Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 08:32 AM EDT

PDB ID	:	1GH6
Title	:	RETINOBLASTOMA POCKET COMPLEXED WITH SV40 LARGE T ANTIGEN
Authors	:	Kim, H.Y.; Cho, Y.
Deposited on	:	2000-11-15
Resolution	:	3.20 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:

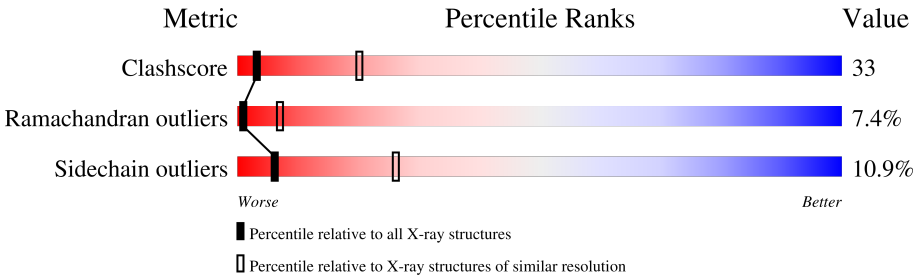
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	114	34% 49% 14% ·
2	B	333	43% 45% 10% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3627 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	114	Total	C	N	O	S	0	0	0
			941	593	153	186	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	expression tag	UNP P03070
A	5	HIS	-	expression tag	UNP P03070
A	6	MET	-	expression tag	UNP P03070

- Molecule 2 is a protein called Retinoblastoma-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	0	0	0
			2686	1732	450	483	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	436	ALA	GLN	conflict	UNP P06400
B	440	ALA	GLU	conflict	UNP P06400
B	578	LEU	-	linker	UNP P06400
B	579	VAL	-	linker	UNP P06400
B	580	PRO	-	linker	UNP P06400
B	581	ARG	-	linker	UNP P06400
B	582	GLY	-	linker	UNP P06400
B	583	SER	-	linker	UNP P06400

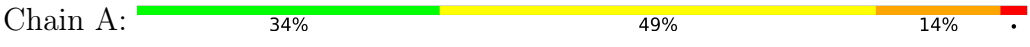
3 Residue-property plots (i)

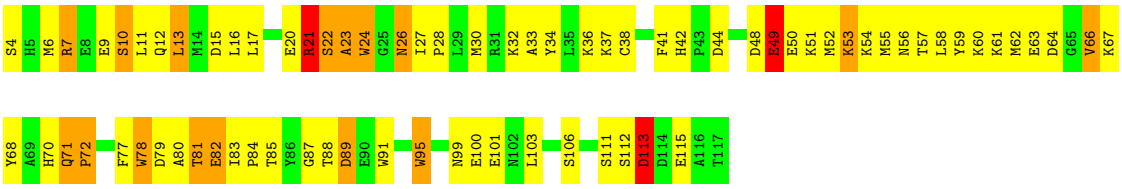
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

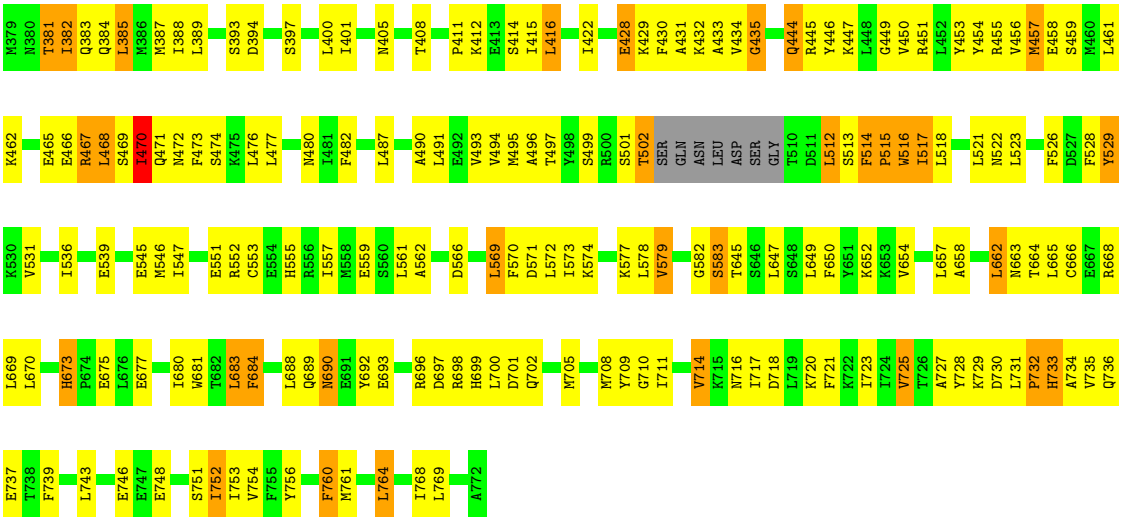
Chain A:





