



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 1SVO / pdb_00001svo
Title : Structure of SV40 large T antigen helicase domain
Authors : Gai, D.; Zhao, R.; Finkielstein, C.V.; Chen, X.S.
Deposited on : 2004-03-29
Resolution : 2.60 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

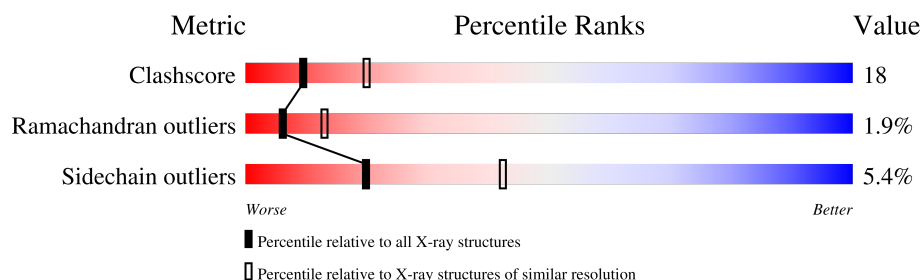
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6056 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	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

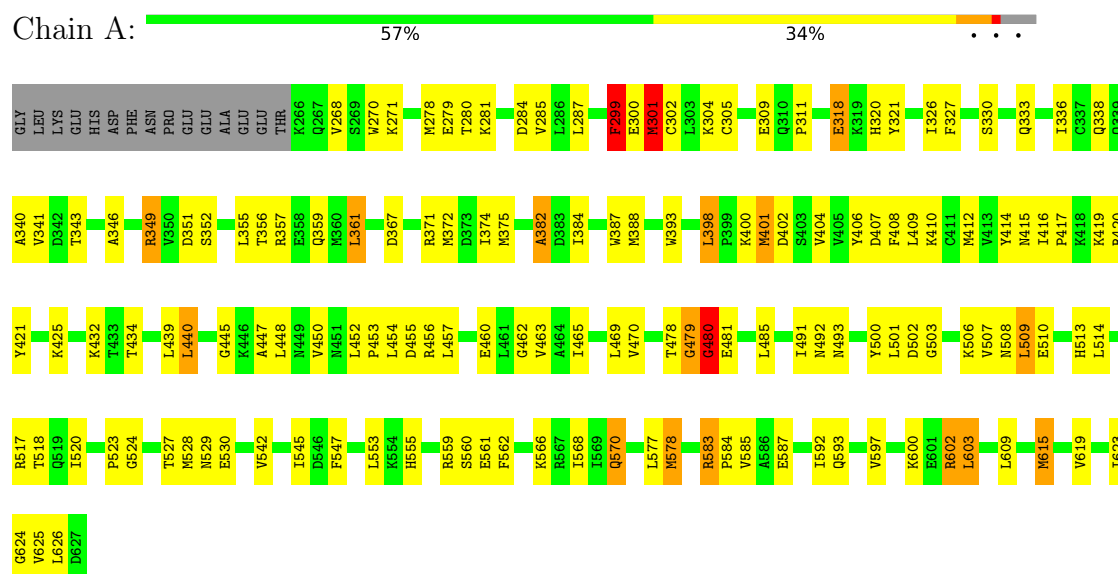
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	85	Total	O	0	0
			85	85		

3 Residue-property plots

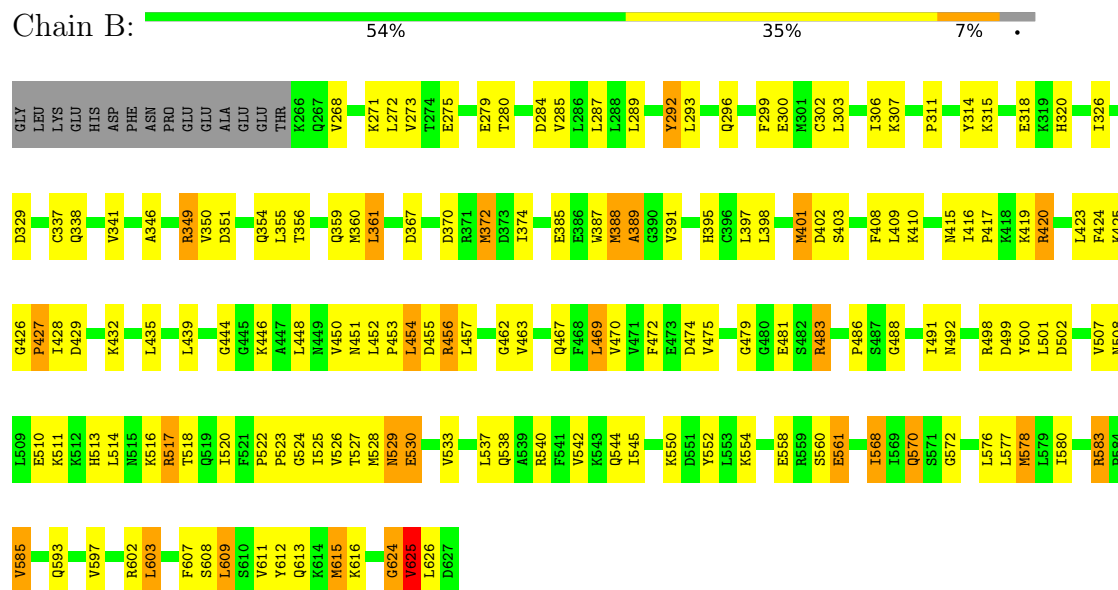
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



• Molecule 1: large T antigen



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.44Å 120.44Å 131.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	90.5 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6056	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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

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	0.67	5/2992 (0.2%)	1.03	13/4030 (0.3%)
1	B	0.67	5/2992 (0.2%)	1.04	20/4030 (0.5%)
All	All	0.67	10/5984 (0.2%)	1.04	33/8060 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	MET	SD-CE	-12.28	1.48	1.79
1	A	615	MET	SD-CE	-12.10	1.49	1.79
1	A	578	MET	SD-CE	-11.44	1.50	1.79
1	B	578	MET	SD-CE	-11.39	1.51	1.79
1	B	360	MET	SD-CE	-10.13	1.54	1.79
1	A	412	MET	SD-CE	-7.16	1.61	1.79
1	A	401	MET	SD-CE	-6.33	1.63	1.79
1	B	388	MET	SD-CE	-6.04	1.64	1.79
1	B	372	MET	SD-CE	-5.41	1.66	1.79
