Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:16 PM GMT

PDB ID	:	1SVL
Title	:	Co-crystal structure of SV40 large T antigen helicase domain and ADP
Authors	:	Gai, D.; Zhao, R.; Finkielstein, C.V.; Chen, X.S.
Deposited on	:	2004-03-29
Resolution	:	1.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

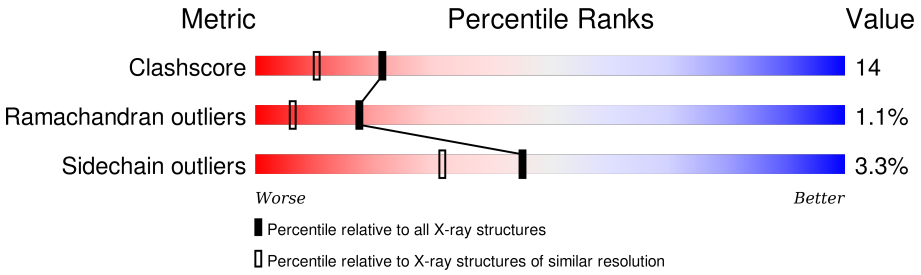
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	69% 26%
1	B	377	67% 27%
1	C	377	73% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9120 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 large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	B	362	Total	C	N	O	S	0	0	0
			2929	1885	492	531	21			
1	C	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			

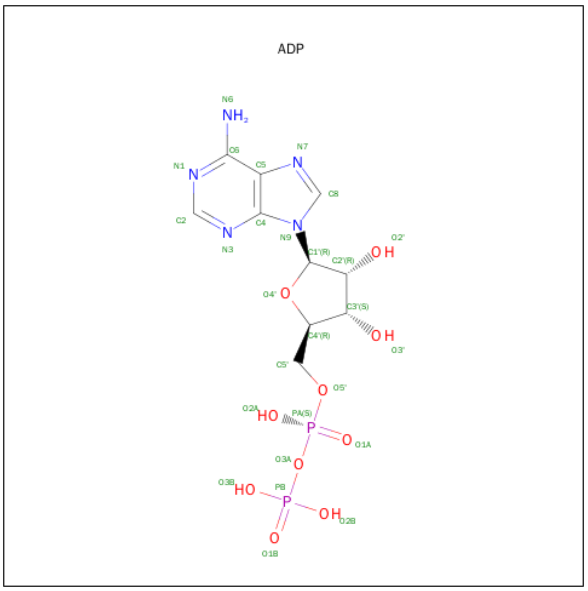
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	59	Total	O	0	0
			59	59		
5	C	109	Total	O	0	0
			109	109		

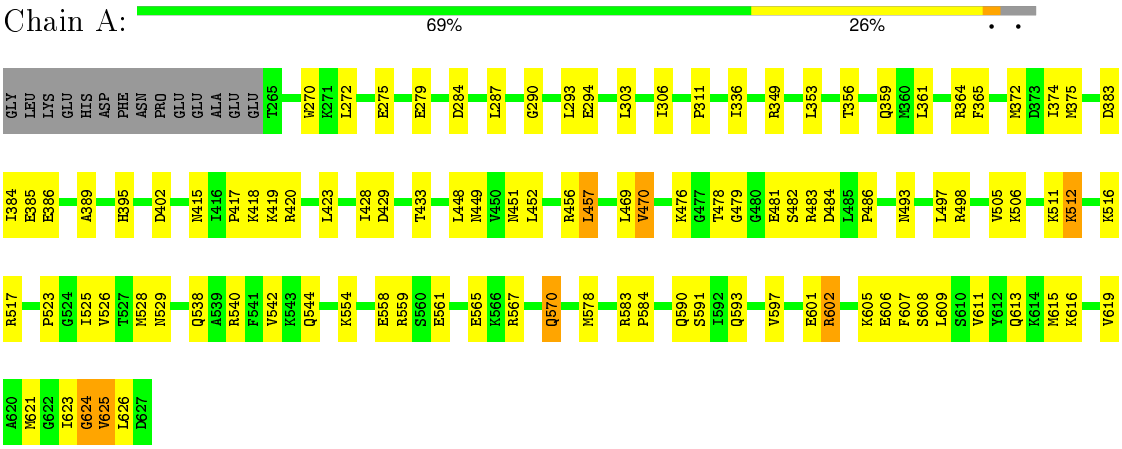
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

