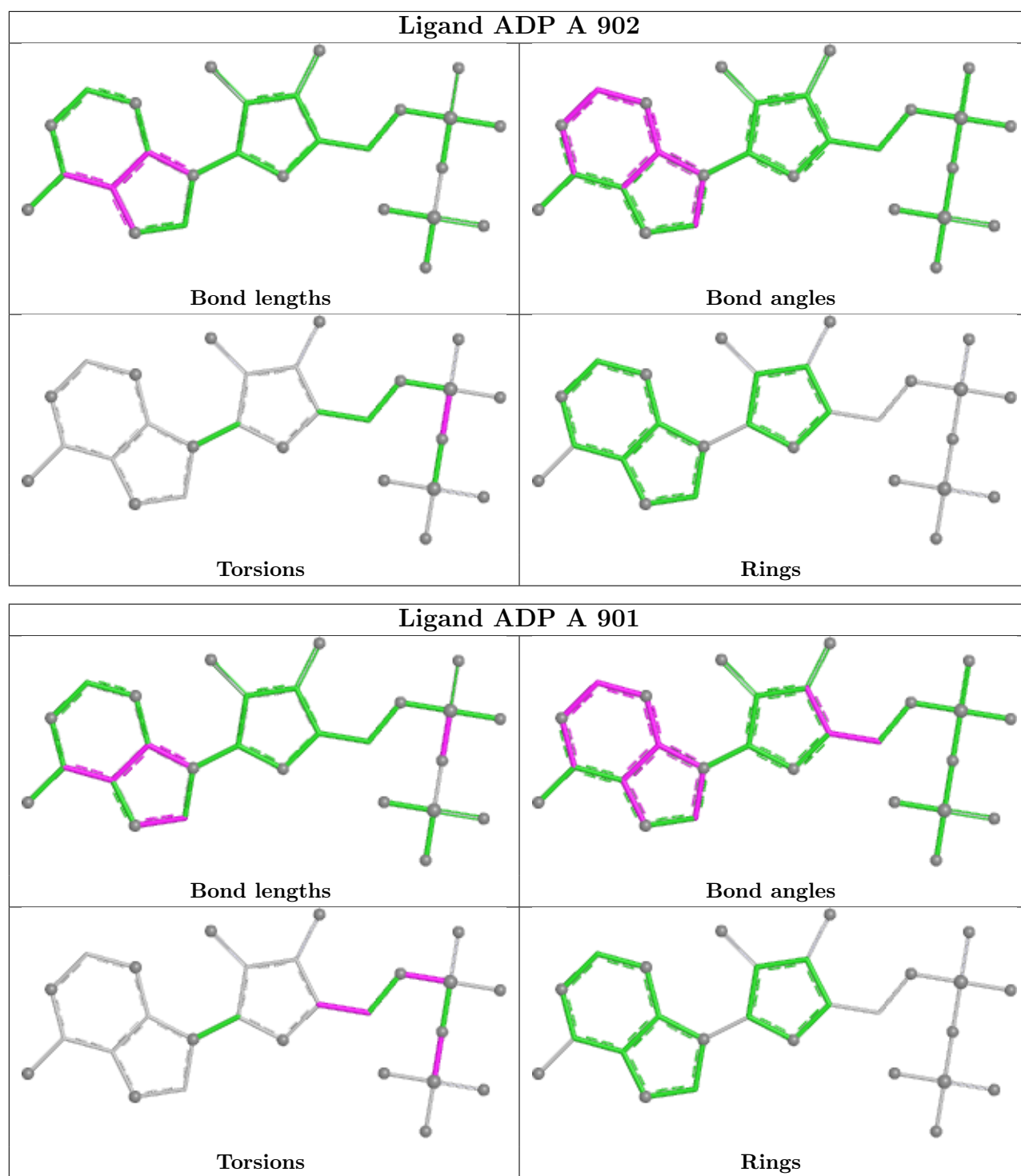
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	902	ADP	3	0
2	B	901	ADP	1	0
2	C	901	ADP	3	0
2	A	901	ADP	1	0

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.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	134:GLN	C	135:GLY	N	1.68