• Molecule 2: Retinoblastoma-associated protein

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	127.13Å 127.13Å 96.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 3.20	Depositor
% Data completeness (in resolution range)	96.0 (19.92-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3627	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.44	0/967	0.72	2/1299 (0.2%)
2	B	0.47	0/2737	0.66	0/3682
All	All	0.46	0/3704	0.67	2/4981 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ALA	N-CA-C	-5.43	96.34	111.00
1	A	72	PRO	N-CA-C	-5.07	98.91	112.10

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	941	0	870	87	0
2	B	2686	0	2748	160	0
All	All	3627	0	3618	242	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 33.

All (242) 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:26:ASN:HD21	1:A:28:PRO:HG2	1.24	1.02
2:B:697:ASP:HB3	2:B:743:LEU:HD22	1.44	0.98
2:B:449:GLY:HA2	2:B:494:VAL:HG21	1.45	0.97
2:B:493:VAL:HG22	2:B:546:MET:HE2	1.44	0.97
2:B:559:GLU:HA	2:B:700:LEU:HD12	1.51	0.93
1:A:71:GLN:HB3	1:A:72:PRO:HD3	1.52	0.92
2:B:552:ARG:HE	2:B:552:ARG:HA	1.38	0.88
2:B:381:THR:HG23	2:B:384:GLN:H	1.38	0.87
1:A:26:ASN:ND2	1:A:28:PRO:HG2	1.91	0.86
2:B:760:PHE:CE2	2:B:764:LEU:HD11	2.11	0.85
1:A:54:LYS:HA	1:A:57:THR:HG22	1.63	0.81
1:A:17:LEU:HA	1:A:55:MET:HE1	1.64	0.79
2:B:428:GLU:HG3	2:B:429:LYS:N	2.01	0.76
1:A:49:GLU:HA	1:A:49:GLU:OE1	1.87	0.74
1:A:99:ASN:HB3	2:B:769:LEU:HD11	1.68	0.74
1:A:51:LYS:O	1:A:51:LYS:HD3	1.89	0.73
2:B:557:ILE:HA	2:B:561:LEU:HB2	1.69	0.72
2:B:514:PHE:HB3	2:B:515:PRO:HD3	1.72	0.71
2:B:665:LEU:HD21	2:B:731:LEU:HD11	1.71	0.70
2:B:382:ILE:O	2:B:382:ILE:HD13	1.91	0.70
1:A:82:GLU:O	1:A:84:PRO:HD3	1.92	0.69
2:B:401:ILE:HG22	2:B:405:ASN:HD21	1.58	0.69
2:B:470:ILE:HG23	2:B:472:ASN:H	1.57	0.69
1:A:41:PHE:CE2	1:A:48:ASP:HB2	2.28	0.69
2:B:467:ARG:O	2:B:468:LEU:HB3	1.92	0.68
2:B:400:LEU:HD13	2:B:400:LEU:O	1.93	0.68
2:B:690:ASN:HD22	2:B:690:ASN:N	1.92	0.68
1:A:13:LEU:HD22	1:A:58:LEU:HB3	1.76	0.68
2:B:512:LEU:N	2:B:512:LEU:HD12	2.08	0.68
2:B:514:PHE:O	2:B:516:TRP:N	2.27	0.67
2:B:577:LYS:C	2:B:578:LEU:HD12	2.14	0.67
2:B:461:LEU:HD11	2:B:477:LEU:HD11	1.76	0.67
2:B:388:ILE:HD12	2:B:389:LEU:N	2.09	0.67
2:B:393:SER:O	2:B:451:ARG:HG2	1.95	0.67