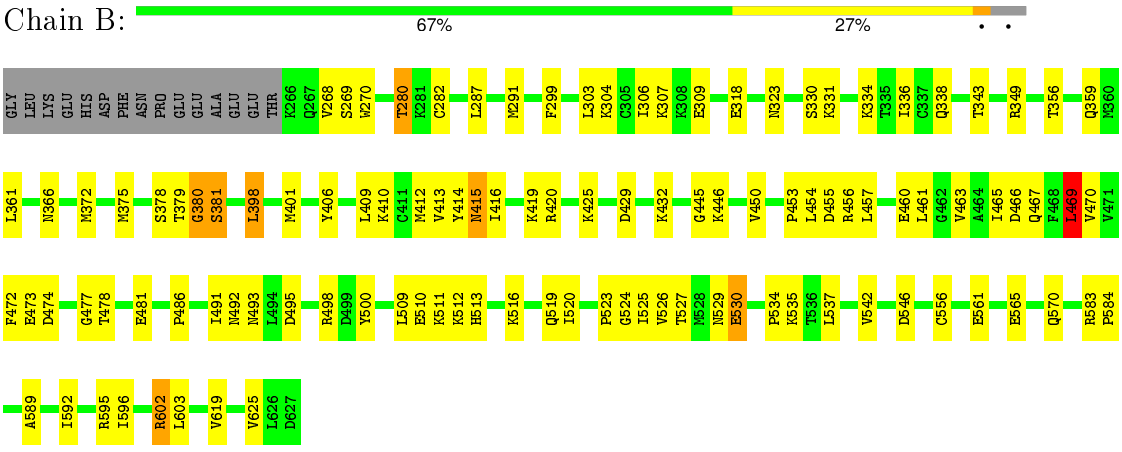
- Molecule 1: large T antigen

Chain A:



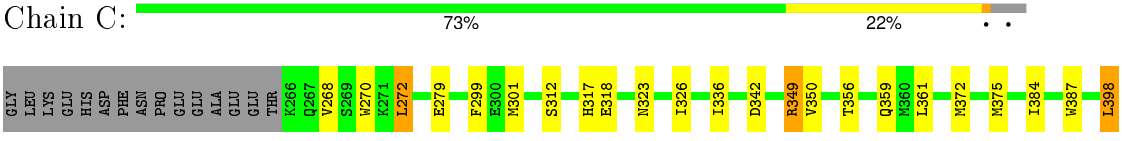
- Molecule 1: large T antigen

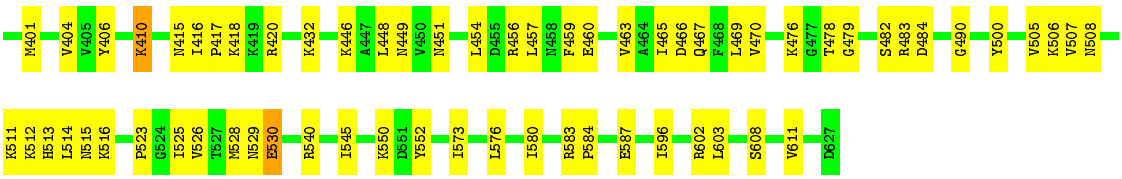
Chain B:



- Molecule 1: large T antigen

Chain C:




M401
V404
Y405
Y406
K410
N415
I416
P417
K418
K419
R420
K432
K446
A447
L448
N449
V450
N451
L454
D455
R456
L457
N458
F459
E460
V463
A464
I465
D466
Q467
F468
L469
V470
K476
G477
T478
G479
S482
R483
D484
G490
Y500
V505
K506
V507
N508
K511
K512
H513
L514
N515
K516
P523
G524
I525
V526
T527
M528
N529
E530
R540
I545
K550
D551
Y552
I573
L576
I580
R583
P584
E587
I596
R602
L603
S608
V611
D627

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.81Å 86.44Å 128.60Å 90.00° 129.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95	Depositor
% Data completeness (in resolution range)	92.5 (30.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9120	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.41	0/2999	0.59	0/4040
1	B	0.40	0/2988	0.58	1/4026 (0.0%)
1	C	0.49	0/2992	0.65	0/4030
All	All	0.44	0/8979	0.60	1/12096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	469	LEU	CA-CB-CG	5.74	128.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2940	0	2989	83	0
1	B	2929	0	2970	105	0
1	C	2933	0	2982	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	1	0
4	C	27	0	12	0	0
5	A	63	0	0	1	0
5	B	59	0	0	0	0
5	C	109	0	0	2	0
All	All	9120	0	8977	252	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 14.

