Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:48 pm BST

PDB ID	:	4AM7
Title	:	ADP-BOUND C-TERMINAL DOMAIN OF ACTIN-RELATED PROTEIN ARP8 FROM S. CEREVISIAE
Authors	:	Wuerges, J.; Saravanan, M.; Bose, D.; Cook, N.J.; Zhang, X.; Wigley, D.B.
Deposited on	:	2012-03-07
Resolution	:	3.25 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 following versions of software and data (see references ⓘ) were used in the production of this report:

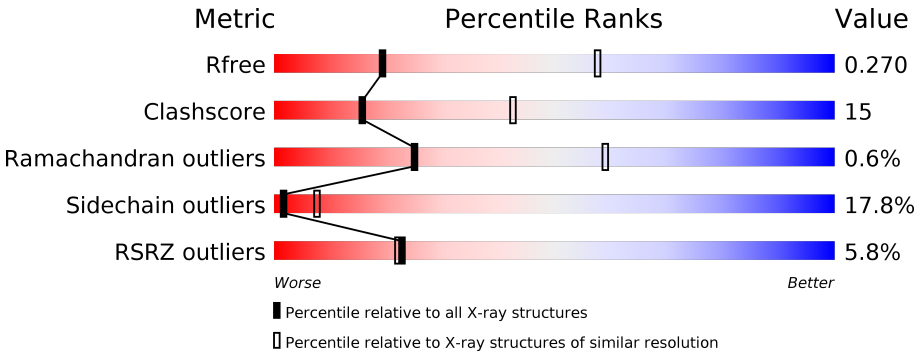
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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 <=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	655	5% 60% 27% 7% • 5%
1	B	655	6% 57% 31% 7% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10126 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 ACTIN-LIKE PROTEIN ARP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			5036	3219	840	963	14			
1	B	623	Total	C	N	O	S	0	0	0
			5036	3219	840	963	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	expression tag	UNP Q12386
A	228	GLY	-	expression tag	UNP Q12386
A	229	SER	-	expression tag	UNP Q12386
A	230	SER	-	expression tag	UNP Q12386
A	231	HIS	-	expression tag	UNP Q12386
A	232	HIS	-	expression tag	UNP Q12386
A	233	HIS	-	expression tag	UNP Q12386
A	234	HIS	-	expression tag	UNP Q12386
A	235	HIS	-	expression tag	UNP Q12386
A	236	HIS	-	expression tag	UNP Q12386
A	237	SER	-	expression tag	UNP Q12386
A	238	SER	-	expression tag	UNP Q12386
A	239	GLY	-	expression tag	UNP Q12386
A	240	LEU	-	expression tag	UNP Q12386
A	241	VAL	-	expression tag	UNP Q12386
A	242	PRO	-	expression tag	UNP Q12386
A	243	ARG	-	expression tag	UNP Q12386
A	244	GLY	-	expression tag	UNP Q12386
A	245	SER	-	expression tag	UNP Q12386
A	246	HIS	-	expression tag	UNP Q12386
A	247	MET	-	expression tag	UNP Q12386
B	227	MET	-	expression tag	UNP Q12386
B	228	GLY	-	expression tag	UNP Q12386
B	229	SER	-	expression tag	UNP Q12386
B	230	SER	-	expression tag	UNP Q12386

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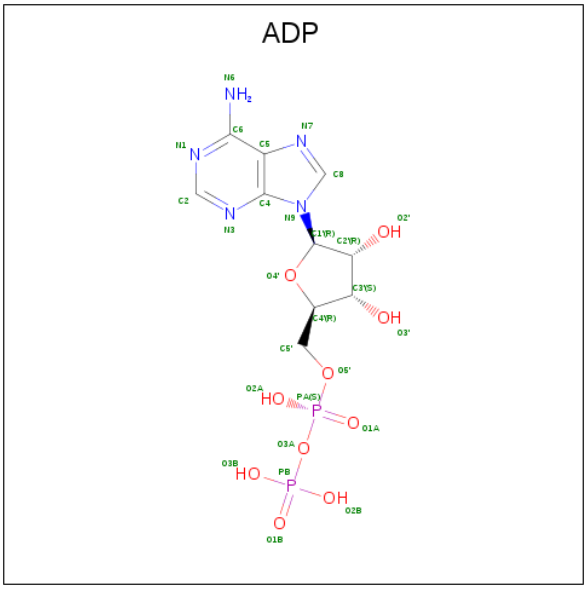
Chain	Residue	Modelled	Actual	Comment	Reference
B	231	HIS	-	expression tag	UNP Q12386
B	232	HIS	-	expression tag	UNP Q12386
B	233	HIS	-	expression tag	UNP Q12386
B	234	HIS	-	expression tag	UNP Q12386
B	235	HIS	-	expression tag	UNP Q12386
B	236	HIS	-	expression tag	UNP Q12386
B	237	SER	-	expression tag	UNP Q12386
B	238	SER	-	expression tag	UNP Q12386
B	239	GLY	-	expression tag	UNP Q12386
B	240	LEU	-	expression tag	UNP Q12386
B	241	VAL	-	expression tag	UNP Q12386
B	242	PRO	-	expression tag	UNP Q12386
B	243	ARG	-	expression tag	UNP Q12386
B	244	GLY	-	expression tag	UNP Q12386
B	245	SER	-	expression tag	UNP Q12386
B	246	HIS	-	expression tag	UNP Q12386
B	247	MET	-	expression tag	UNP Q12386

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



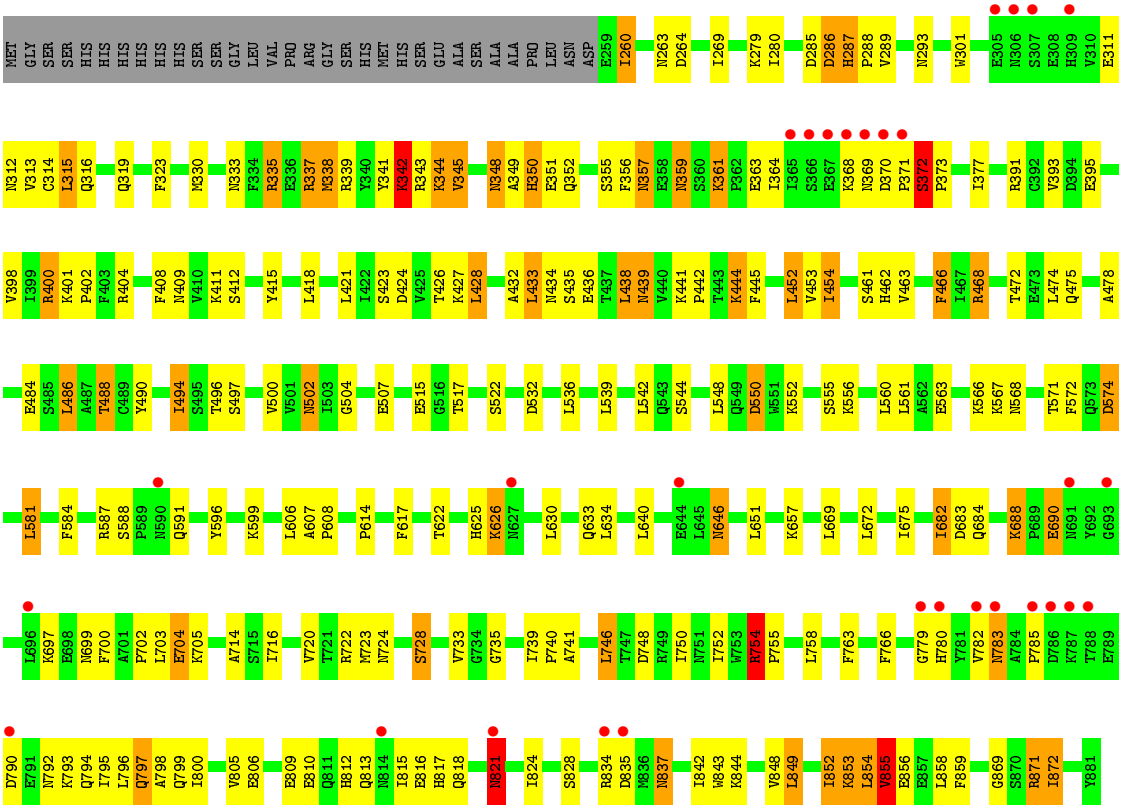
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