1:A:13:LEU:HD12	1:A:13:LEU:O	1.94	0.67
1:A:54:LYS:HA	1:A:57:THR:CG2	2.24	0.65
2:B:668:ARG:HH22	2:B:730:ASP:HB2	1.61	0.65
2:B:428:GLU:HG3	2:B:429:LYS:H	1.60	0.65
2:B:496:ALA:HA	2:B:499:SER:HB3	1.79	0.65
1:A:63:GLU:O	1:A:66:VAL:HG12	1.96	0.65
2:B:735:VAL:HG12	2:B:737:GLU:H	1.63	0.64
1:A:60:LYS:HD2	1:A:83:ILE:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:GLU:HG2	2:B:462:LYS:HE3	1.79	0.64
1:A:103:LEU:HD21	2:B:714:VAL:HG13	1.80	0.63
1:A:95:TRP:CE3	1:A:95:TRP:HA	2.33	0.63
2:B:493:VAL:HG13	2:B:546:MET:SD	2.38	0.63
2:B:388:ILE:HD12	2:B:388:ILE:C	2.18	0.63
2:B:559:GLU:HA	2:B:700:LEU:CD1	2.27	0.62
1:A:71:GLN:OE1	1:A:71:GLN:HA	1.98	0.62
2:B:552:ARG:HA	2:B:552:ARG:NE	2.13	0.61
1:A:21:ARG:O	1:A:21:ARG:HG3	2.01	0.61
1:A:37:LYS:HG2	1:A:55:MET:HE2	1.82	0.61
1:A:41:PHE:HE2	1:A:48:ASP:HB2	1.64	0.61
2:B:729:LYS:NZ	2:B:736:GLN:HB3	2.15	0.61
1:A:81:THR:HG22	1:A:82:GLU:N	2.17	0.60
2:B:683:LEU:HD12	2:B:711:ILE:HG12	1.84	0.59
1:A:67:LYS:HA	1:A:78:TRP:CG	2.38	0.59
1:A:34:TYR:HE2	1:A:56:ASN:HA	1.67	0.59
2:B:385:LEU:O	2:B:388:ILE:HG13	2.02	0.59
2:B:401:ILE:HG22	2:B:405:ASN:ND2	2.17	0.59
1:A:95:TRP:HA	1:A:95:TRP:HE3	1.68	0.58
2:B:574:LYS:HG2	2:B:692:TYR:OH	2.03	0.58
2:B:645:THR:O	2:B:645:THR:HG23	2.03	0.58
2:B:514:PHE:O	2:B:515:PRO:C	2.41	0.58
1:A:26:ASN:ND2	1:A:28:PRO:CG	2.66	0.58
2:B:476:LEU:HD11	2:B:482:PHE:CD1	2.39	0.58
2:B:764:LEU:O	2:B:768:ILE:HG13	2.04	0.58
2:B:577:LYS:O	2:B:578:LEU:HD12	2.04	0.58
2:B:572:LEU:HD23	2:B:647:LEU:HD12	1.86	0.58
2:B:716:ASN:O	2:B:717:ILE:HD13	2.04	0.57
2:B:394:ASP:CG	2:B:451:ARG:HE	2.07	0.57
2:B:411:PRO:O	2:B:414:SER:HB3	2.05	0.57
2:B:578:LEU:O	2:B:579:VAL:HB	2.05	0.57
1:A:71:GLN:CB	1:A:72:PRO:HD3	2.32	0.56
2:B:493:VAL:HA	2:B:546:MET:CE	2.36	0.56
1:A:52:MET:HE1	1:A:91:TRP:HZ3	1.71	0.56
1:A:26:ASN:HD22	1:A:26:ASN:C	2.08	0.56
2:B:570:PHE:O	2:B:572:LEU:N	2.39	0.56
2:B:698:ARG:NH1	2:B:743:LEU:O	2.40	0.55
1:A:48:ASP:O	1:A:50:GLU:N	2.39	0.55
1:A:99:ASN:C	1:A:101:GLU:N	2.59	0.55
2:B:572:LEU:CD2	2:B:647:LEU:HD12	2.36	0.55
2:B:449:GLY:HA3	2:B:491:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:VAL:HA	2:B:546:MET:HE1	1.88	0.55
2:B:415:ILE:HD12	2:B:416:LEU:N	2.21	0.54
1:A:38:CYS:SG	1:A:91:TRP:HH2	2.31	0.54