All (252) 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:C:372:MET:HA	1:C:375:MET:HE3	1.42	0.98
1:B:269:SER:H	1:B:323:ASN:HD21	1.11	0.96
1:A:311:PRO:HG2	1:A:374:ILE:HD13	1.53	0.90
1:A:486:PRO:HG2	1:B:498:ARG:HH22	1.37	0.88
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.14	0.87
1:C:451:ASN:HD21	1:C:476:LYS:H	1.20	0.87
1:B:512:LYS:HG3	1:B:513:HIS:H	1.39	0.86
1:C:529:ASN:O	1:C:530:GLU:HB2	1.75	0.84
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.93	0.83
1:B:366:ASN:HD22	1:B:595:ARG:HH11	1.28	0.82
1:B:474:ASP:H	1:B:527:THR:HG23	1.44	0.80
1:C:415:ASN:HD21	1:C:420:ARG:HH11	1.32	0.78
1:B:474:ASP:H	1:B:527:THR:CG2	1.97	0.77
1:C:465:ILE:HD13	1:C:516:LYS:HB2	1.68	0.76
1:C:446:LYS:HG2	1:C:467:GLN:HE21	1.51	0.76
1:C:446:LYS:HG2	1:C:467:GLN:NE2	2.01	0.75
1:A:415:ASN:HD21	1:A:420:ARG:NH1	1.85	0.75
1:B:280:THR:HG22	1:B:282:CYS:HB2	1.70	0.74
1:B:453:PRO:HD2	1:B:456:ARG:HD2	1.68	0.74
1:A:419:LYS:HA	1:A:542:VAL:HG11	1.70	0.72
1:A:415:ASN:ND2	1:A:420:ARG:HH11	1.87	0.71
1:A:498:ARG:HG3	1:A:540:ARG:HE	1.54	0.70
1:B:473:GLU:OE2	1:B:527:THR:HG21	1.91	0.70
1:B:510:GLU:HB2	1:B:516:LYS:HG2	1.73	0.70
1:A:383:ASP:OD2	1:A:386:GLU:HG3	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLY:O	1:B:446:LYS:HD2	1.91	0.70
1:B:425:LYS:HE2	1:B:530:GLU:HA	1.72	0.70
1:A:517:ARG:HB2	1:A:517:ARG:NH1	2.08	0.68
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.27	0.68
1:A:609:LEU:O	1:A:613:GLN:HG3	1.93	0.67
1:A:419:LYS:HA	1:A:542:VAL:CG1	2.24	0.67
1:B:419:LYS:HA	1:B:542:VAL:HG11	1.77	0.67
1:C:500:TYR:CZ	1:C:507:VAL:HG11	2.30	0.66
1:B:491:ILE:HD11	1:B:534:PRO:HD3	1.78	0.66
1:A:538:GLN:HE22	1:A:544:GLN:NE2	1.95	0.65
1:A:311:PRO:CG	1:A:374:ILE:HD13	2.26	0.65
1:B:420:ARG:HB3	1:B:523:PRO:HB3	1.79	0.65
1:A:415:ASN:HD22	1:A:420:ARG:HG2	1.62	0.65
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.61	0.64
1:B:466:ASP:H	1:B:519:GLN:HE22	1.46	0.64
1:C:401:MET:O	1:C:401:MET:HE2	1.98	0.64
1:C:454:LEU:HD12	1:C:457:LEU:HD23	1.80	0.63
1:B:419:LYS:HA	1:B:542:VAL:CG1	2.29	0.63
1:B:366:ASN:HD22	1:B:595:ARG:NH1	1.96	0.62
1:A:415:ASN:ND2	1:A:420:ARG:HG2	2.15	0.62
1:B:473:GLU:HA	1:B:527:THR:HG22	1.82	0.61
1:A:619:VAL:HG22	1:A:625:VAL:HG22	1.81	0.61
1:C:356:THR:OG1	1:C:359:GLN:HG3	1.99	0.61
1:B:556:CYS:SG	1:B:625:VAL:HG13	2.40	0.61
1:A:511:LYS:O	1:A:512:LYS:HB3	2.00	0.60
1:B:334:LYS:HE2	1:C:342:ASP:OD1	2.02	0.60