1	A	372	MET	SD-CE	-5.08	1.66	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	GLY	N-CA-C	-8.23	104.53	115.32
1	B	389	ALA	N-CA-C	-7.29	103.04	112.23
1	A	583	ARG	N-CA-C	7.14	119.94	110.08
1	B	517	ARG	N-CA-C	6.84	119.93	110.35
1	A	623	ILE	N-CA-C	6.65	120.19	113.47
1	A	517	ARG	N-CA-C	6.63	118.86	110.24
1	B	529	ASN	N-CA-C	6.58	120.01	112.57
1	B	520	ILE	N-CA-C	-6.46	101.22	109.30
1	A	480	GLY	N-CA-C	6.45	128.45	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	625	VAL	N-CA-C	6.40	120.00	111.17
1	A	388	MET	N-CA-C	-6.28	105.11	112.89
1	B	524	GLY	N-CA-C	6.28	118.61	110.45
1	B	444	GLY	N-CA-C	-6.25	103.42	112.17
1	B	501	LEU	N-CA-C	5.91	117.52	111.14
1	B	388	MET	N-CA-C	-5.81	106.02	113.23
1	B	585	VAL	N-CA-C	5.67	116.32	110.36
1	A	299	PHE	N-CA-C	-5.64	105.89	112.89
1	A	524	GLY	N-CA-C	5.41	119.58	111.42
1	B	626	LEU	N-CA-C	5.38	119.47	113.02
1	B	568	ILE	N-CA-C	5.35	116.41	111.81
1	B	456	ARG	N-CA-C	-5.33	107.32	112.97
1	B	583	ARG	N-CA-C	5.29	117.97	110.24
1	B	403	SER	N-CA-C	-5.29	105.57	112.23
1	A	501	LEU	N-CA-C	5.29	117.47	111.02
1	A	382	ALA	N-CA-C	5.27	117.72	110.35
1	A	626	LEU	N-CA-C	5.24	119.39	113.15
1	B	479	GLY	N-CA-C	-5.23	105.24	111.36
1	A	520	ILE	N-CA-C	-5.11	102.15	108.89
1	A	421	TYR	N-CA-C	5.09	117.73	109.24
1	B	292	TYR	N-CA-C	5.08	116.81	111.28
1	A	481	GLU	N-CA-C	-5.07	107.09	113.28
1	B	401	MET	N-CA-C	5.02	116.76	111.28
1	B	391	VAL	N-CA-C	-5.01	105.61	110.42

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	2933	0	2982	105	0
1	B	2933	0	2982	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	103	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	85	0	0	6	0
All	All	6056	0	5964	212	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 18.