2:B:579:VAL:HG13	2:B:579:VAL:O	2.07	0.54
2:B:705:MET:O	2:B:708:MET:HB2	2.08	0.54
2:B:751:SER:O	2:B:754:VAL:N	2.40	0.54
2:B:428:GLU:C	2:B:430:PHE:H	2.11	0.54
2:B:692:TYR:CD1	2:B:693:GLU:N	2.76	0.54
2:B:445:ARG:HG3	2:B:445:ARG:HH11	1.72	0.54
1:A:26:ASN:HD22	1:A:28:PRO:HD2	1.72	0.54
1:A:13:LEU:HD12	1:A:13:LEU:C	2.29	0.53
2:B:450:VAL:O	2:B:453:TYR:HB3	2.09	0.53
1:A:99:ASN:C	1:A:101:GLU:H	2.11	0.53
2:B:497:THR:C	2:B:499:SER:H	2.12	0.52
2:B:400:LEU:HD23	2:B:458:GLU:HA	1.92	0.52
1:A:33:ALA:O	1:A:36:LYS:N	2.41	0.52
1:A:54:LYS:CA	1:A:57:THR:HG22	2.37	0.52
1:A:80:ALA:O	1:A:81:THR:OG1	2.26	0.52
1:A:13:LEU:HD22	1:A:58:LEU:CB	2.39	0.52
1:A:49:GLU:O	1:A:53:LYS:HE3	2.10	0.52
2:B:714:VAL:HG11	2:B:768:ILE:HG22	1.91	0.52
1:A:38:CYS:HG	1:A:91:TRP:HH2	1.58	0.52
1:A:71:GLN:HB3	1:A:72:PRO:CD	2.31	0.52
2:B:490:ALA:O	2:B:493:VAL:N	2.43	0.51
2:B:668:ARG:HD2	2:B:669:LEU:CD1	2.41	0.51
1:A:26:ASN:O	1:A:30:MET:HG3	2.10	0.51
1:A:57:THR:HG23	1:A:58:LEU:N	2.26	0.51
2:B:455:ARG:NH1	2:B:539:GLU:OE2	2.43	0.51
2:B:649:LEU:O	2:B:652:LYS:HB3	2.11	0.51
1:A:53:LYS:HD2	1:A:87:GLY:O	2.10	0.51
1:A:9:GLU:HA	1:A:12:GLN:HB3	1.92	0.50
1:A:34:TYR:CE2	1:A:56:ASN:HA	2.47	0.50
1:A:48:ASP:O	1:A:52:MET:N	2.45	0.50
2:B:518:LEU:HD21	2:B:528:PHE:HB2	1.93	0.50
2:B:693:GLU:OE1	2:B:696:ARG:HD2	2.12	0.50
1:A:37:LYS:HG2	1:A:55:MET:CE	2.41	0.50
2:B:669:LEU:CD2	2:B:723:ILE:HG22	2.42	0.50
2:B:582:GLY:O	2:B:583:SER:HB3	2.12	0.50
2:B:673:HIS:HB2	2:B:675:GLU:OE2	2.11	0.50
2:B:381:THR:HG23	2:B:384:GLN:N	2.18	0.49
2:B:491:LEU:O	2:B:495:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ILE:CD1	2:B:521:LEU:HD23	2.43	0.49
2:B:454:TYR:O	2:B:455:ARG:C	2.51	0.49
2:B:496:ALA:C	2:B:499:SER:HB3	2.33	0.49
2:B:465:GLU:O	2:B:469:SER:HA	2.13	0.49
1:A:24:TRP:O	1:A:30:MET:SD	2.70	0.49
1:A:52:MET:HA	1:A:55:MET:HB3	1.95	0.49
1:A:67:LYS:HE3	1:A:68:TYR:CE1	2.48	0.49
1:A:101:GLU:C	1:A:103:LEU:H	2.15	0.49
1:A:103:LEU:CD2	2:B:714:VAL:HG13	2.43	0.48
2:B:501:SER:O	2:B:502:THR:HB	2.12	0.48
2:B:513:SER:O	2:B:515:PRO:HD2	2.12	0.48
2:B:472:ASN:O	2:B:473:PHE:HB2	2.12	0.48
1:A:88:THR:O	1:A:89:ASP:C	2.51	0.48
2:B:752:ILE:HG23	2:B:753:ILE:N	2.28	0.48
2:B:725:VAL:HG13	2:B:739:PHE:CZ	2.48	0.48
2:B:756:TYR:CE1	2:B:761:MET:HB2	2.49	0.48