1:A:389:ALA:HB1	1:A:625:VAL:HG11	1.82	0.59
1:C:349:ARG:HH11	1:C:349:ARG:HB2	1.66	0.59
1:A:395:HIS:HD2	1:A:616:LYS:NZ	1.99	0.59
1:C:584:PRO:HG2	1:C:587:GLU:HG3	1.85	0.59
1:A:621:MET:HB2	1:A:623:ILE:HG13	1.85	0.59
1:B:416:ILE:O	1:B:420:ARG:HG3	2.02	0.59
1:C:448:LEU:HG	1:C:470:VAL:HG13	1.84	0.59
1:A:624:GLY:O	1:A:626:LEU:N	2.36	0.59
1:C:401:MET:HE3	1:C:401:MET:HA	1.84	0.58
1:A:590:GLN:NE2	1:A:591:SER:H	2.02	0.57
1:C:268:VAL:HG22	1:C:326:ILE:HG22	1.86	0.57
1:B:445:GLY:C	1:B:446:LYS:HD2	2.25	0.57
1:A:275:GLU:O	1:A:279:GLU:HG2	2.04	0.57
1:A:498:ARG:HG3	1:A:540:ARG:NE	2.20	0.56
1:C:583:ARG:HD3	1:C:587:GLU:OE1	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:HG22	1:B:526:VAL:N	2.20	0.56
1:C:478:THR:HG22	1:C:479:GLY:N	2.21	0.56
1:C:576:LEU:O	1:C:580:ILE:HG12	2.06	0.56
1:C:449:ASN:O	1:C:460:GLU:HG2	2.06	0.56
1:B:446:LYS:HG2	1:B:463:VAL:HG12	1.87	0.56
1:C:540:ARG:NH2	5:C:225:HOH:O	2.38	0.55
1:B:306:ILE:HG13	1:B:307:LYS:N	2.22	0.55
1:C:525:ILE:HG22	1:C:526:VAL:N	2.20	0.55
1:C:398:LEU:HD21	1:C:545:ILE:HG21	1.88	0.55
1:B:592:ILE:HG12	1:B:596:ILE:CD1	2.37	0.55
1:A:429:ASP:HA	4:A:800:ADP:H5'1	1.88	0.55
1:B:469:LEU:C	1:B:469:LEU:HD23	2.27	0.55
1:B:491:ILE:HD11	1:B:534:PRO:CD	2.37	0.55
1:C:401:MET:HE3	1:C:404:VAL:HB	1.89	0.54
1:C:469:LEU:HD12	1:C:469:LEU:C	2.28	0.54
1:B:450:VAL:HG22	1:B:450:VAL:O	2.07	0.54
1:A:479:GLY:H	1:A:481:GLU:HG3	1.71	0.54
1:B:412:MET:HE3	1:B:469:LEU:HB2	1.88	0.54
1:A:284:ASP:HB3	1:A:287:LEU:HB3	1.88	0.54
1:C:401:MET:CE	1:C:404:VAL:HB	2.38	0.54
1:A:449:ASN:O	1:A:452:LEU:HD13	2.07	0.54
1:A:517:ARG:HB2	1:A:517:ARG:CZ	2.37	0.54
1:B:280:THR:CG2	1:B:282:CYS:HB2	2.37	0.53
1:C:268:VAL:CG2	1:C:326:ILE:HG22	2.37	0.53
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.90	0.53
1:A:615:MET:O	1:A:619:VAL:HG23	2.09	0.53
1:B:412:MET:HE1	1:B:523:PRO:HG2	1.91	0.52
1:C:415:ASN:HD21	1:C:420:ARG:NH1	2.03	0.52
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.72	0.52
1:C:483:ARG:N	1:C:483:ARG:HD2	2.25	0.52
1:B:493:ASN:N	1:B:493:ASN:HD22	2.07	0.52
1:B:410:LYS:HA	1:B:413:VAL:HG12	1.92	0.51
1:C:482:SER:OG	1:C:483:ARG:HD2	2.10	0.51
1:B:512:LYS:HG3	1:B:513:HIS:ND1	2.25	0.51
1:B:472:PHE:HB2	1:B:526:VAL:HG22	1.92	0.51
1:A:602:ARG:O	1:A:605:LYS:HG2	2.11	0.51
1:A:361:LEU:HD11	1:A:365:PHE:CZ	2.45	0.51
1:A:512:LYS:O	1:A:512:LYS:HG2	2.11	0.51
1:B:299:PHE:CZ	1:B:318:GLU:HB2	2.46	0.51