All (212) 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:402:ASP:HA	1:A:578:MET:HE3	1.52	0.91
1:A:356:THR:H	1:A:359:GLN:HE21	1.18	0.88
1:B:402:ASP:HA	1:B:578:MET:HE3	1.57	0.86
1:A:450:VAL:HG13	1:A:457:LEU:HD11	1.59	0.82
1:B:446:LYS:HG2	1:B:467:GLN:NE2	1.95	0.81
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.27	0.81
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.97	0.80
1:A:311:PRO:HG2	1:A:374:ILE:HD13	1.64	0.79
1:B:533:VAL:HG13	1:B:537:LEU:HD23	1.64	0.78
1:B:446:LYS:HG2	1:B:467:GLN:HE21	1.48	0.77
1:B:560:SER:OG	1:B:624:GLY:HA2	1.86	0.76
1:B:483:ARG:H	1:B:483:ARG:HD2	1.51	0.76
1:B:284:ASP:HB3	1:B:287:LEU:HB3	1.69	0.75
1:A:432:LYS:HE2	1:A:527:THR:HG23	1.69	0.74
1:A:415:ASN:ND2	1:A:420:ARG:HD2	2.02	0.72
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.35	0.72
1:B:508:ASN:ND2	1:B:518:THR:HG23	2.05	0.72
1:A:285:VAL:HG21	1:A:338:GLN:NE2	2.05	0.72
1:B:450:VAL:HG13	1:B:457:LEU:HD11	1.72	0.72
1:B:311:PRO:HG2	1:B:374:ILE:HD13	1.73	0.70
1:A:356:THR:OG1	1:A:359:GLN:HG3	1.92	0.70
1:B:350:VAL:O	1:B:354:GLN:HG3	1.92	0.69
1:A:356:THR:H	1:A:359:GLN:NE2	1.91	0.69
1:A:491:ILE:CD1	1:A:528:MET:HE2	2.23	0.69
1:A:398:LEU:HB2	1:A:401:MET:HE2	1.74	0.67
1:A:491:ILE:HD11	1:A:528:MET:HE2	1.78	0.65
1:A:415:ASN:HD21	1:A:420:ARG:HD2	1.62	0.64
1:B:538:GLN:HE22	1:B:544:GLN:NE2	1.95	0.64
1:A:453:PRO:HG2	1:A:456:ARG:NH1	2.12	0.64
1:A:407:ASP:O	1:A:410:LYS:HG2	1.98	0.63
1:B:453:PRO:HG2	1:B:456:ARG:HD2	1.80	0.63
1:B:529:ASN:O	1:B:530:GLU:HB2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ALA:O	1:A:448:LEU:HD23	1.98	0.63
1:A:416:ILE:O	1:A:420:ARG:HG2	1.99	0.63
1:B:609:LEU:HD13	1:B:613:GLN:HG2	1.81	0.62
1:B:415:ASN:HD21	1:B:420:ARG:NH1	1.98	0.62
1:A:400:LYS:O	1:A:404:VAL:HG23	2.00	0.62
1:B:415:ASN:ND2	1:B:523:PRO:HG3	2.16	0.61
1:B:285:VAL:HG22	1:B:341:VAL:HG21	1.82	0.60
1:B:419:LYS:HA	1:B:542:VAL:HB	1.81	0.60
1:A:419:LYS:HA	1:A:542:VAL:HB	1.85	0.59
1:A:299:PHE:C	1:A:301:MET:H	2.10	0.59
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.02	0.59
1:A:420:ARG:HB3	1:A:523:PRO:HB3	1.83	0.59
1:B:351:ASP:HB3	1:B:355:LEU:HD12	1.85	0.58
1:A:500:TYR:CE2	1:A:507:VAL:HG11	2.38	0.58