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	815/842 (96%)	0.99	68 (8%) 17 19	43, 57, 70, 79	6 (0%)
1	B	813/842 (96%)	0.97	75 (9%) 14 16	30, 56, 70, 88	7 (0%)
1	C	814/842 (96%)	0.87	69 (8%) 16 18	28, 56, 69, 81	9 (1%)
All	All	2442/2526 (96%)	0.94	212 (8%) 16 17	28, 56, 70, 88	22 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	4.9
1	A	654	LEU	4.7
1	A	656	PHE	4.7
1	A	806	GLY	4.6
1	C	152	PRO	4.6
1	A	72	TYR	4.5
1	C	588[A]	ARG	4.5
1	C	491	THR	4.1
1	B	454	GLY	4.1
1	B	72	TYR	3.9
1	C	660	VAL	3.9
1	B	132	PRO	3.8
1	C	654	LEU	3.8
1	B	749	GLY	3.8
1	B	81	GLY	3.7
1	B	660	VAL	3.7
1	A	343	PRO	3.7
1	A	336	ALA	3.6
1	B	674	ALA	3.6
1	B	73	ALA	3.6
1	C	655	LEU	3.5
1	B	603	ALA	3.5
1	A	73	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	77	PHE	3.4
1	A	321	SER	3.3
1	A	128	GLY	3.3
1	A	102	GLY	3.2
1	C	150	ALA	3.2
1	A	142	PHE	3.2
1	A	11	PRO	3.2
1	C	73	ALA	3.1
1	B	627	TYR	3.1
1	B	669	GLY	3.1
1	B	618	ALA	3.1
1	B	10	PHE	3.0
1	B	77	PHE	2.9
1	B	632	PHE	2.9
1	C	249	PRO	3.0
1	A	657	LEU	2.9
1	C	340	LYS	2.9
1	A	334	GLY	2.9
1	A	131	PRO	2.9
1	C	343	PRO	2.9
1	B	706	ALA	2.9
1	A	347	ILE	2.9
1	C	274	MET	2.9
1	C	161	TYR	2.8
1	A	79	GLN	2.8
1	C	272	ALA	2.8
1	C	348	ALA	2.8
1	C	247[A]	MET	2.8
1	C	327	TYR	2.8
1	B	702	ALA	2.8
1	B	80	ALA	2.8
1	C	494	HIS	2.8
1	C	806	GLY	2.8
1	B	651	MET	2.8
1	C	335	HIS	2.7
1	B	8	PRO	2.7
1	A	291	HIS	2.7
1	A	649	TRP	2.7
1	B	637	LYS	2.7
1	B	265	THR	2.7
1	B	709	ARG	2.7
1	B	806	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	PRO	2.7
1	C	144	PRO	2.7
1	A	653	GLU	2.6
1	A	136	ILE	2.6
1	C	337	GLU	2.6
1	C	138	TYR	2.6
1	B	578	GLY	2.6
1	C	487	ALA	2.6
1	A	130	TYR	2.6
1	B	11	PRO	2.6
1	A	341	ASN	2.5
1	C	656	PHE	2.5
1	B	686	ILE	2.5
1	A	327	TYR	2.5
1	A	126	ARG	2.5
1	C	339	VAL	2.5
1	B	629	ALA	2.5
1	A	689	VAL	2.5
1	A	385	LEU	2.5
1	A	100	ALA	2.5
1	B	577	GLY	2.5
1	A	761	THR	2.4
1	B	105	THR	2.4
1	A	690	LEU	2.4
1	C	277	ARG	2.4
1	B	619	THR	2.4
1	B	453	VAL	2.4
1	C	77	PHE	2.4
1	A	76	LEU	2.4
1	A	554	GLN	2.4
1	A	248[A]	GLU	2.4
1	C	344	GLU	2.4
1	A	658	PRO	2.4
1	C	146	THR	2.4
1	C	262	VAL	2.4
1	C	132	PRO	2.3
1	C	669	GLY	2.3
1	A	267	ALA	2.3
1	B	299	ALA	2.3
1	B	636	VAL	2.3
1	A	295	LEU	2.3
1	B	677	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	329	GLU	2.3
1	B	703	ASP	2.3
1	C	341	ASN	2.3
1	A	627	TYR	2.3
1	B	71	PRO	2.3
1	C	131	PRO	2.3
1	C	251	TYR	2.3
1	A	572	GLY	2.3
1	C	80	ALA	2.3
1	C	76	LEU	2.3
1	C	288	PRO	2.3
1	C	814	GLY	2.3
1	A	272	ALA	2.3
1	B	164	THR	2.3
1	C	136	ILE	2.3
1	B	701	PHE	2.3
1	B	289	LEU	2.3
1	B	621	LEU	2.3
1	A	301	ASN	2.3
1	B	74	ARG	2.3
1	B	241[A]	ARG	2.3
1	C	492	GLU	2.3
1	A	686	ILE	2.3
1	A	339	VAL	2.3
1	B	15	PHE	2.2
1	C	488	ASP	2.2
1	A	333	PRO	2.2
1	A	139	ALA	2.2
1	A	354	ALA	2.2
1	B	642	GLU	2.2
1	A	748	SER	2.2
1	C	125	SER	2.2
1	B	707	ILE	2.2
1	A	302	VAL	2.2
1	A	513	LEU	2.2
1	A	679	VAL	2.2
1	B	476	VAL	2.2
1	C	304	PHE	2.2
1	A	514	ASP	2.2
1	C	223	ASP	2.2
1	A	277	ARG	2.2
1	A	602	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	147	PRO	2.2
1	C	577	GLY	2.2
1	B	678	GLU	2.2
1	B	617	ALA	2.2
1	A	522	LEU	2.2
1	B	263	LEU	2.2
1	B	615	LEU	2.2
1	C	44	VAL	2.2
1	B	620	PRO	2.2
1	A	133	GLY	2.2
1	A	345	GLN	2.2
1	A	125	SER	2.2
1	B	163	VAL	2.2
1	C	804	ASP	2.2
1	C	11	PRO	2.2
1	A	344	GLU	2.2
1	C	72	TYR	2.1
1	B	157	LEU	2.1
1	B	312	LEU	2.1
1	B	685	ASN	2.1
1	C	453	VAL	2.1
1	A	293	LYS	2.1
1	B	752	GLY	2.1
1	C	156	GLY	2.1
1	B	242	ALA	2.1
1	B	659	SER	2.1
1	C	271	SER	2.1
1	C	328	ALA	2.1
1	C	484	TYR	2.1
1	B	699	ASP	2.1
1	B	490	HIS	2.1
1	B	689	VAL	2.1
1	B	491	THR	2.1
1	C	101	ARG	2.1
1	C	346	ALA	2.1
1	B	610	ASP	2.1
1	B	672	TYR	2.1
1	C	130	TYR	2.1
1	B	198	VAL	2.1
1	C	206	VAL	2.1
1	B	801	TRP	2.1
1	C	115	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	622	ALA	2.1
1	B	662	ALA	2.1
1	A	655	LEU	2.1
1	C	583	ILE	2.1
1	C	607	GLY	2.1
1	C	74	ARG	2.1
1	A	89	ASP	2.0
1	B	347	ILE	2.0
1	C	347	ILE	2.0
1	A	138	TYR	2.0
1	B	650	VAL	2.0
1	A	749	GLY	2.0
1	A	340	LYS	2.0
1	B	100	ALA	2.0
1	B	79	GLN	2.0
1	A	78	ASN	2.0
1	A	243	LEU	2.0
1	C	203	ASP	2.0
1	A	842	ARG	2.0
1	B	625	ARG	2.0
1	B	614	LYS	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.