1:B:366:ASN:ND2	1:B:595:ARG:HH11	2.04	0.50
1:C:583:ARG:CD	1:C:587:GLU:OE1	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:MET:CE	1:B:469:LEU:HB2	2.42	0.50
1:B:270:TRP:CE2	1:B:336:ILE:HG12	2.47	0.50
1:B:512:LYS:HG3	1:B:513:HIS:N	2.18	0.50
1:A:597:VAL:O	1:A:601:GLU:HG3	2.12	0.50
1:A:457:LEU:HD11	1:A:493:ASN:HB3	1.93	0.50
1:B:477:GLY:HA2	1:B:491:ILE:HG22	1.94	0.49
1:A:372:MET:HA	1:A:375:MET:HG2	1.95	0.49
1:A:561:GLU:O	1:A:565:GLU:HG3	2.12	0.49
1:C:525:ILE:CG2	1:C:526:VAL:N	2.74	0.49
1:C:465:ILE:CD1	1:C:516:LYS:HB2	2.39	0.49
1:B:303:LEU:HA	1:B:306:ILE:HG12	1.94	0.49
1:A:559:ARG:HH11	1:A:559:ARG:HG3	1.77	0.49
1:B:478:THR:O	1:B:481:GLU:HG3	2.11	0.49
1:B:491:ILE:HG23	1:B:492:ASN:N	2.27	0.49
1:B:406:TYR:O	1:B:410:LYS:HG2	2.12	0.49
1:C:401:MET:CE	1:C:401:MET:HA	2.43	0.49
1:C:483:ARG:HD2	1:C:483:ARG:H	1.78	0.49
1:B:398:LEU:HD22	1:B:401:MET:HE1	1.95	0.49
1:A:511:LYS:O	1:A:512:LYS:CB	2.61	0.48
1:C:459:PHE:HE1	1:C:513:HIS:H	1.60	0.48
1:A:602:ARG:HB2	1:A:605:LYS:NZ	2.28	0.48
1:A:608:SER:O	1:A:611:VAL:HG22	2.13	0.48
1:A:385:GLU:HA	1:A:607:PHE:CZ	2.44	0.48
1:A:593:GLN:O	1:A:597:VAL:HG23	2.13	0.48
1:B:378:SER:C	1:B:380:GLY:N	2.67	0.48
1:A:433:THR:HB	4:A:800:ADP:O2A	2.13	0.48
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.14	0.48
1:C:608:SER:OG	1:C:611:VAL:HG23	2.12	0.48
1:B:477:GLY:HA2	1:B:491:ILE:CG2	2.43	0.48
1:A:505:VAL:HG13	5:A:119:HOH:O	2.14	0.48
1:B:412:MET:HE2	1:B:469:LEU:HG	1.96	0.47
1:B:460:GLU:O	1:B:463:VAL:HG23	2.14	0.47
1:B:291:MET:HA	1:B:291:MET:CE	2.44	0.47
1:B:291:MET:HE3	1:C:350:VAL:CG2	2.44	0.47
1:B:415:ASN:HD22	1:B:420:ARG:HD2	1.77	0.47
1:B:446:LYS:HD3	1:B:467:GLN:CD	2.33	0.47
1:A:554:LYS:O	1:A:558:GLU:HG3	2.14	0.47
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.49	0.47
1:A:493:ASN:O	1:A:497:LEU:HG	2.14	0.47
1:A:478:THR:HA	1:A:481:GLU:OE2	2.14	0.47
1:C:272:LEU:HD23	1:C:323:ASN:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.50	0.47
1:B:410:LYS:HA	1:B:413:VAL:CG1	2.44	0.47
1:A:448:LEU:HG	1:A:470:VAL:HG22	1.97	0.47
1:A:402:ASP:HA	1:A:578:MET:CE	2.44	0.47
1:B:429:ASP:HA	4:B:800:ADP:H5'1	1.98	0.46
1:C:299:PHE:CE1	1:C:318:GLU:HG2	2.51	0.46
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.30	0.46
1:A:384:ILE:HG21	1:A:606:GLU:OE1	2.15	0.46
1:A:476:LYS:HE3	1:A:486:PRO:HB2	1.96	0.46
1:C:432:LYS:HE3	1:C:528:MET:O	2.16	0.46