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.65	0.58
1:A:529:ASN:O	1:A:530:GLU:HB2	2.03	0.58
1:B:469:LEU:C	1:B:469:LEU:HD12	2.29	0.58
1:B:432:LYS:HE2	1:B:527:THR:HG23	1.85	0.58
1:A:268:VAL:HG22	1:A:326:ILE:HG22	1.85	0.57
1:B:389:ALA:HB1	1:B:625:VAL:HG21	1.86	0.57
1:A:583:ARG:HD2	1:A:587:GLU:OE1	2.05	0.57
1:B:272:LEU:HD22	1:B:320:HIS:CE1	2.40	0.56
1:B:450:VAL:HG12	1:B:450:VAL:O	2.04	0.56
1:A:508:ASN:ND2	1:A:518:THR:HG23	2.20	0.56
1:A:327:PHE:CZ	1:A:333:GLN:HB3	2.41	0.56
1:A:434:THR:HG23	1:A:570:GLN:HG3	1.88	0.55
1:A:462:GLY:HA3	1:A:510:GLU:O	2.06	0.55
1:B:452:LEU:HB3	1:B:453:PRO:CD	2.37	0.55
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.41	0.55
1:B:453:PRO:HD2	1:B:456:ARG:HB2	1.89	0.55
1:B:268:VAL:HG22	1:B:326:ILE:HG22	1.89	0.55
1:A:480:GLY:O	1:A:485:LEU:HB2	2.08	0.54
1:A:508:ASN:HD22	1:A:518:THR:HG23	1.73	0.54
1:A:432:LYS:HB3	1:A:547:PHE:CD1	2.43	0.54
1:A:469:LEU:HD12	1:A:469:LEU:C	2.33	0.54
1:A:398:LEU:HD21	1:A:545:ILE:HG21	1.89	0.54
1:A:432:LYS:HE3	1:A:528:MET:O	2.08	0.54
1:B:508:ASN:N	1:B:508:ASN:HD22	2.05	0.54
1:A:351:ASP:HB3	1:A:355:LEU:HD12	1.90	0.53
1:A:508:ASN:HD22	1:A:508:ASN:N	2.04	0.53
1:B:432:LYS:HE3	1:B:528:MET:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:VAL:HG21	1:B:597:VAL:HG22	1.90	0.53
1:A:284:ASP:HB3	1:A:287:LEU:HB3	1.91	0.53
1:A:615:MET:HB3	1:A:625:VAL:CG1	2.39	0.53
1:B:500:TYR:CE2	1:B:507:VAL:HG11	2.44	0.53
1:B:425:LYS:HE2	1:B:530:GLU:HA	1.91	0.53
1:A:361:LEU:HD11	1:A:409:LEU:HD22	1.90	0.52
1:B:424:PHE:CE1	1:B:545:ILE:HD12	2.45	0.52
1:B:303:LEU:HG	3:B:118:HOH:O	2.10	0.52
1:B:538:GLN:NE2	1:B:544:GLN:NE2	2.58	0.52
1:B:608:SER:OG	1:B:611:VAL:HG23	2.09	0.51
1:A:346:ALA:HB2	1:B:289:LEU:HD23	1.92	0.51
1:B:462:GLY:HA3	1:B:510:GLU:O	2.11	0.51
1:A:583:ARG:HD3	1:A:584:PRO:HD2	1.92	0.51
1:B:397:LEU:O	1:B:398:LEU:HD12	2.10	0.51
1:B:602:ARG:HG3	1:B:602:ARG:HH11	1.75	0.51
1:B:307:LYS:HD3	3:B:88:HOH:O	2.11	0.50
1:A:375:MET:HB3	1:A:382:ALA:CB	2.40	0.50
1:A:299:PHE:CE1	1:A:318:GLU:HG2	2.47	0.50
1:B:387:TRP:CE3	1:B:568:ILE:HG23	2.46	0.50
1:A:393:TRP:CE2	1:A:553:LEU:HD22	2.46	0.49
1:A:507:VAL:O	1:A:518:THR:HA	2.11	0.49
1:A:602:ARG:HG3	1:A:602:ARG:HH11	1.77	0.49
1:B:454:LEU:O	1:B:454:LEU:HG	2.12	0.49