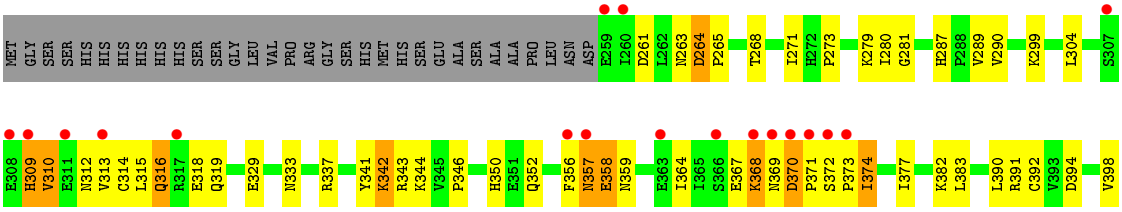
• Molecule 1: ACTIN-LIKE PROTEIN ARP8

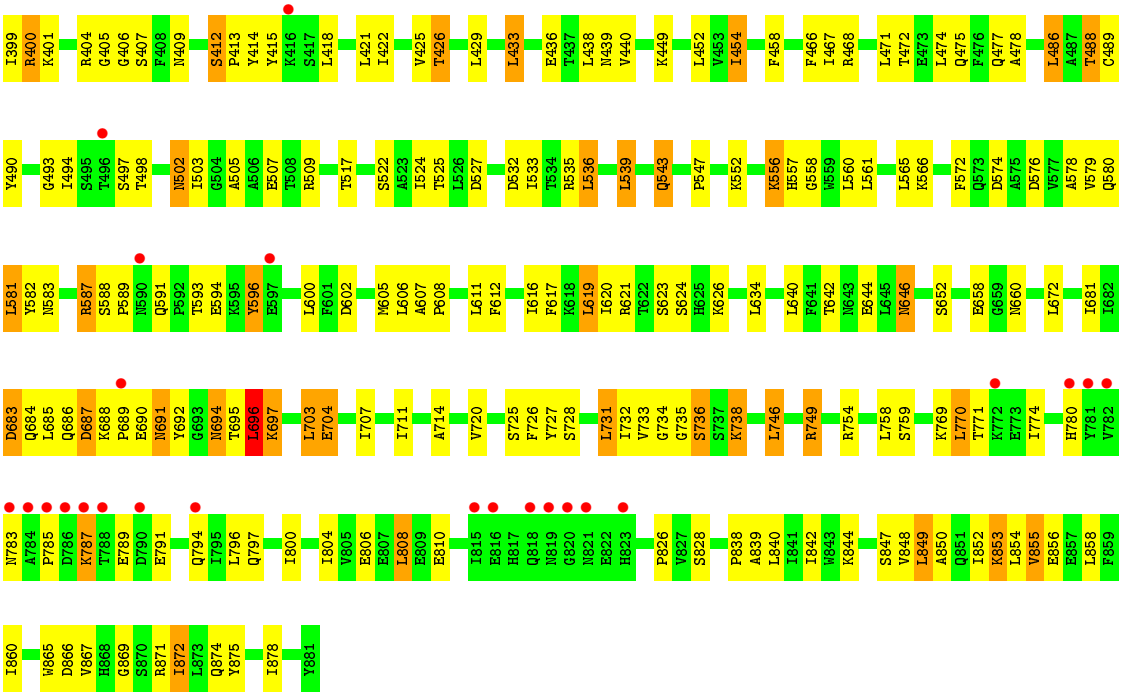
Chain A:



• Molecule 1: ACTIN-LIKE PROTEIN ARP8

Chain B:




I399 R400 K401 R404 G405 G406 S407 F408 N409 S412 P413 Y414 Y415 K416 S417 L418 L421 I422 V425 T426 L429 L433 E436 T437 L438 N439 V440 K449 L452 V453 I454 F458 F466 I467 R468 L471 T472 E473 L474 Q475 F476 Q477 A478 L486 A487 T488 C489
Y490 G493 I494 S495 T496 S497 T498 N502 I503 G504 A505 A506 E507 T508 R509 T517 S522 A523 I524 T525 L526 D527 D532 I533 T534 R535 L536 L539 Q543 P547 K552 K556 H557 G558 W559 L560 L561 L565 K566 F572 Q573 D574 A575 D576 V577 A578 V579 Q580
L581 Y582 N583 R587 S588 P589 N590 Q591 P592 T593 E594 K595 Y596 E597 L600 F601 D602 M605 L606 A607 P608 L611 F612 I616 F617 K618 L619 I620 R621 T622 S623 S624 H625 K626 L634 L640 P641 T642 N643 E644 L645 M646 S652 E658 G659 M660 L672 I681 I682
D683 Q684 L685 Q686 D687 K688 P689 E690 N691 Y692 G693 M694 T695 L696 K697 L703 E704 I707 I711 A714 V720 S725 F726 Y727 S728 L731 I732 V733 G734 G735 S736 S737 K738 L746 R749 R754 L758 S759 K769 L770 T771 K772 E773 I774 H780 Y781 V782
N783 A784 P785 D786 K787 T788 E789 D790 E791 Q794 T795 L796 Q797 I800 I804 V805 E806 E807 L808 E809 E810 I815 E816 H817 Q818 N819 G820 N821 E822 H823 P826 V827 S828 P838 A839 L840 I841 I842 W843 K844 S847 V848 L849 A850 Q851 I852 K853 L854 V855 E856 E857 L858 F859
I860 W865 D866 V867 H868 G869 S870 R871 I872 L873 Q874 Y875 I878 Y881

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.72Å 89.80Å 149.65Å 90.00° 114.37° 90.00°	Depositor
Resolution (Å)	19.81 – 3.25 19.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.81-3.25) 96.5 (19.81-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.219 , 0.284 0.215 , 0.270	Depositor DCC
R_{free} test set	1301 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	98.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10126	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.65	0/5149	0.77	6/6982 (0.1%)
1	B	0.54	0/5149	0.70	4/6982 (0.1%)
All	All	0.60	0/10298	0.74	10/13964 (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	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	LYS	N-CA-C	6.07	127.39	111.00
1	A	335	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	350	HIS	N-CA-C	5.73	126.47	111.00
1	B	370	ASP	N-CA-C	5.58	126.06	111.00
1	A	858	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	581	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	493	GLY	N-CA-C	-5.28	99.90	113.10
1	B	581	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	754	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	696	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ALA	Peptide
1	A	688	LYS	Peptide
1	A	690	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5036	0	4985	159	0
1	B	5036	0	4985	138	0
2	A	27	0	12	4	0
2	B	27	0	12	1	0
All	All	10126	0	9994	296	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 15.