1:A:483:ARG:O	1:A:483:ARG:HG2	2.16	0.46
1:A:525:ILE:HG22	1:A:526:VAL:N	2.31	0.46
1:C:611:VAL:HG21	5:C:52:HOH:O	2.15	0.46
1:C:514:LEU:HD23	1:C:516:LYS:NZ	2.31	0.46
1:C:478:THR:HG22	1:C:479:GLY:H	1.80	0.45
1:A:290:GLY:O	1:A:294:GLU:HG3	2.16	0.45
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.63	0.45
1:A:482:SER:C	1:A:484:ASP:H	2.19	0.45
1:B:602:ARG:O	1:B:602:ARG:HD3	2.16	0.45
1:B:291:MET:HA	1:B:291:MET:HE2	1.98	0.45
1:C:416:ILE:O	1:C:420:ARG:HG2	2.17	0.45
1:A:516:LYS:O	1:A:517:ARG:HB2	2.16	0.45
1:A:361:LEU:O	1:A:364:ARG:HB3	2.16	0.45
1:B:372:MET:HA	1:B:375:MET:HG2	1.98	0.45
1:B:420:ARG:HB3	1:B:523:PRO:CB	2.45	0.45
1:B:331:LYS:HD2	1:C:270:TRP:CE2	2.52	0.45
1:B:456:ARG:HB2	1:B:456:ARG:HH11	1.82	0.44
1:B:457:LEU:O	1:B:461:LEU:HG	2.17	0.44
1:A:356:THR:OG1	1:A:359:GLN:HG3	2.16	0.44
1:B:465:ILE:O	1:B:466:ASP:HB2	2.16	0.44
1:C:448:LEU:HD22	1:C:463:VAL:HB	1.99	0.44
1:B:493:ASN:ND2	1:B:493:ASN:N	2.65	0.44
1:A:583:ARG:HA	1:A:584:PRO:HD3	1.85	0.44
1:B:619:VAL:HG22	1:B:625:VAL:HG12	1.98	0.44
1:C:384:ILE:HG13	1:C:384:ILE:O	2.18	0.44
1:C:417:PRO:O	1:C:418:LYS:HB2	2.16	0.44
1:A:449:ASN:ND2	1:A:452:LEU:HD11	2.33	0.44
1:B:561:GLU:O	1:B:565:GLU:HG3	2.17	0.44
1:C:372:MET:CA	1:C:375:MET:HE3	2.30	0.44
1:B:469:LEU:HD23	1:B:470:VAL:N	2.32	0.44
1:B:592:ILE:HG12	1:B:596:ILE:HD13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ASP:HA	1:B:537:LEU:HD13	1.99	0.43
1:A:479:GLY:H	1:A:481:GLU:CG	2.32	0.43
1:B:299:PHE:CE2	1:B:318:GLU:HB2	2.53	0.43
1:B:425:LYS:O	1:B:546:ASP:HA	2.18	0.43
1:C:507:VAL:HG12	1:C:508:ASN:N	2.33	0.43
1:C:416:ILE:O	1:C:420:ARG:CG	2.67	0.43
1:A:538:GLN:HE22	1:A:544:GLN:HE21	1.64	0.43
1:C:451:ASN:HD22	1:C:490:GLY:H	1.65	0.43
1:B:412:MET:CE	1:B:523:PRO:HG2	2.49	0.43
1:B:268:VAL:HG21	1:B:330:SER:HB2	1.99	0.43
1:A:451:ASN:C	1:A:452:LEU:HD12	2.39	0.43
1:A:417:PRO:O	1:A:418:LYS:HB2	2.18	0.43
1:B:592:ILE:O	1:B:596:ILE:HD13	2.19	0.43
1:B:450:VAL:HG23	1:B:457:LEU:HD11	2.01	0.43
1:B:583:ARG:HA	1:B:584:PRO:HD3	1.81	0.43
1:B:500:TYR:HE2	1:B:509:LEU:HD21	1.84	0.43
1:B:453:PRO:HB2	1:B:455:ASP:OD1	2.19	0.42
1:B:378:SER:C	1:B:380:GLY:H	2.22	0.42
1:C:415:ASN:ND2	1:C:420:ARG:HH11	2.06	0.42
1:C:448:LEU:HG	1:C:470:VAL:CG1	2.49	0.42
1:B:529:ASN:O	1:B:530:GLU:C	2.57	0.42
1:C:580:ILE:CD1	1:C:596:ILE:HD12	2.50	0.42
1:C:482:SER:C	1:C:484:ASP:H	2.23	0.42
1:A:419:LYS:CA	1:A:542:VAL:HG11	2.45	0.42