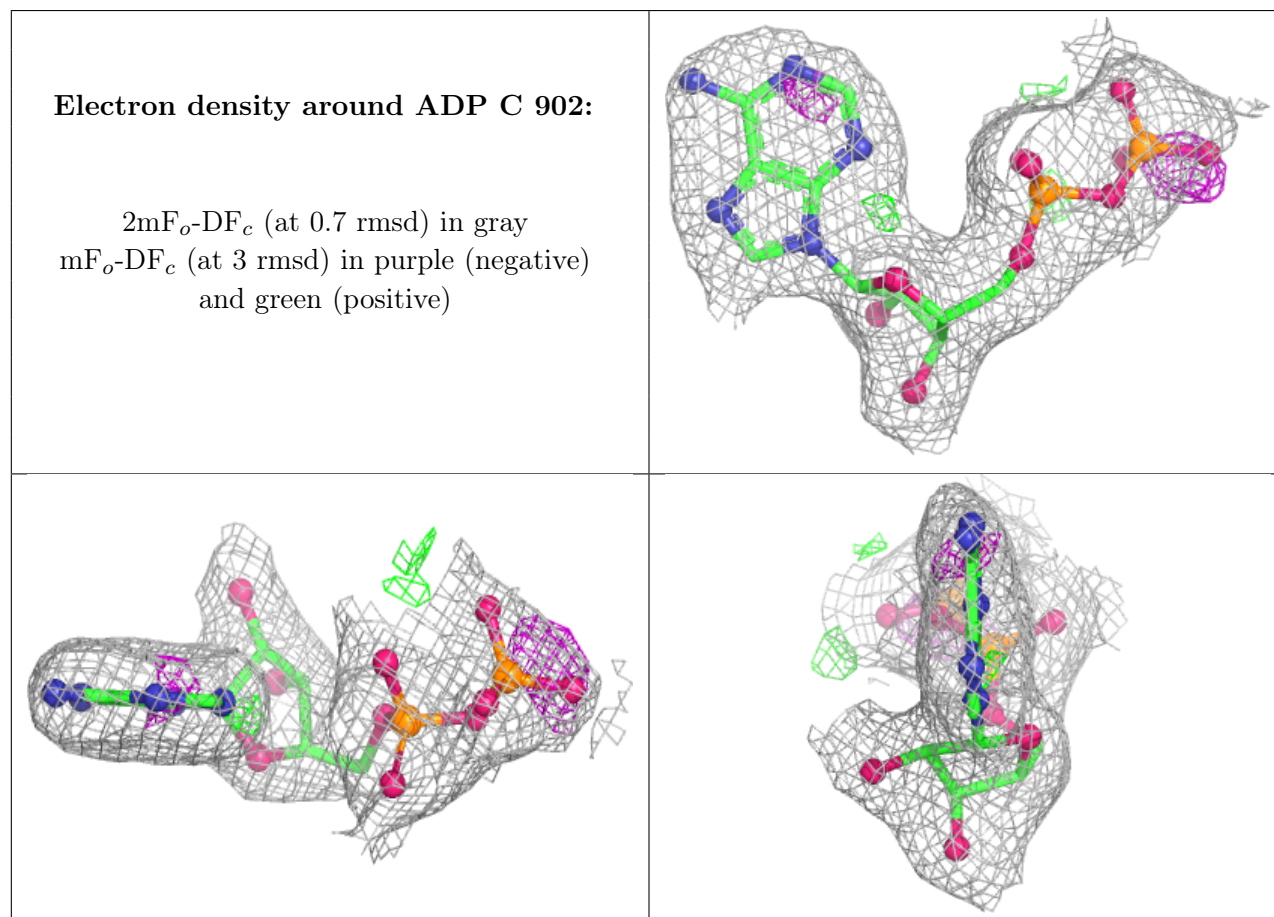
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	903	1/1	0.91	0.16	70,70,70,70	1
3	ZN	B	904	1/1	0.92	0.15	59,59,59,59	1