All (296) 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:335:ARG:HB3	1:A:339:ARG:HH12	1.06	1.18
1:A:335:ARG:HB3	1:A:339:ARG:NH1	1.73	1.03
1:A:315:LEU:HG	1:A:316:GLN:H	1.27	0.97
1:A:790:ASP:HB2	1:A:793:LYS:HB2	1.44	0.97
1:A:372:SER:HB3	1:A:373:PRO:HD2	1.48	0.94
1:B:372:SER:HB2	1:B:373:PRO:HD2	1.50	0.92
1:B:535:ARG:HD3	1:B:620:ILE:HG22	1.53	0.91
1:A:790:ASP:CB	1:A:793:LYS:HB2	2.01	0.91
1:B:642:THR:HG22	1:B:644:GLU:HB2	1.52	0.90
1:A:434:ASN:ND2	1:A:441:LYS:HE2	1.89	0.86
1:B:587:ARG:HD3	1:B:589:PRO:HD3	1.58	0.85
1:A:688:LYS:HB3	1:A:690:GLU:HB3	1.59	0.84
1:B:684:GLN:O	1:B:688:LYS:HB2	1.77	0.84
1:A:315:LEU:HG	1:A:316:GLN:N	1.93	0.82
1:A:795:ILE:HA	1:A:798:ALA:HB3	1.60	0.82
1:A:785:PRO:HB2	1:A:793:LYS:HD2	1.62	0.81
1:A:372:SER:HB3	1:A:373:PRO:CD	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ASP:O	1:B:689:PRO:HD3	1.83	0.78
1:A:434:ASN:HD21	1:A:441:LYS:HE2	1.45	0.78
1:B:488:THR:HG22	1:B:842:ILE:HG12	1.67	0.77
1:B:731:LEU:HD22	1:B:733:VAL:HG23	1.67	0.76
1:B:860:ILE:HG23	1:B:872:ILE:HD12	1.67	0.74
1:B:524:ILE:HD11	1:B:652:SER:HB3	1.69	0.74
1:A:849:LEU:HD22	1:A:855:VAL:HG13	1.69	0.73
1:B:527:ASP:O	1:B:621:ARG:NH2	2.21	0.73
1:B:505:ALA:HA	2:B:1882:ADP:O3'	1.88	0.73
1:A:502:ASN:HD22	1:A:502:ASN:C	1.92	0.72
1:B:358:GLU:HB2	1:B:594:GLU:HG2	1.69	0.72
1:A:522:SER:HB3	1:A:714:ALA:HB2	1.72	0.70
1:A:735:GLY:HA3	2:A:1882:ADP:H5'2	1.74	0.70
1:B:374:ILE:H	1:B:374:ILE:HD12	1.57	0.70
2:A:1882:ADP:O2A	2:A:1882:ADP:O1B	2.07	0.69
1:A:817:HIS:HD2	1:A:818:GLN:N	1.89	0.69
1:B:333:ASN:HD21	1:B:749:ARG:HH21	1.43	0.67
1:A:279:LYS:N	1:A:279:LYS:HD2	2.10	0.66
1:A:783:ASN:H	1:A:783:ASN:HD22	1.42	0.66
1:A:490:TYR:HE1	1:A:494:ILE:HD12	1.60	0.66
1:B:557:HIS:HB2	1:B:587:ARG:HB3	1.78	0.65
1:B:704:GLU:HA	1:B:707:ILE:HD12	1.80	0.63
1:B:532:ASP:HB3	1:B:617:PHE:CD1	2.33	0.63
1:A:372:SER:CB	1:A:373:PRO:CD	2.77	0.63
1:A:279:LYS:HD2	1:A:279:LYS:H	1.64	0.62
1:A:869:GLY:O	1:A:872:ILE:HD13	1.99	0.62
1:B:642:THR:CG2	1:B:644:GLU:HB2	2.28	0.62
1:B:738:LYS:HD3	1:B:838:PRO:HG3	1.81	0.62
1:A:315:LEU:CG	1:A:316:GLN:N	2.62	0.62
1:A:343:ARG:HG3	1:A:344:LYS:N	2.15	0.62
1:A:400:ARG:NH1	1:A:424:ASP:OD2	2.32	0.61
1:B:372:SER:HB2	1:B:373:PRO:CD	2.29	0.61
1:A:368:LYS:HG2	1:A:369:ASN:H	1.65	0.61
1:A:688:LYS:CB	1:A:690:GLU:HB3	2.29	0.61
1:B:502:ASN:HD22	1:B:502:ASN:C	2.04	0.61
1:A:286:ASP:OD1	1:A:286:ASP:N	2.29	0.60
1:A:817:HIS:CD2	1:A:818:GLN:N	2.69	0.60
1:A:809:GLU:O	1:A:813:GLN:HG3	2.02	0.60
1:B:535:ARG:HD3	1:B:620:ILE:CG2	2.29	0.60
1:B:587:ARG:HD3	1:B:589:PRO:CD	2.29	0.60
1:A:370:ASP:H	1:A:371:PRO:HD3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASP:HB3	1:A:617:PHE:CD1	2.37	0.60
1:A:702:PRO:HB2	1:A:704:GLU:OE1	2.01	0.60
1:B:733:VAL:HG12	1:B:734:GLY:N	2.16	0.60
1:A:488:THR:HB	1:A:842:ILE:HD13	1.84	0.59
1:B:261:ASP:HB3	1:B:477:GLN:OE1	2.02	0.59
1:A:293:ASN:O	1:A:401:LYS:HG2	2.03	0.58
1:A:337:ARG:NH2	1:A:748:ASP:OD2	2.27	0.58
1:A:484:GLU:O	1:A:488:THR:HG22	2.04	0.58
1:B:806:GLU:O	1:B:810:GLU:HB2	2.03	0.58
1:B:333:ASN:ND2	1:B:749:ARG:HH21	2.01	0.57
1:A:567:LYS:HE3	2:A:1882:ADP:N7	2.20	0.57
1:A:454:ILE:HD11	1:A:463:VAL:HG13	1.86	0.57
1:B:400:ARG:HD3	1:B:415:TYR:CZ	2.40	0.57
1:B:263:ASN:HD22	1:B:856:GLU:HA	1.70	0.57
1:A:795:ILE:HA	1:A:798:ALA:CB	2.34	0.57
1:B:787:LYS:HE2	1:B:796:LEU:HD22	1.86	0.57
1:B:572:PHE:CZ	1:B:608:PRO:HB2	2.39	0.57
1:A:690:GLU:O	1:A:690:GLU:HG3	2.05	0.57
1:B:280:ILE:HD11	1:B:429:LEU:HD22	1.87	0.57
1:B:503:ILE:HG22	1:B:736:SER:HB3	1.87	0.57
1:B:547:PRO:HB2	1:B:596:TYR:CE1	2.41	0.56
1:B:524:ILE:CD1	1:B:652:SER:HB3	2.35	0.56
1:A:409:ASN:HD21	1:A:412:SER:HB2	1.69	0.56
1:B:468:ARG:O	1:B:472:THR:HB	2.05	0.56
1:A:797:GLN:HA	1:A:800:ILE:HG22	1.87	0.56
1:A:854:LEU:O	1:A:856:GLU:N	2.38	0.56
1:B:281:GLY:HA2	1:B:438:LEU:HD21	1.87	0.56
1:B:642:THR:HG22	1:B:644:GLU:CB	2.32	0.56
1:B:732:ILE:HD11	1:B:746:LEU:HD12	1.88	0.56
1:A:646:ASN:HD22	1:A:646:ASN:H	1.54	0.55
1:B:522:SER:HB3	1:B:714:ALA:HB2	1.88	0.55
1:B:343:ARG:NH1	1:B:578:ALA:HB2	2.21	0.55
1:B:390:LEU:O	1:B:556:LYS:HG3	2.07	0.55
1:A:779:GLY:O	1:A:782:VAL:HG13	2.07	0.55
1:B:733:VAL:CG1	1:B:734:GLY:N	2.70	0.55
1:A:313:VAL:HG12	1:A:552:LYS:HD3	1.88	0.54
1:A:584:PHE:CE1	1:A:596:TYR:HB2	2.43	0.54
1:B:849:LEU:HD22	1:B:855:VAL:HG13	1.89	0.54
1:A:361:LYS:HD3	1:A:363:GLU:HB2	1.90	0.54
1:A:370:ASP:N	1:A:371:PRO:HD3	2.22	0.53
1:A:490:TYR:CE1	1:A:494:ILE:HD12	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ARG:NH1	1:B:591:GLN:OE1	2.42	0.53