1:C:529:ASN:O	1:C:530:GLU:CB	2.53	0.42
1:B:419:LYS:CA	1:B:542:VAL:HG11	2.48	0.42
1:B:304:LYS:HA	1:B:309:GLU:OE1	2.19	0.42
1:B:589:ALA:O	1:B:592:ILE:HG22	2.20	0.42
1:A:590:GLN:CD	1:A:590:GLN:N	2.73	0.41
1:B:413:VAL:HG13	1:B:414:TYR:N	2.35	0.41
1:C:550:LYS:HD3	1:C:552:TYR:OH	2.20	0.41
1:A:428:ILE:HD13	1:A:529:ASN:OD1	2.20	0.41
1:B:412:MET:HE2	1:B:469:LEU:CG	2.50	0.41
1:A:420:ARG:HG2	1:A:523:PRO:HB3	2.02	0.41
1:A:361:LEU:O	1:A:361:LEU:HD13	2.20	0.41
1:A:469:LEU:HD12	1:A:469:LEU:C	2.41	0.41
1:B:511:LYS:O	1:B:512:LYS:HB3	2.21	0.41
1:C:511:LYS:HG2	1:C:512:LYS:HG3	2.02	0.41
1:B:409:LEU:O	1:B:413:VAL:HG12	2.19	0.41
1:B:380:GLY:O	1:B:381:SER:HB2	2.21	0.41
1:A:590:GLN:HE21	1:A:591:SER:H	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:CG2	1:B:526:VAL:N	2.84	0.41
1:C:550:LYS:HD3	1:C:552:TYR:CZ	2.56	0.41
1:B:416:ILE:O	1:B:420:ARG:CG	2.67	0.41
1:A:498:ARG:HD3	1:A:540:ARG:HH21	1.86	0.41
1:B:465:ILE:HA	1:B:519:GLN:NE2	2.36	0.41
1:B:379:THR:O	1:B:380:GLY:O	2.38	0.41
1:A:402:ASP:HA	1:A:578:MET:HE1	2.02	0.41
1:A:293:LEU:CD1	1:B:343:THR:HG23	2.51	0.41
1:A:567:ARG:HA	1:A:570:GLN:OE1	2.21	0.41
1:A:559:ARG:NH1	1:A:559:ARG:HG3	2.35	0.41
1:C:387:TRP:CZ3	1:C:573:ILE:HB	2.56	0.41
1:C:505:VAL:HG12	1:C:506:LYS:O	2.21	0.40
1:A:303:LEU:HA	1:A:306:ILE:HG22	2.03	0.40
1:C:406:TYR:CZ	1:C:410:LYS:HD3	2.57	0.40
1:B:432:LYS:HB3	1:B:527:THR:OG1	2.22	0.40
1:A:528:MET:HG2	1:A:529:ASN:O	2.22	0.40
1:B:470:VAL:O	1:B:524:GLY:HA3	2.21	0.40
1:B:535:LYS:HB2	1:B:535:LYS:HE3	1.93	0.40
1:B:453:PRO:C	1:B:455:ASP:H	2.24	0.40
1:B:510:GLU:HG3	1:B:510:GLU:O	2.20	0.40
1:A:395:HIS:HD2	1:A:616:LYS:HZ3	1.67	0.40
1:A:505:VAL:CG1	1:A:506:LYS:N	2.84	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	361/377 (96%)	341 (94%)	16 (4%)	4 (1%)	17 6
1	B	360/377 (96%)	337 (94%)	18 (5%)	5 (1%)	14 4
1	C	360/377 (96%)	344 (96%)	13 (4%)	3 (1%)	24 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1081/1131 (96%)	1022 (94%)	47 (4%)	12 (1%)	17 6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	VAL
1	B	380	GLY
1	A	456	ARG
1	A	512	LYS
1	B	381	SER
1	B	530	GLU
1	C	530	GLU
1	B	454	LEU
1	C	456	ARG
1	C	515	ASN
1	A	624	GLY
1	B	486	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/336 (96%)	316 (98%)	8 (2%)	55 45
1	B	322/336 (96%)	310 (96%)	12 (4%)	41 27
1	C	323/336 (96%)	311 (96%)	12 (4%)	41 27
All	All	969/1008 (96%)	937 (97%)	32 (3%)	45 32