1:A:48:ASP:C	1:A:50:GLU:N	2.66	0.48
2:B:547:ILE:O	2:B:551:GLU:HG3	2.13	0.48
2:B:514:PHE:HB3	2:B:515:PRO:CD	2.42	0.47
2:B:526:PHE:O	2:B:529:TYR:HB3	2.13	0.47
2:B:536:ILE:HD13	2:B:547:ILE:HG23	1.96	0.47
2:B:663:ASN:O	2:B:664:THR:C	2.53	0.47
1:A:77:PHE:CE2	1:A:79:ASP:HB2	2.49	0.47
1:A:99:ASN:O	1:A:101:GLU:N	2.47	0.47
2:B:669:LEU:HD11	2:B:727:ALA:HB2	1.96	0.47
1:A:16:LEU:HD11	1:A:55:MET:HA	1.97	0.47
2:B:553:CYS:O	2:B:557:ILE:HG13	2.15	0.47
2:B:468:LEU:HD23	2:B:468:LEU:O	2.15	0.47
2:B:491:LEU:O	2:B:495:MET:CB	2.64	0.46
2:B:521:LEU:O	2:B:522:ASN:HB3	2.15	0.46
2:B:385:LEU:CD2	2:B:389:LEU:HG	2.45	0.46
2:B:434:VAL:O	2:B:435:GLY:C	2.54	0.46
2:B:669:LEU:HD21	2:B:723:ILE:HG22	1.96	0.46
1:A:42:HIS:C	1:A:44:ASP:H	2.18	0.46
2:B:512:LEU:N	2:B:512:LEU:CD1	2.79	0.46
2:B:760:PHE:CD2	2:B:764:LEU:HD11	2.50	0.46
1:A:13:LEU:HD21	1:A:59:TYR:HA	1.98	0.46
2:B:688:LEU:O	2:B:692:TYR:HB3	2.15	0.46
2:B:690:ASN:N	2:B:690:ASN:ND2	2.62	0.46
2:B:528:PHE:O	2:B:531:VAL:HG12	2.16	0.46
2:B:431:ALA:C	2:B:433:ALA:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:669:LEU:HD12	2:B:669:LEU:N	2.31	0.46
2:B:709:TYR:HD2	2:B:756:TYR:CE2	2.34	0.46
2:B:728:TYR:CE2	2:B:734:ALA:HB1	2.51	0.46
2:B:570:PHE:C	2:B:572:LEU:N	2.69	0.45
1:A:7:ARG:O	1:A:10:SER:HB3	2.16	0.45
2:B:689:GLN:C	2:B:690:ASN:HD22	2.19	0.45
1:A:112:SER:O	1:A:113:ASP:O	2.34	0.45
2:B:456:VAL:O	2:B:457:MET:C	2.54	0.45
2:B:732:PRO:O	2:B:733:HIS:HB3	2.16	0.45
2:B:415:ILE:HD12	2:B:415:ILE:C	2.36	0.45
1:A:103:LEU:HD21	2:B:714:VAL:CG1	2.46	0.45
2:B:699:HIS:O	2:B:700:LEU:C	2.55	0.45
2:B:444:GLN:HE21	2:B:444:GLN:HB2	1.64	0.45
2:B:456:VAL:O	2:B:459:SER:N	2.49	0.45
1:A:20:GLU:O	1:A:22:SER:N	2.49	0.45
2:B:384:GLN:O	2:B:388:ILE:HG23	2.16	0.45
2:B:476:LEU:HD11	2:B:482:PHE:CE1	2.52	0.45
2:B:662:LEU:O	2:B:662:LEU:HD23	2.17	0.45
1:A:52:MET:HE1	1:A:91:TRP:CZ3	2.51	0.45
2:B:699:HIS:O	2:B:702:GLN:HB2	2.18	0.44
1:A:81:THR:O	1:A:82:GLU:HB3	2.17	0.44
1:A:57:THR:HG23	1:A:58:LEU:H	1.80	0.44
1:A:27:ILE:N	1:A:28:PRO:HD2	2.33	0.43
2:B:449:GLY:CA	2:B:494:VAL:HG21	2.32	0.43
2:B:669:LEU:CD1	2:B:669:LEU:N	2.81	0.43
2:B:552:ARG:NH2	2:B:555:HIS:ND1	2.65	0.43
1:A:70:HIS:O	1:A:71:GLN:C	2.56	0.43
1:A:77:PHE:HE2	1:A:79:ASP:HB2	1.82	0.43
2:B:662:LEU:CD2	2:B:666:CYS:SG	3.06	0.43