1:B:279:LYS:HG3	1:B:290:VAL:HG22	1.91	0.53
1:B:797:GLN:HA	1:B:800:ILE:HG12	1.90	0.53
1:A:607:ALA:HB3	1:A:608:PRO:CD	2.39	0.53
1:A:289:VAL:HG23	1:A:438:LEU:HD21	1.91	0.53
1:A:724:ASN:O	1:A:728:SER:OG	2.27	0.53
1:A:817:HIS:HD2	1:A:818:GLN:H	1.54	0.53
1:A:816:GLU:HA	1:A:816:GLU:OE1	2.08	0.53
1:B:486:LEU:O	1:B:489:CYS:HB2	2.08	0.53
1:B:390:LEU:O	1:B:556:LYS:CG	2.57	0.52
1:B:273:PRO:HG2	1:B:406:GLY:HA2	1.92	0.52
1:B:552:LYS:O	1:B:558:GLY:HA3	2.09	0.52
1:A:728:SER:HA	1:A:828:SER:HB2	1.92	0.52
1:A:834:ARG:HH11	1:A:834:ARG:HG2	1.75	0.52
1:A:854:LEU:O	1:A:855:VAL:C	2.49	0.52
1:B:684:GLN:O	1:B:688:LYS:N	2.43	0.52
1:B:467:ILE:HG22	1:B:471:LEU:HD12	1.91	0.52
1:B:703:LEU:HD22	1:B:707:ILE:HD11	1.92	0.52
1:A:364:ILE:HD12	1:A:373:PRO:HB3	1.91	0.51
1:A:844:LYS:O	1:A:848:VAL:HG23	2.10	0.51
1:B:312:ASN:HB3	1:B:394:ASP:OD1	2.11	0.51
1:A:488:THR:HG21	1:A:500:VAL:HG11	1.91	0.51
1:A:817:HIS:CD2	1:A:818:GLN:H	2.28	0.51
1:B:612:PHE:HE2	1:B:746:LEU:HD23	1.74	0.51
1:B:372:SER:CB	1:B:373:PRO:HD2	2.34	0.51
1:A:785:PRO:CB	1:A:793:LYS:HD2	2.36	0.51
1:A:588:SER:HB2	1:A:591:GLN:H	1.76	0.51
1:B:844:LYS:O	1:B:847:SER:HB2	2.11	0.51
1:A:427:LYS:NZ	1:B:867:VAL:O	2.40	0.50
1:B:486:LEU:HD13	1:B:490:TYR:CE1	2.46	0.50
1:A:315:LEU:HD21	1:A:542:LEU:CD1	2.42	0.50
1:B:524:ILE:CG1	1:B:652:SER:HB3	2.42	0.50
1:B:770:LEU:CD2	1:B:808:LEU:HB3	2.41	0.50
1:A:439:ASN:HD22	1:A:439:ASN:C	2.14	0.50
1:A:474:LEU:O	1:A:475:GLN:HB2	2.12	0.50
1:A:490:TYR:HE1	1:A:494:ILE:CD1	2.24	0.50
1:B:804:ILE:O	1:B:808:LEU:HB2	2.12	0.50
1:B:733:VAL:HG13	1:B:838:PRO:O	2.11	0.50
1:A:344:LYS:O	1:A:345:VAL:HG13	2.12	0.50
1:A:563:GLU:O	1:A:567:LYS:HB2	2.12	0.49
1:B:728:SER:HA	1:B:828:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HD2	1:A:568:ASN:OD1	2.12	0.49
1:B:409:ASN:ND2	1:B:412:SER:HB2	2.27	0.49
1:A:675:ILE:HG23	1:A:716:ILE:HD13	1.95	0.49
1:A:352:GLN:OE1	1:A:599:LYS:O	2.30	0.49
1:A:754:ARG:HD2	1:A:758:LEU:O	2.13	0.49
1:A:688:LYS:HB3	1:A:690:GLU:CB	2.39	0.49
1:B:309:HIS:O	1:B:309:HIS:CG	2.66	0.49
1:B:341:TYR:HB3	1:B:342:LYS:HD2	1.95	0.49
1:B:646:ASN:C	1:B:646:ASN:HD22	2.15	0.49
1:B:731:LEU:HD23	1:B:732:ILE:N	2.28	0.49
1:A:755:PRO:HG2	1:A:758:LEU:HD12	1.95	0.48
1:B:858:LEU:HD13	1:B:878:ILE:HB	1.95	0.48
1:A:869:GLY:O	1:A:872:ILE:CD1	2.62	0.48
1:A:426:THR:HB	1:A:474:LEU:HD21	1.95	0.48
1:B:681:ILE:O	1:B:685:LEU:HG	2.12	0.48
1:B:489:CYS:O	1:B:494:ILE:HB	2.14	0.48
1:A:335:ARG:NH1	1:A:339:ARG:HH22	2.11	0.48
1:A:418:LEU:HD11	1:A:634:LEU:HG	1.95	0.48
1:A:424:ASP:O	1:A:428:LEU:HB2	2.14	0.48
1:B:318:GLU:HG2	1:B:543:GLN:HE21	1.79	0.48
1:B:503:ILE:HD11	1:B:703:LEU:HD11	1.95	0.48
1:A:348:ASN:O	1:A:350:HIS:ND1	2.47	0.47
1:A:468:ARG:O	1:A:472:THR:HB	2.14	0.47
1:A:855:VAL:HB	1:A:859:PHE:CE2	2.49	0.47
1:B:426:THR:HB	1:B:474:LEU:HD11	1.96	0.47
1:A:402:PRO:HG2	1:A:428:LEU:HD12	1.96	0.47
1:A:330:MET:HE3	1:A:606:LEU:O	2.14	0.47
1:A:818:GLN:HG3	1:A:818:GLN:O	2.15	0.47
1:A:852:ILE:HB	1:A:853:LYS:HD2	1.96	0.47
1:B:405:GLY:C	1:B:407:SER:H	2.17	0.47
1:B:533:ILE:HD11	1:B:611:LEU:HD21	1.97	0.47
1:A:504:GLY:HA3	2:A:1882:ADP:O3A	2.15	0.47
1:A:418:LEU:HD13	1:A:633:GLN:HB3	1.96	0.47
1:A:550:ASP:N	1:A:550:ASP:OD1	2.42	0.47
1:A:795:ILE:O	1:A:799:GLN:N	2.42	0.47
1:B:433:LEU:O	1:B:438:LEU:O	2.32	0.47
1:B:299:LYS:HE2	1:B:310:VAL:HG11	1.96	0.47
1:B:634:LEU:HD23	1:B:634:LEU:HA	1.80	0.47
1:B:454:ILE:HG23	1:B:458:PHE:HB3	1.97	0.47
1:A:400:ARG:HD3	1:A:415:TYR:CZ	2.50	0.46
1:A:812:HIS:HA	1:A:815:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LYS:HD3	1:A:697:LYS:HB3	1.98	0.46
1:B:704:GLU:OE2	1:B:749:ARG:HG2	2.15	0.46
1:A:834:ARG:HG2	1:A:834:ARG:NH1	2.30	0.46
1:B:316:GLN:HB3	1:B:539:LEU:HD23	1.98	0.46
1:B:850:ALA:HA	1:B:855:VAL:HG11	1.96	0.46
1:A:614:PRO:HG2	1:A:700:PHE:O	2.16	0.46
1:B:754:ARG:HE	1:B:759:SER:HB3	1.80	0.46
1:A:502:ASN:ND2	1:A:502:ASN:C	2.65	0.46
1:B:343:ARG:HG3	1:B:344:LYS:N	2.30	0.46
1:B:374:ILE:H	1:B:374:ILE:CD1	2.23	0.46
1:A:837:ASN:HD22	1:A:837:ASN:C	2.18	0.46
1:B:399:ILE:CD1	1:B:556:LYS:HE3	2.46	0.46
1:A:280:ILE:HG23	1:A:280:ILE:O	2.16	0.46
1:B:616:ILE:HA	1:B:619:LEU:HD22	1.98	0.45
1:A:646:ASN:HD22	1:A:646:ASN:N	2.14	0.45
1:A:690:GLU:O	1:A:690:GLU:CG	2.65	0.45
1:B:261:ASP:HB3	1:B:477:GLN:CD	2.36	0.45
1:A:359:ASN:HD22	1:A:359:ASN:N	2.13	0.45
1:A:626:LYS:H	1:A:626:LYS:HD3	1.81	0.45
1:A:748:ASP:O	1:A:752:ILE:HG13	2.15	0.45
1:B:490:TYR:CE1	1:B:494:ILE:HD12	2.51	0.45