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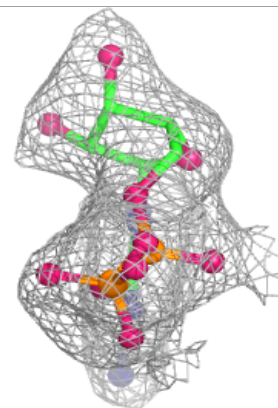
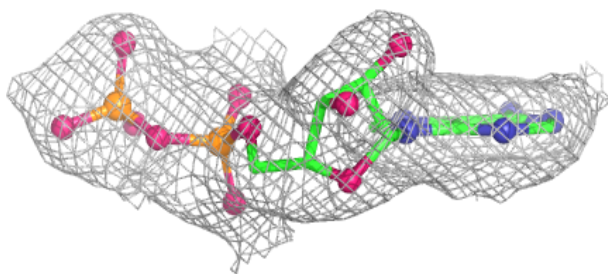
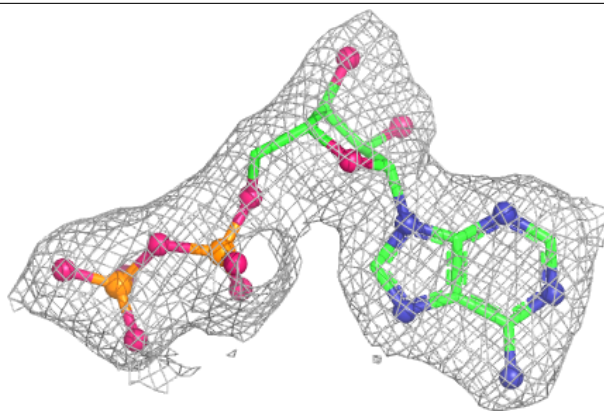
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	905	1/1	0.92	0.13	42,42,42,42	0
2	ADP	C	902	27/27	0.93	0.09	39,45,56,57	0
2	ADP	B	902	27/27	0.95	0.08	46,50,58,59	0
2	ADP	C	901	27/27	0.95	0.08	48,55,56,57	1
2	ADP	A	901	27/27	0.96	0.06	43,55,56,57	0
2	ADP	B	901	27/27	0.96	0.07	35,40,42,43	0
2	ADP	A	902	27/27	0.97	0.06	36,39,45,47	0
3	ZN	A	903	1/1	0.98	0.07	59,59,59,59	1
3	ZN	C	904	1/1	0.99	0.02	66,66,66,66	1
3	ZN	B	903	1/1	0.99	0.03	71,71,71,71	0
3	ZN	A	904	1/1	1.00	0.02	55,55,55,55	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.