1:A:16:LEU:HD13	1:A:55:MET:HB2	2.00	0.43
2:B:428:GLU:C	2:B:430:PHE:N	2.71	0.43
2:B:493:VAL:CG2	2:B:546:MET:HE2	2.31	0.43
2:B:680:ILE:HD13	2:B:708:MET:HA	2.00	0.43
2:B:710:GLY:O	2:B:714:VAL:HG22	2.18	0.43
1:A:52:MET:CE	1:A:91:TRP:HZ3	2.32	0.43
1:A:101:GLU:C	1:A:103:LEU:N	2.71	0.43
2:B:408:THR:H	2:B:474:SER:HB2	1.84	0.43
2:B:746:GLU:C	2:B:748:GLU:H	2.21	0.43
1:A:67:LYS:HB2	1:A:78:TRP:CD1	2.54	0.42
2:B:751:SER:O	2:B:752:ILE:C	2.57	0.42
2:B:400:LEU:HB2	2:B:458:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:TRP:O	2:B:684:PHE:HB3	2.19	0.42
2:B:446:TYR:O	2:B:447:LYS:C	2.58	0.42
2:B:654:VAL:O	2:B:657:LEU:N	2.52	0.42
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.92	0.42
2:B:422:ILE:HG21	2:B:521:LEU:HD11	2.01	0.42
2:B:496:ALA:CA	2:B:499:SER:HB3	2.45	0.42
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.80	0.42
2:B:752:ILE:CG2	2:B:753:ILE:N	2.82	0.42
2:B:657:LEU:O	2:B:658:ALA:C	2.58	0.42
1:A:33:ALA:O	1:A:34:TYR:C	2.58	0.42
2:B:381:THR:C	2:B:383:GLN:N	2.73	0.41
2:B:397:SER:HB3	2:B:458:GLU:OE1	2.19	0.41
1:A:64:ASP:C	1:A:66:VAL:H	2.23	0.41
1:A:84:PRO:O	1:A:85:THR:C	2.59	0.41
2:B:445:ARG:HG3	2:B:445:ARG:NH1	2.35	0.41
2:B:517:ILE:HD11	2:B:521:LEU:HD23	2.02	0.41
1:A:88:THR:HG23	1:A:89:ASP:N	2.34	0.41
2:B:400:LEU:HD21	2:B:457:MET:HG2	2.02	0.41
1:A:24:TRP:CH2	1:A:62:MET:HE2	2.56	0.41
2:B:699:HIS:CE1	2:B:701:ASP:CG	2.94	0.41
2:B:668:ARG:HH22	2:B:730:ASP:CB	2.32	0.41
1:A:6:MET:SD	1:A:62:MET:HE3	2.60	0.41
2:B:516:TRP:O	2:B:518:LEU:N	2.53	0.41
2:B:569:LEU:O	2:B:573:ILE:HG13	2.21	0.41
1:A:48:ASP:O	1:A:49:GLU:C	2.59	0.41
1:A:81:THR:CG2	1:A:82:GLU:N	2.81	0.41
2:B:514:PHE:O	2:B:517:ILE:HG22	2.20	0.41
2:B:650:PHE:O	2:B:654:VAL:HG23	2.21	0.41
2:B:670:LEU:HD23	2:B:670:LEU:HA	1.92	0.41
2:B:725:VAL:HG13	2:B:739:PHE:CE2	2.55	0.41
2:B:570:PHE:O	2:B:573:ILE:N	2.54	0.40
1:A:6:MET:HE1	1:A:61:LYS:HE2	2.02	0.40
2:B:561:LEU:O	2:B:562:ALA:C	2.58	0.40
1:A:100:GLU:HG3	2:B:761:MET:HE1	2.04	0.40
1:A:41:PHE:CD1	1:A:41:PHE:C	2.95	0.40
2:B:692:TYR:HD1	2:B:693:GLU:N	2.19	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	112/114 (98%)	75 (67%)	23 (20%)	14 (12%)	0 1
2	B	322/333 (97%)	232 (72%)	72 (22%)	18 (6%)	2 14
All	All	434/447 (97%)	307 (71%)	95 (22%)	32 (7%)	1 7