1:A:370:ASP:N	1:A:371:PRO:CD	2.80	0.45
1:B:449:LYS:HG2	1:B:478:ALA:HB3	1.98	0.45
1:A:357:ASN:HB3	1:A:596:TYR:CZ	2.52	0.45
1:B:350:HIS:C	1:B:352:GLN:H	2.20	0.45
1:B:412:SER:HA	1:B:413:PRO:HD3	1.69	0.45
1:B:536:LEU:HD11	1:B:616:ILE:HD13	1.98	0.45
1:B:502:ASN:C	1:B:502:ASN:ND2	2.70	0.45
1:B:694:ASN:HB2	1:B:697:LYS:HG2	1.98	0.45
1:A:402:PRO:O	1:A:409:ASN:HB3	2.17	0.44
1:A:651:LEU:HD22	1:A:682:ILE:CG2	2.48	0.44
1:A:702:PRO:HG2	1:A:705:LYS:HE3	1.99	0.44
1:A:746:LEU:HD22	1:A:750:ILE:HD11	2.00	0.44
1:A:263:ASN:HD22	1:A:856:GLU:HA	1.83	0.44
1:A:411:LYS:HG2	1:A:626:LYS:HB3	1.99	0.44
1:A:288:PRO:HB3	1:A:843:TRP:CE2	2.51	0.44
1:A:871:ARG:CG	1:A:871:ARG:HH11	2.30	0.44
1:B:727:TYR:HB3	1:B:826:PRO:O	2.17	0.44
1:A:452:LEU:HD11	1:A:466:PHE:CD2	2.53	0.44
1:B:497:SER:HB3	1:B:726:PHE:CE1	2.53	0.44
1:A:607:ALA:HB3	1:A:608:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:GLY:O	1:B:872:ILE:HG12	2.16	0.44
1:B:602:ASP:OD2	1:B:606:LEU:HD11	2.18	0.44
1:B:865:TRP:HA	1:B:872:ILE:HD11	1.99	0.44
1:A:364:ILE:HG21	1:A:587:ARG:NH1	2.33	0.44
1:B:421:LEU:O	1:B:425:VAL:HG23	2.18	0.44
1:B:735:GLY:CA	1:B:839:ALA:HB2	2.48	0.44
1:A:260:ILE:H	1:A:260:ILE:HG13	1.49	0.43
1:A:338:MET:HE1	1:A:574:ASP:O	2.18	0.43
1:A:740:PRO:O	1:A:741:ALA:HB3	2.18	0.43
1:B:418:LEU:HG	1:B:422:ILE:HD12	2.01	0.43
1:B:683:ASP:O	1:B:687:ASP:HB3	2.19	0.43
1:A:368:LYS:HG2	1:A:369:ASN:N	2.33	0.43
1:A:269:ILE:HD13	1:A:433:LEU:HD11	2.01	0.43
1:A:682:ILE:HG13	1:A:683:ASP:N	2.32	0.43
1:B:426:THR:HB	1:B:474:LEU:HD21	2.00	0.43
1:A:452:LEU:HD22	1:A:453:VAL:O	2.19	0.43
1:A:454:ILE:CD1	1:A:463:VAL:HG13	2.47	0.43
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.78	0.43
1:A:572:PHE:CZ	1:A:608:PRO:HB2	2.53	0.43
1:A:739:ILE:HA	1:A:740:PRO:HD3	1.87	0.43
1:A:763:PHE:O	1:A:766:PHE:HB3	2.19	0.43
1:B:691:ASN:N	1:B:691:ASN:HD22	2.16	0.43
1:B:852:ILE:HG13	1:B:853:LYS:NZ	2.34	0.43
1:A:812:HIS:O	1:A:816:GLU:HG2	2.19	0.43
1:A:821:ASN:HD22	1:A:821:ASN:C	2.22	0.43
1:B:264:ASP:HA	1:B:265:PRO:HD3	1.86	0.43
1:B:280:ILE:HD11	1:B:429:LEU:CD2	2.48	0.43
1:B:497:SER:HB2	1:B:725:SER:OG	2.18	0.43
1:B:691:ASN:H	1:B:691:ASN:HD22	1.67	0.43
1:A:408:PHE:HB2	1:A:462:HIS:CE1	2.53	0.42
1:B:572:PHE:HA	1:B:605:MET:HG3	2.01	0.42
1:B:343:ARG:HH11	1:B:578:ALA:HB2	1.84	0.42
1:B:738:LYS:HA	1:B:738:LYS:HD2	1.35	0.42
1:A:263:ASN:HD22	1:A:856:GLU:HG3	1.84	0.42
1:B:356:PHE:HD1	1:B:357:ASN:HD22	1.68	0.42
1:A:377:ILE:O	1:A:393:VAL:HG22	2.20	0.42
1:A:805:VAL:O	1:A:809:GLU:HB3	2.20	0.42
1:A:853:LYS:H	1:A:853:LYS:HD2	1.85	0.42
1:B:711:ILE:HG12	1:B:726:PHE:HB3	2.02	0.42
1:A:341:TYR:HB2	1:A:342:LYS:HG2	2.01	0.42
1:A:442:PRO:O	1:A:445:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:SER:CB	1:A:714:ALA:HB2	2.48	0.42
1:B:607:ALA:HB3	1:B:608:PRO:HD3	2.02	0.42
1:B:783:ASN:O	1:B:785:PRO:HD3	2.19	0.42
1:B:364:ILE:HD12	1:B:593:THR:HG21	2.02	0.41
1:A:301:TRP:HB3	1:B:875:TYR:HB3	2.01	0.41
1:A:435:SER:O	1:A:436:GLU:C	2.59	0.41
1:A:651:LEU:HB2	1:A:682:ILE:HG22	2.02	0.41
1:A:806:GLU:HA	1:A:809:GLU:HB3	2.02	0.41
1:B:557:HIS:CB	1:B:587:ARG:HB3	2.48	0.41
1:A:806:GLU:O	1:A:810:GLU:HB3	2.20	0.41
1:B:271:ILE:HG22	1:B:273:PRO:HD3	2.01	0.41
1:A:421:LEU:C	1:A:421:LEU:HD23	2.41	0.41
1:A:444:LYS:HB3	1:A:444:LYS:HE2	1.81	0.41
1:B:316:GLN:NE2	1:B:316:GLN:HA	2.36	0.41
1:B:400:ARG:HB3	1:B:414:TYR:HB2	2.01	0.41
1:B:696:LEU:HD23	1:B:696:LEU:H	1.85	0.41
1:A:409:ASN:ND2	1:A:412:SER:HB2	2.35	0.41
1:A:280:ILE:HG21	1:A:432:ALA:HB1	2.02	0.41
1:A:684:GLN:O	1:A:688:LYS:HB2	2.21	0.41
1:B:265:PRO:O	1:B:268:THR:HB	2.21	0.41
1:B:731:LEU:HD23	1:B:732:ILE:H	1.86	0.41
1:B:758:LEU:HA	1:B:758:LEU:HD23	1.91	0.41
1:B:582:TYR:CG	1:B:583:ASN:N	2.88	0.41
1:B:844:LYS:O	1:B:848:VAL:HG23	2.21	0.41
1:A:319:GLN:HB3	1:A:323:PHE:CD1	2.56	0.41
1:A:478:ALA:HB1	1:A:859:PHE:HB3	2.02	0.41
1:B:368:LYS:HE3	1:B:369:ASN:H	1.86	0.41
1:B:849:LEU:O	1:B:852:ILE:HG22	2.21	0.41
1:A:285:ASP:HB3	1:A:287:HIS:O	2.21	0.40
1:A:494:ILE:HG12	1:A:494:ILE:O	2.22	0.40
1:A:818:GLN:O	1:A:818:GLN:CG	2.69	0.40
1:B:433:LEU:HD13	1:B:433:LEU:HA	1.81	0.40
1:B:561:LEU:O	1:B:565:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	621/655 (95%)	542 (87%)	76 (12%)	3 (0%)	29	62
1	B	621/655 (95%)	534 (86%)	83 (13%)	4 (1%)	25	59
All	All	1242/1310 (95%)	1076 (87%)	159 (13%)	7 (1%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	PRO
1	B	371	PRO
1	A	372	SER
1	A	855	VAL
1	B	691	ASN
1	A	821	ASN
1	B	579	VAL