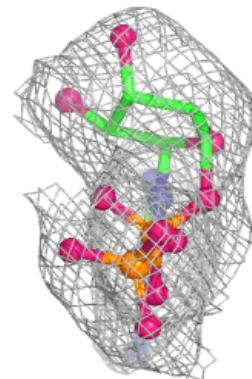
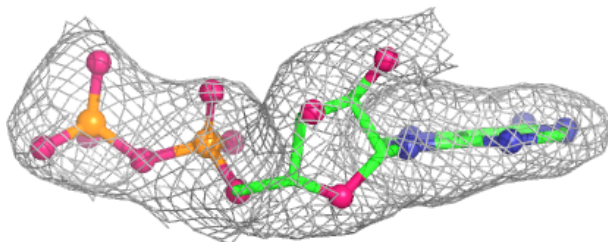
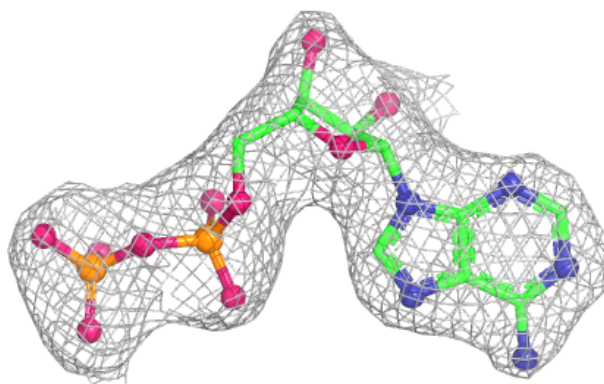


Electron density around ADP B 902:

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

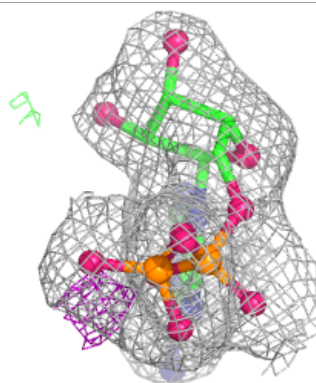
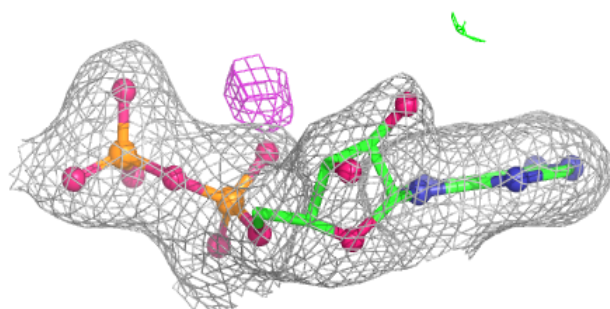
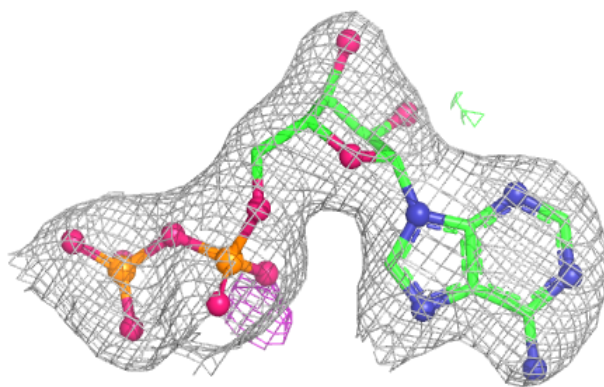
**Electron density around ADP C 901:**