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

Mol	Chain	Res	Type
1	A	272	LEU
1	A	349	ARG
1	A	353	LEU
1	A	423	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	LEU
1	A	470	VAL
1	A	570	GLN
1	A	602	ARG
1	B	280	THR
1	B	287	LEU
1	B	338	GLN
1	B	349	ARG
1	B	361	LEU
1	B	398	LEU
1	B	415	ASN
1	B	469	LEU
1	B	520	ILE
1	B	570	GLN
1	B	602	ARG
1	B	603	LEU
1	C	272	LEU
1	C	279	GLU
1	C	301	MET
1	C	312	SER
1	C	317	HIS
1	C	349	ARG
1	C	361	LEU
1	C	398	LEU
1	C	410	LYS
1	C	466	ASP
1	C	602	ARG
1	C	603	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	310	GLN
1	A	333	GLN
1	A	338	GLN
1	A	354	GLN
1	A	395	HIS
1	A	415	ASN
1	A	458	ASN
1	A	544	GLN
1	A	590	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	296	GLN
1	B	323	ASN
1	B	333	GLN
1	B	354	GLN
1	B	366	ASN
1	B	415	ASN
1	B	493	ASN
1	B	519	GLN
1	B	538	GLN
1	B	613	GLN
1	C	296	GLN
1	C	317	HIS
1	C	363	ASN
1	C	415	ASN
1	C	451	ASN
1	C	467	GLN
1	C	508	ASN
1	C	544	GLN
1	C	555	HIS
1	C	613	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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	ADP	A	800	3	22,29,29	1.17	3 (13%)	27,45,45	2.67	4 (14%)
4	ADP	B	800	3	22,29,29	1.22	2 (9%)	27,45,45	2.69	6 (22%)
4	ADP	C	800	3	22,29,29	1.33	2 (9%)	27,45,45	2.90	6 (22%)

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
4	ADP	A	800	3	-	0/12/32/32	0/3/3/3
4	ADP	B	800	3	-	0/12/32/32	0/3/3/3
4	ADP	C	800	3	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	ADP	C5-N7	-2.23	1.31	1.39
4	B	800	ADP	PA-O2A	-2.20	1.45	1.54
4	A	800	ADP	PA-O2A	-2.01	1.46	1.54
4	C	800	ADP	PA-O1A	-2.00	1.43	1.51
4	B	800	ADP	O4'-C1'	2.27	1.44	1.41
4	A	800	ADP	O4'-C1'	2.40	1.44	1.41
4	C	800	ADP	O4'-C1'	2.90	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	800	ADP	N3-C2-N1	-13.64	118.45	128.89
4	B	800	ADP	N3-C2-N1	-12.72	119.16	128.89
4	A	800	ADP	N3-C2-N1	-12.71	119.16	128.89
4	A	800	ADP	C4-C5-N7	-2.50	107.18	109.48
4	C	800	ADP	O4'-C4'-C5'	-2.36	100.87	109.32
4	B	800	ADP	C4-C5-N7	-2.20	107.46	109.48
4	C	800	ADP	C4-C5-N7	-2.03	107.61	109.48
4	B	800	ADP	O4'-C4'-C5'	-2.03	102.07	109.32
4	A	800	ADP	C2-N1-C6	2.00	122.34	118.77
4	B	800	ADP	C2-N1-C6	2.07	122.47	118.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	800	ADP	O3A-PA-O5'	2.17	108.69	102.94
4	A	800	ADP	C4'-O4'-C1'	2.17	112.11	109.72
4	B	800	ADP	C4'-O4'-C1'	2.41	112.36	109.72
4	C	800	ADP	C2-N1-C6	2.43	123.11	118.77
4	C	800	ADP	C4'-O4'-C1'	2.48	112.45	109.72
4	C	800	ADP	O3A-PA-O5'	2.70	110.11	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	ADP	2	0
4	B	800	ADP	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.