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	569/595 (96%)	473 (83%)	96 (17%)	2	9
1	B	569/595 (96%)	462 (81%)	107 (19%)	1	6
All	All	1138/1190 (96%)	935 (82%)	203 (18%)	2	7

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ILE
1	A	264	ASP
1	A	286	ASP
1	A	287	HIS
1	A	311	GLU
1	A	312	ASN
1	A	314	CYS
1	A	315	LEU
1	A	333	ASN
1	A	337	ARG
1	A	338	MET
1	A	342	LYS
1	A	344	LYS
1	A	345	VAL
1	A	348	ASN
1	A	351	GLU
1	A	355	SER
1	A	356	PHE
1	A	357	ASN
1	A	359	ASN
1	A	361	LYS
1	A	372	SER
1	A	391	ARG
1	A	395	GLU
1	A	398	VAL
1	A	400	ARG
1	A	404	ARG
1	A	423	SER
1	A	428	LEU
1	A	433	LEU
1	A	438	LEU
1	A	439	ASN
1	A	444	LYS
1	A	452	LEU
1	A	454	ILE
1	A	461	SER
1	A	466	PHE
1	A	468	ARG
1	A	486	LEU
1	A	488	THR
1	A	494	ILE
1	A	496	THR
1	A	497	SER

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Mol	Chain	Res	Type
1	A	502	ASN
1	A	507	GLU
1	A	515	GLU
1	A	517	THR
1	A	536	LEU
1	A	539	LEU
1	A	544	SER
1	A	548	LEU
1	A	550	ASP
1	A	555	SER
1	A	556	LYS
1	A	560	LEU
1	A	561	LEU
1	A	566	LYS
1	A	571	THR
1	A	574	ASP
1	A	581	LEU
1	A	622	THR
1	A	625	HIS
1	A	626	LYS
1	A	630	LEU
1	A	640	LEU
1	A	646	ASN
1	A	669	LEU
1	A	672	LEU
1	A	682	ILE
1	A	699	ASN
1	A	703	LEU
1	A	704	GLU
1	A	720	VAL
1	A	722	ARG
1	A	723	MET
1	A	728	SER
1	A	733	VAL
1	A	746	LEU
1	A	754	ARG
1	A	780	HIS
1	A	783	ASN
1	A	792	ASN
1	A	794	GLN
1	A	796	LEU
1	A	797	GLN

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Mol	Chain	Res	Type
1	A	821	ASN
1	A	824	ILE
1	A	835	ASP
1	A	837	ASN
1	A	849	LEU
1	A	852	ILE
1	A	853	LYS
1	A	854	LEU
1	A	855	VAL
1	A	871	ARG
1	A	872	ILE
1	B	264	ASP
1	B	287	HIS
1	B	289	VAL
1	B	304	LEU
1	B	309	HIS
1	B	310	VAL
1	B	313	VAL
1	B	314	CYS
1	B	315	LEU
1	B	316	GLN
1	B	319	GLN
1	B	329	GLU
1	B	337	ARG
1	B	342	LYS
1	B	357	ASN
1	B	358	GLU
1	B	359	ASN
1	B	367	GLU
1	B	368	LYS
1	B	370	ASP
1	B	374	ILE
1	B	377	ILE
1	B	382	LYS
1	B	383	LEU
1	B	391	ARG
1	B	392	CYS
1	B	398	VAL
1	B	400	ARG
1	B	401	LYS
1	B	404	ARG
1	B	412	SER

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Mol	Chain	Res	Type
1	B	426	THR
1	B	433	LEU
1	B	436	GLU
1	B	439	ASN
1	B	440	VAL
1	B	452	LEU
1	B	454	ILE
1	B	466	PHE
1	B	475	GLN
1	B	486	LEU
1	B	488	THR
1	B	498	THR
1	B	502	ASN
1	B	507	GLU
1	B	509	ARG
1	B	517	THR
1	B	525	THR
1	B	536	LEU
1	B	539	LEU
1	B	543	GLN
1	B	556	LYS
1	B	560	LEU
1	B	566	LYS
1	B	574	ASP
1	B	576	ASP
1	B	580	GLN
1	B	581	LEU
1	B	587	ARG
1	B	588	SER
1	B	596	TYR
1	B	600	LEU
1	B	619	LEU
1	B	623	SER
1	B	624	SER
1	B	626	LYS
1	B	640	LEU
1	B	646	ASN
1	B	658	GLU
1	B	660	ASN
1	B	672	LEU
1	B	683	ASP
1	B	686	GLN

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Mol	Chain	Res	Type
1	B	687	ASP
1	B	690	GLU
1	B	692	TYR
1	B	694	ASN
1	B	695	THR
1	B	696	LEU
1	B	697	LYS
1	B	703	LEU
1	B	704	GLU
1	B	720	VAL
1	B	731	LEU
1	B	736	SER
1	B	738	LYS
1	B	746	LEU
1	B	749	ARG
1	B	769	LYS
1	B	770	LEU
1	B	771	THR
1	B	774	ILE
1	B	780	HIS
1	B	787	LYS
1	B	789	GLU
1	B	791	GLU
1	B	794	GLN
1	B	808	LEU
1	B	840	LEU
1	B	849	LEU
1	B	853	LYS
1	B	854	LEU
1	B	855	VAL
1	B	866	ASP
1	B	871	ARG
1	B	872	ILE
1	B	874	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	306	ASN
1	A	348	ASN
1	A	359	ASN

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Mol	Chain	Res	Type
1	A	434	ASN
1	A	439	ASN
1	A	447	GLN
1	A	502	ASN
1	A	646	ASN
1	A	686	GLN
1	A	699	ASN
1	A	783	ASN
1	A	792	ASN
1	A	794	GLN
1	A	817	HIS
1	A	837	ASN
1	B	316	GLN
1	B	333	ASN
1	B	369	ASN
1	B	434	ASN
1	B	439	ASN
1	B	502	ASN
1	B	543	GLN
1	B	583	ASN
1	B	590	ASN
1	B	646	ASN
1	B	666	ASN
1	B	680	ASN
1	B	686	GLN
1	B	691	ASN
1	B	794	GLN
1	B	818	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	1882	-	24,29,29	1.23	2 (8%)	29,45,45	2.01	11 (37%)
2	ADP	B	1882	-	24,29,29	1.52	3 (12%)	29,45,45	1.76	10 (34%)