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

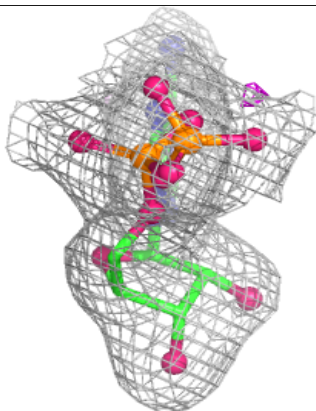
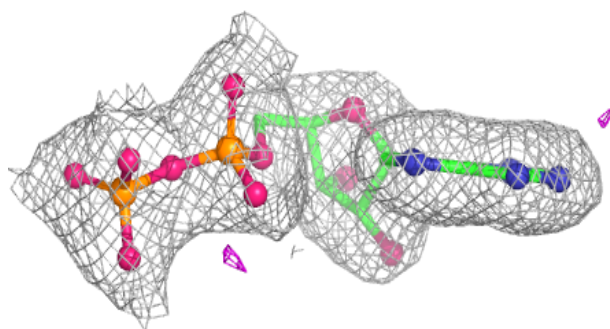
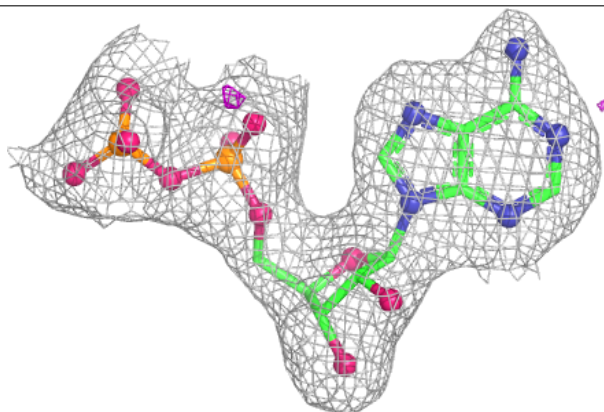


Electron density around ADP A 901:

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

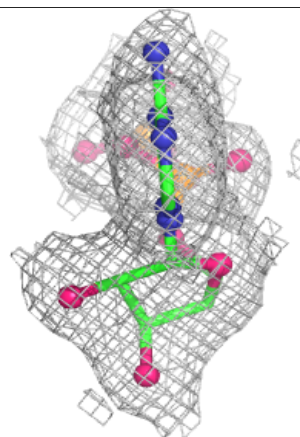
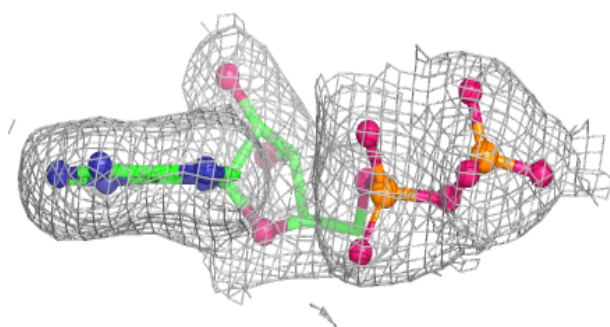
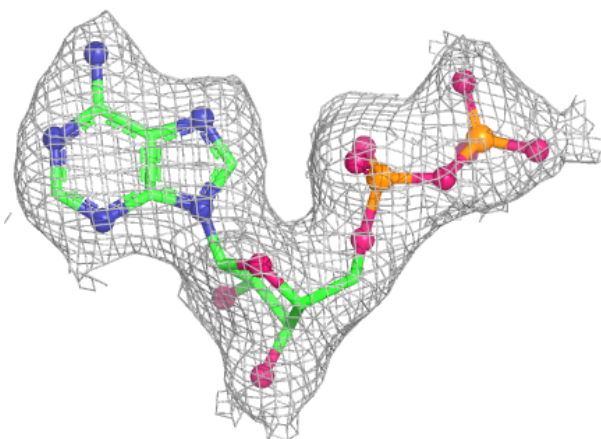
**Electron density around ADP B 901:**

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



Electron density around ADP A 902:

$2mF_o - DF_c$ (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.