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	THR
1	A	111	SER
1	A	113	ASP
1	A	115	GLU
2	B	466	GLU
2	B	470	ILE
2	B	514	PHE
2	B	516	TRP
2	B	579	VAL
2	B	718	ASP
1	A	22	SER
1	A	49	GLU
1	A	82	GLU
2	B	412	LYS
2	B	435	GLY
2	B	517	ILE
2	B	571	ASP
2	B	733	HIS
1	A	21	ARG
1	A	78	TRP
2	B	515	PRO
2	B	732	PRO
2	B	760	PHE
1	A	10	SER
1	A	15	ASP

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Mol	Chain	Res	Type
1	A	23	ALA
1	A	24	TRP
1	A	66	VAL
2	B	432	LYS
2	B	457	MET
2	B	583	SER
2	B	752	ILE

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	100/100 (100%)	87 (87%)	13 (13%)	4	19
2	B	303/309 (98%)	272 (90%)	31 (10%)	7	29
All	All	403/409 (98%)	359 (89%)	44 (11%)	6	26

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	ARG
1	A	11	LEU
1	A	13	LEU
1	A	21	ARG
1	A	26	ASN
1	A	49	GLU
1	A	53	LYS
1	A	71	GLN
1	A	89	ASP
1	A	95	TRP
1	A	106	SER
1	A	113	ASP
2	B	381	THR
2	B	382	ILE
2	B	385	LEU

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Mol	Chain	Res	Type
2	B	387	MET
2	B	416	LEU
2	B	428	GLU
2	B	444	GLN
2	B	467	ARG
2	B	468	LEU
2	B	470	ILE
2	B	471	GLN
2	B	480	ASN
2	B	487	LEU
2	B	502	THR
2	B	512	LEU
2	B	523	LEU
2	B	529	TYR
2	B	545	GLU
2	B	566	ASP
2	B	569	LEU
2	B	662	LEU
2	B	673	HIS
2	B	677	GLU
2	B	683	LEU
2	B	684	PHE
2	B	690	ASN
2	B	714	VAL
2	B	720	LYS
2	B	721	PHE
2	B	725	VAL
2	B	764	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	26	ASN
1	A	93	GLN
1	A	99	ASN
2	B	380	ASN
2	B	383	GLN
2	B	390	ASN
2	B	405	ASN
2	B	444	GLN
2	B	471	GLN

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Mol	Chain	Res	Type
2	B	480	ASN
2	B	690	ASN
2	B	736	GLN
2	B	762	GLN
2	B	770	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.