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	A	1882	-	-	6/12/32/32	0/3/3/3
2	ADP	B	1882	-	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1882	ADP	C2-N3	3.38	1.37	1.32
2	B	1882	ADP	C5-C4	3.27	1.49	1.40
2	A	1882	ADP	C2-N3	2.93	1.36	1.32
2	A	1882	ADP	C5-C4	2.71	1.48	1.40
2	B	1882	ADP	C8-N7	2.14	1.38	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1882	ADP	N6-C6-N1	3.78	126.42	118.57
2	B	1882	ADP	N3-C2-N1	-3.50	123.21	128.68
2	A	1882	ADP	O5'-PA-O1A	-3.43	95.67	109.07
2	A	1882	ADP	N3-C2-N1	-3.31	123.51	128.68
2	A	1882	ADP	C5-C6-N6	-3.23	115.44	120.35
2	A	1882	ADP	O3A-PB-O1B	-2.86	95.32	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1882	ADP	O3B-PB-O3A	2.83	114.11	104.64
2	A	1882	ADP	O2A-PA-O1A	2.76	125.89	112.24
2	A	1882	ADP	O2B-PB-O3A	-2.72	95.51	104.64
2	B	1882	ADP	C1'-N9-C4	-2.68	121.93	126.64
2	B	1882	ADP	O3'-C3'-C2'	-2.67	103.19	111.82
2	B	1882	ADP	C2'-C3'-C4'	2.63	107.74	102.64
2	A	1882	ADP	PA-O3A-PB	-2.50	124.26	132.83
2	A	1882	ADP	O4'-C1'-C2'	-2.42	103.39	106.93
2	A	1882	ADP	O2B-PB-O1B	2.37	119.97	110.68
2	B	1882	ADP	O3B-PB-O1B	2.35	119.89	110.68
2	B	1882	ADP	N6-C6-N1	2.35	123.45	118.57
2	B	1882	ADP	O2A-PA-O1A	2.29	123.56	112.24
2	B	1882	ADP	O5'-PA-O1A	-2.16	100.62	109.07
2	B	1882	ADP	PA-O3A-PB	-2.13	125.50	132.83
2	B	1882	ADP	O2'-C2'-C1'	-2.13	102.99	110.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1882	ADP	C5'-O5'-PA-O1A
2	A	1882	ADP	C5'-O5'-PA-O2A
2	B	1882	ADP	C5'-O5'-PA-O1A
2	B	1882	ADP	C5'-O5'-PA-O2A
2	A	1882	ADP	C5'-O5'-PA-O3A
2	A	1882	ADP	PB-O3A-PA-O2A
2	A	1882	ADP	PB-O3A-PA-O1A
2	B	1882	ADP	C5'-O5'-PA-O3A
2	B	1882	ADP	PB-O3A-PA-O1A
2	A	1882	ADP	O4'-C4'-C5'-O5'
2	B	1882	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

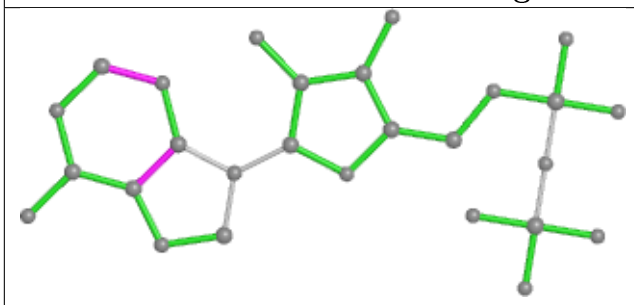
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1882	ADP	4	0
2	B	1882	ADP	1	0

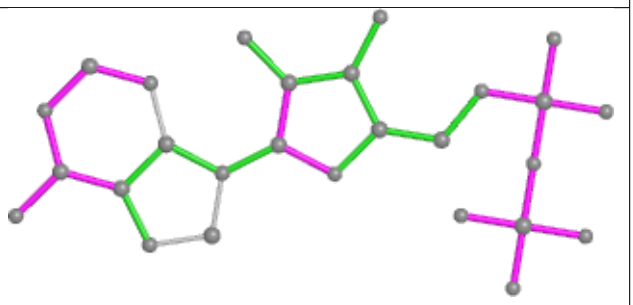
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