1:A:384:ILE:HD11	1:A:603:LEU:HD11	1.93	0.49
1:A:478:THR:O	1:A:479:GLY:C	2.55	0.49
1:B:423:LEU:HD11	1:B:528:MET:HE3	1.95	0.49
1:A:615:MET:HB3	1:A:625:VAL:HG12	1.95	0.49
1:A:450:VAL:HG12	1:A:493:ASN:HB2	1.95	0.48
1:B:507:VAL:C	1:B:508:ASN:HD22	2.21	0.48
1:B:428:ILE:HG12	1:B:429:ASP:OD1	2.13	0.48
1:B:498:ARG:HB2	1:B:540:ARG:HE	1.79	0.48
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.78	0.48
1:A:375:MET:C	1:A:382:ALA:HB3	2.39	0.48
1:A:555:HIS:HB3	1:A:559:ARG:NH1	2.28	0.48
1:A:305:CYS:HB2	3:A:184:HOH:O	2.13	0.48
1:A:585:VAL:HG23	3:A:168:HOH:O	2.13	0.48
1:B:349:ARG:HH11	1:B:349:ARG:HB2	1.78	0.48
1:A:455:ASP:CG	1:B:456:ARG:HH12	2.22	0.48
1:A:375:MET:O	1:A:382:ALA:HB3	2.14	0.48
1:B:513:HIS:O	1:B:514:LEU:HG	2.14	0.47
1:B:311:PRO:HG2	1:B:374:ILE:CD1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:VAL:HG21	1:B:526:VAL:HG13	1.96	0.47
1:B:273:VAL:HG22	1:B:292:TYR:CE2	2.49	0.47
1:B:550:LYS:HD3	1:B:552:TYR:OH	2.15	0.47
1:A:285:VAL:HG22	1:A:341:VAL:HG21	1.97	0.47
1:B:511:LYS:HB3	1:B:516:LYS:HG3	1.96	0.47
1:A:425:LYS:HE2	1:A:530:GLU:HA	1.96	0.47
1:B:367:ASP:O	1:B:370:ASP:HB2	2.15	0.47
1:B:537:LEU:O	1:B:540:ARG:HB2	2.13	0.47
1:B:446:LYS:HB2	3:B:62:HOH:O	2.15	0.47
1:B:285:VAL:HG21	1:B:338:GLN:HE22	1.79	0.47
1:A:615:MET:O	1:A:619:VAL:HG23	2.15	0.46
1:B:602:ARG:HG3	1:B:602:ARG:NH1	2.30	0.46
1:B:388:MET:HE3	1:B:603:LEU:HD21	1.96	0.46
1:A:593:GLN:O	1:A:597:VAL:HG23	2.14	0.46
1:A:299:PHE:CZ	1:A:318:GLU:HG2	2.51	0.46
1:A:440:LEU:HD21	1:A:445:GLY:O	2.16	0.46
1:A:268:VAL:HG21	1:A:330:SER:HB2	1.98	0.46
1:A:285:VAL:HG21	1:A:338:GLN:HE22	1.80	0.46
1:A:299:PHE:C	1:A:301:MET:N	2.74	0.46
1:A:356:THR:HG23	1:A:359:GLN:NE2	2.31	0.46
1:A:302:CYS:SG	1:A:305:CYS:N	2.88	0.46
1:A:402:ASP:HA	1:A:578:MET:CE	2.36	0.46
1:A:583:ARG:CD	1:A:587:GLU:OE1	2.63	0.46
1:A:304:LYS:HG2	1:A:309:GLU:OE1	2.17	0.45
1:B:385:GLU:HG2	1:B:607:PHE:HE2	1.81	0.45
1:B:401:MET:HG3	1:B:578:MET:HE1	1.99	0.45
1:A:414:TYR:O	1:A:415:ASN:C	2.59	0.45
1:B:576:LEU:O	1:B:580:ILE:HG13	2.16	0.45
1:A:506:LYS:NZ	1:A:506:LYS:HB2	2.31	0.45
1:B:285:VAL:HG21	1:B:338:GLN:NE2	2.32	0.45
1:B:329:ASP:HA	3:B:20:HOH:O	2.17	0.45
1:A:280:THR:O	1:A:281:LYS:HB2	2.17	0.45