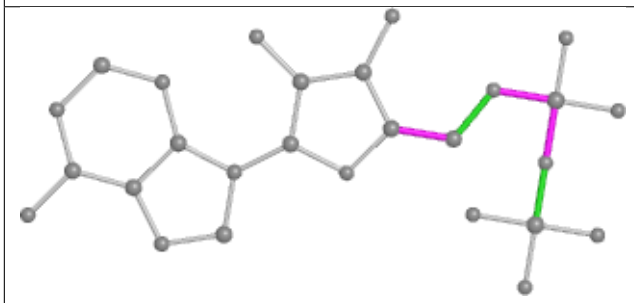
Ligand ADP A 1882



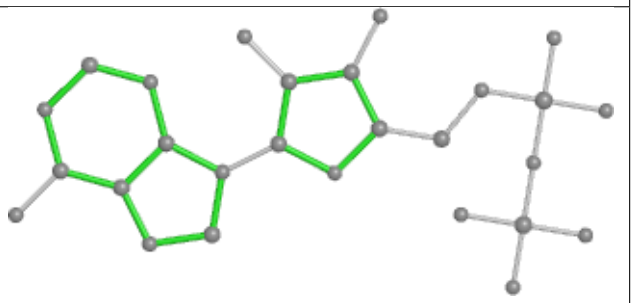
Bond lengths



Bond angles

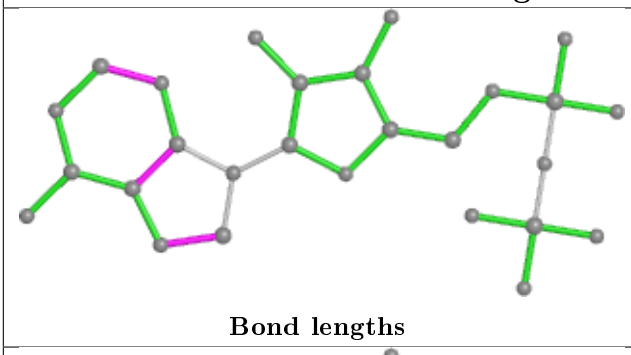


Torsions

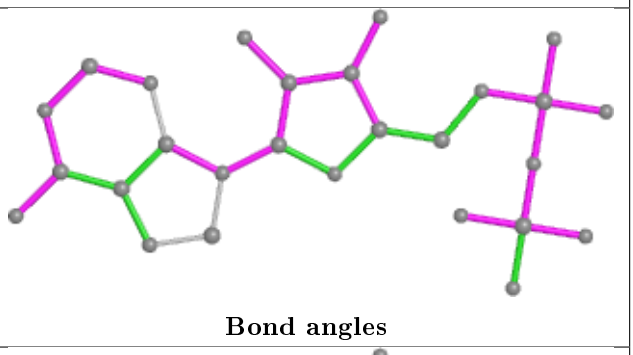


Rings

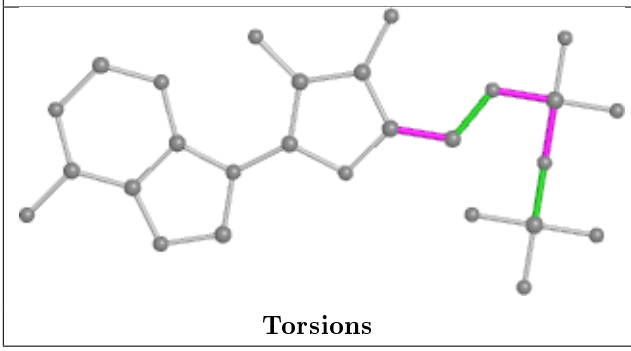
Ligand ADP B 1882



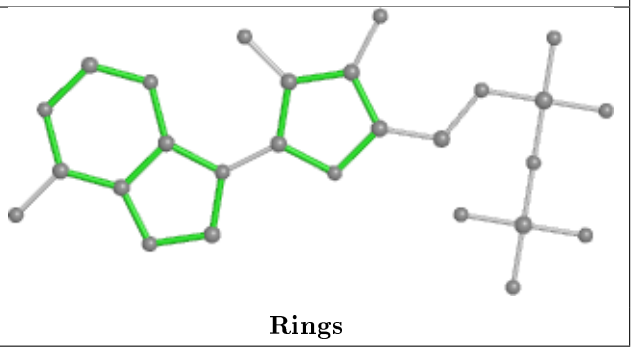
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	623/655 (95%)	-0.10	30 (4%)	30	28	61, 97, 174, 284	0
1	B	623/655 (95%)	0.11	42 (6%)	17	17	76, 124, 221, 295	0
All	All	1246/1310 (95%)	0.01	72 (5%)	23	22	61, 110, 212, 295	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	786	ASP	8.6
1	B	782	VAL	7.7
1	B	373	PRO	6.6
1	B	787	LYS	6.6
1	B	689	PRO	5.8
1	A	366	SER	5.8
1	B	818	GLN	5.5
1	A	368	LYS	5.5
1	B	781	TYR	5.4
1	A	371	PRO	5.4
1	B	369	ASN	5.3
1	B	821	ASN	5.3
1	A	370	ASP	5.2
1	A	782	VAL	5.2
1	B	372	SER	4.8
1	B	819	ASN	4.7
1	B	820	GLY	4.4
1	A	786	ASP	4.3
1	A	780	HIS	4.3
1	B	307	SER	4.3
1	A	787	LYS	4.3
1	B	785	PRO	4.2
1	A	309	HIS	4.2
1	B	780	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	369	ASN	4.1
1	B	590	ASN	4.1
1	B	371	PRO	4.0
1	A	788	THR	3.5
1	A	367	GLU	3.5
1	B	368	LYS	3.4
1	B	790	ASP	3.3
1	B	823	HIS	3.3
1	B	356	PHE	3.3
1	B	259	GLU	3.2
1	B	788	THR	3.0
1	B	308	GLU	3.0
1	B	815	ILE	2.9
1	A	783	ASN	2.8
1	B	357	ASN	2.8
1	B	816	GLU	2.8
1	B	370	ASP	2.7
1	A	644	GLU	2.7
1	A	365	ILE	2.6
1	B	496	THR	2.6
1	A	834	ARG	2.6
1	B	313	VAL	2.6
1	B	366	SER	2.6
1	B	311	GLU	2.5
1	A	307	SER	2.5
1	B	317	ARG	2.5
1	A	691	ASN	2.4
1	A	305	GLU	2.4
1	A	779	GLY	2.4
1	A	821	ASN	2.4
1	B	309	HIS	2.3
1	A	785	PRO	2.3
1	B	363	GLU	2.2
1	B	772	LYS	2.2
1	A	306	ASN	2.2
1	A	696	LEU	2.2
1	B	597	GLU	2.2
1	B	794	GLN	2.2
1	B	260	ILE	2.1
1	A	790	ASP	2.1
1	A	835	ASP	2.1
1	A	693	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	814	ASN	2.1
1	A	590	ASN	2.1
1	A	627	ASN	2.1
1	B	416	LYS	2.0
1	B	784	ALA	2.0
1	B	783	ASN	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 carbohydrates in this entry.

6.4 Ligands (i)

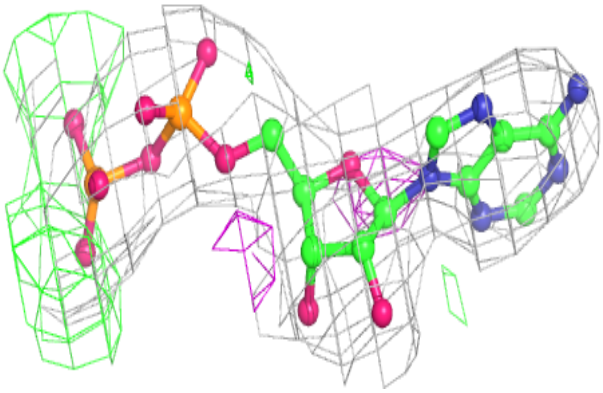
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

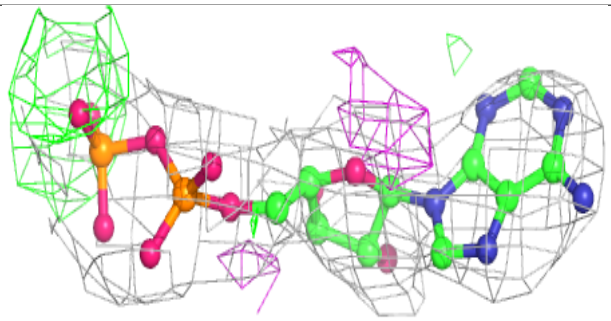
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	1882	27/27	0.85	0.24	83,89,91,91	0
2	ADP	B	1882	27/27	0.88	0.22	92,96,98,99	0

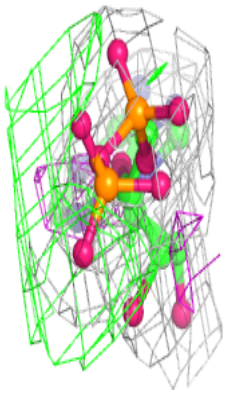
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1882:

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

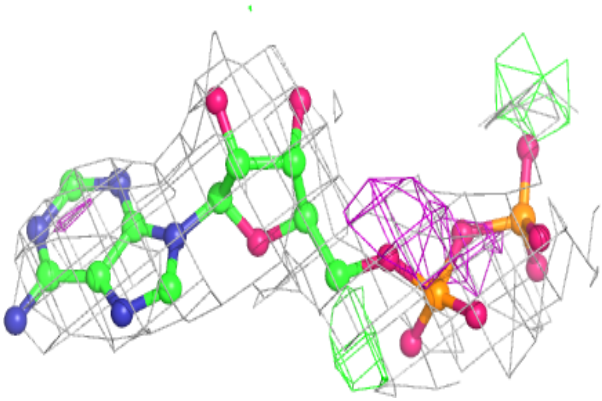


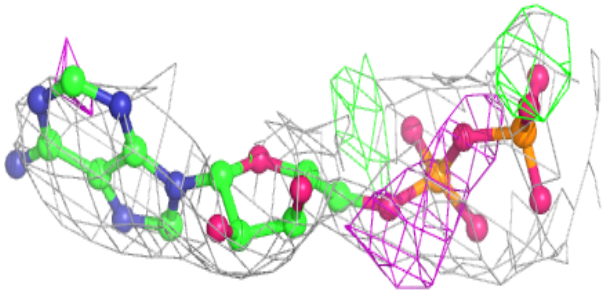


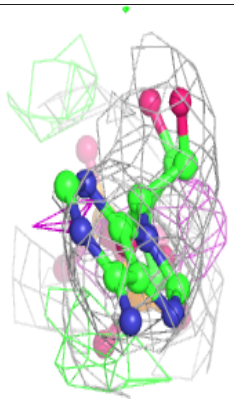


Electron density around ADP B 1882:

$2mF_o$-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.