1:A:371:ARG:O	1:A:375:MET:HG3	2.17	0.45
1:B:560:SER:HG	1:B:624:GLY:HA2	1.80	0.45
1:B:280:THR:HG22	1:B:280:THR:O	2.17	0.44
1:B:448:LEU:HD21	1:B:463:VAL:HB	1.99	0.44
1:B:450:VAL:HG21	1:B:472:PHE:CD1	2.52	0.44
1:B:612:TYR:HA	1:B:615:MET:HE3	1.98	0.44
1:B:609:LEU:HD13	1:B:609:LEU:O	2.16	0.44
1:B:337:CYS:O	1:B:341:VAL:HG23	2.16	0.44
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TRP:CE3	1:A:568:ILE:HG23	2.52	0.44
1:A:432:LYS:HE2	1:A:527:THR:CG2	2.41	0.44
1:A:417:PRO:HA	1:A:502:ASP:O	2.17	0.44
1:B:293:LEU:O	1:B:296:GLN:HG2	2.18	0.44
1:B:525:ILE:HG22	1:B:526:VAL:N	2.32	0.44
1:B:612:TYR:HA	1:B:615:MET:CE	2.47	0.44
1:B:522:PRO:HA	1:B:523:PRO:HD3	1.81	0.44
1:B:561:GLU:CD	1:B:561:GLU:H	2.25	0.44
1:B:585:VAL:HG13	1:B:593:GLN:HB3	2.00	0.44
1:B:346:ALA:O	1:B:350:VAL:HG23	2.17	0.43
1:A:448:LEU:HD22	1:A:463:VAL:HB	1.99	0.43
1:B:451:ASN:O	1:B:452:LEU:HD23	2.18	0.43
1:A:448:LEU:HG	1:A:470:VAL:HG13	1.99	0.43
1:A:450:VAL:C	1:A:452:LEU:H	2.26	0.43
1:B:372:MET:HE3	1:B:577:LEU:HG	2.00	0.43
1:A:281:LYS:HE3	1:A:367:ASP:OD1	2.17	0.43
1:A:465:ILE:HD11	1:A:509:LEU:HB3	2.00	0.43
1:B:314:TYR:CE1	1:B:315:LYS:HG3	2.53	0.43
1:B:388:MET:CE	1:B:603:LEU:HD21	2.47	0.43
1:B:609:LEU:HD22	1:B:609:LEU:HA	1.78	0.43
1:A:356:THR:HG23	1:A:359:GLN:HE21	1.83	0.43
1:B:385:GLU:HG2	1:B:607:PHE:CE2	2.53	0.43
1:B:508:ASN:HD21	1:B:518:THR:HG23	1.80	0.43
1:B:554:LYS:O	1:B:558:GLU:HG3	2.19	0.43
1:B:395:HIS:CE1	1:B:616:LYS:HZ1	2.37	0.43
1:A:402:ASP:CA	1:A:578:MET:HE3	2.37	0.42
1:A:320:HIS:O	1:A:321:TYR:C	2.63	0.42
1:A:271:LYS:HE2	3:A:142:HOH:O	2.18	0.42
1:A:349:ARG:O	1:A:352:SER:HB3	2.20	0.42
1:A:408:PHE:CD2	1:A:439:LEU:HD22	2.53	0.42
1:A:406:TYR:CE1	1:A:587:GLU:HG2	2.53	0.42
1:A:450:VAL:HG12	1:A:450:VAL:O	2.19	0.42
1:A:304:LYS:HA	1:A:309:GLU:HG3	2.00	0.42
1:B:299:PHE:CE2	1:B:318:GLU:HG3	2.55	0.42
1:A:560:SER:OG	1:A:624:GLY:HA2	2.20	0.42
1:B:561:GLU:CD	1:B:561:GLU:N	2.77	0.42
1:B:361:LEU:HD11	1:B:409:LEU:HD22	2.02	0.42
1:B:491:ILE:CD1	1:B:528:MET:HE2	2.50	0.42
1:A:398:LEU:HB2	1:A:401:MET:CE	2.47	0.41
1:B:401:MET:HE1	1:B:435:LEU:HD22	2.02	0.41
1:A:600:LYS:HG2	3:A:171:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:VAL:HG22	3:B:62:HOH:O	2.20	0.41
1:B:275:GLU:O	1:B:279:GLU:HG3	2.19	0.41
1:A:508:ASN:ND2	1:A:508:ASN:N	2.68	0.41
1:A:513:HIS:O	1:A:514:LEU:HG	2.20	0.41
1:B:570:GLN:HG2	3:B:21:HOH:O	2.20	0.41
1:B:612:TYR:O	1:B:615:MET:HB2	2.21	0.41
1:A:562:PHE:O	1:A:566:LYS:HB2	2.21	0.41
1:B:302:CYS:O	1:B:306:ILE:HG13	2.21	0.41
1:A:460:GLU:O	1:A:463:VAL:HG23	2.21	0.41
1:B:453:PRO:C	1:B:455:ASP:H	2.29	0.40
1:B:426:GLY:O	1:B:427:PRO:O	2.40	0.40
1:A:340:ALA:O	1:A:343:THR:HB	2.21	0.40
1:A:440:LEU:HD21	1:A:445:GLY:C	2.47	0.40
1:B:408:PHE:CD2	1:B:439:LEU:HD22	2.56	0.40
1:B:410:LYS:HD3	1:B:410:LYS:HA	1.93	0.40
1:B:416:ILE:HA	1:B:417:PRO:HD3	1.98	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	360/377 (96%)	329 (91%)	24 (7%)	7 (2%)	6	13
1	B	360/377 (96%)	337 (94%)	16 (4%)	7 (2%)	6	13
All	All	720/754 (96%)	666 (92%)	40 (6%)	14 (2%)	6	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	GLY
1	B	427	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	454	LEU
1	A	479	GLY
1	B	481	GLU
1	B	488	GLY
1	A	300	GLU
1	B	486	PRO
1	A	301	MET
1	B	530	GLU
1	A	503	GLY
1	A	561	GLU
1	B	454	LEU
1	B	624	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	323/336 (96%)	306 (95%)	17 (5%)	20	43
1	B	323/336 (96%)	305 (94%)	18 (6%)	19	40
All	All	646/672 (96%)	611 (95%)	35 (5%)	20	42

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

Mol	Chain	Res	Type
1	A	278	MET
1	A	279	GLU
1	A	299	PHE
1	A	301	MET
1	A	318	GLU
1	A	349	ARG
1	A	361	LEU
1	A	398	LEU
1	A	440	LEU
1	A	492	ASN
1	A	509	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	570	GLN
1	A	577	LEU
1	A	592	ILE
1	A	602	ARG
1	A	603	LEU
1	A	609	LEU
1	B	271	LYS
1	B	300	GLU
1	B	349	ARG
1	B	361	LEU
1	B	420	ARG
1	B	469	LEU
1	B	474	ASP
1	B	483	ARG
1	B	492	ASN
1	B	499	ASP
1	B	502	ASP
1	B	517	ARG
1	B	561	GLU
1	B	570	GLN
1	B	583	ARG
1	B	603	LEU
1	B	609	LEU
1	B	625	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	338	GLN
1	A	359	GLN
1	A	415	ASN
1	A	467	GLN
1	A	496	ASN
1	A	508	ASN
1	A	529	ASN
1	A	544	GLN
1	B	333	GLN
1	B	338	GLN
1	B	415	ASN
1	B	467	GLN
1	B	489	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	508	ASN
1	B	529	ASN
1	B	538	GLN
1	B	544	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.