



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:45 AM UTC

PDB ID : 1PI6 / pdb_00001pi6
Title : YEAST ACTIN INTERACTING PROTEIN 1 (Aip1), ORTHORHOMBIC CRYSTAL FORM
Authors : Voegtli, W.C.; Madrona, A.Y.; Wilson, D.K.
Deposited on : 2003-05-29
Resolution : 2.50 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

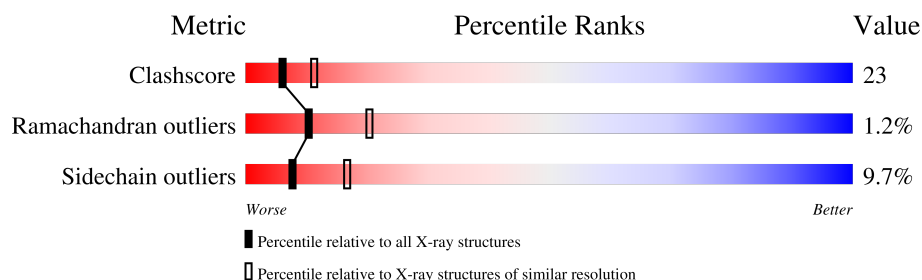
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	615	 60% 32% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4808 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 interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4675	2944	794	923	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	ARG	HIS	engineered mutation	UNP P46680

- 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		

- Molecule 3 is water.

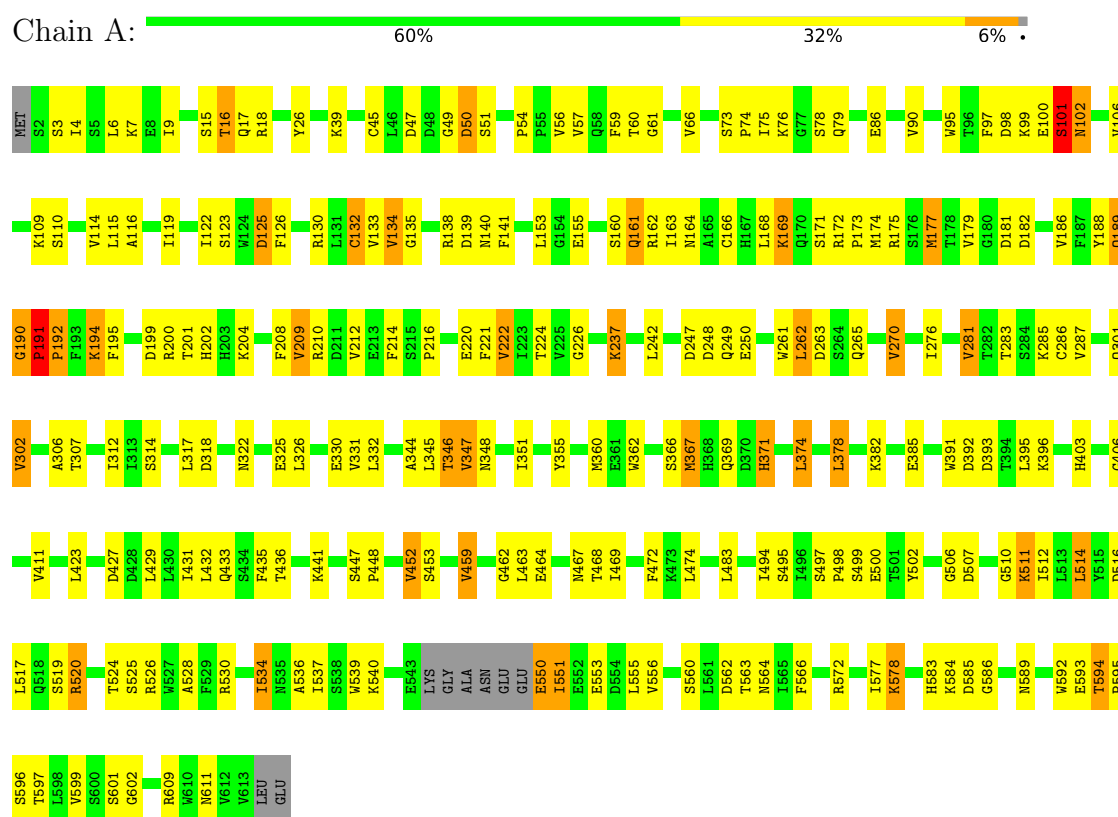
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		

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: Actin interacting protein 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.12Å 154.43Å 62.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.82 – 2.50	Depositor
% Data completeness (in resolution range)	91.4 (24.82-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.64	4/4774 (0.1%)	1.47	36/6475 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	SER	C-N	-24.68	1.03	1.33
1	A	190	GLY	N-CA	20.26	1.72	1.44
1	A	191	PRO	N-CD	17.99	1.73	1.47
1	A	191	PRO	N-CA	-5.12	1.38	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	PRO	CA-C-N	47.88	179.68	119.84
1	A	191	PRO	C-N-CA	47.88	179.68	119.84
1	A	189	GLN	CA-C-N	-27.79	78.24	121.87
1	A	189	GLN	C-N-CA	-27.79	78.24	121.87
1	A	190	GLY	CA-C-N	21.43	178.44	127.00
1	A	190	GLY	C-N-CA	21.43	178.44	127.00
1	A	190	GLY	C-N-CD	-18.30	80.33	120.60
1	A	191	PRO	C-N-CD	-11.86	76.37	125.00
1	A	3	SER	CA-C-N	9.32	136.96	122.70
1	A	3	SER	C-N-CA	9.32	136.96	122.70
1	A	586	GLY	N-CA-C	8.14	122.39	111.72
1	A	435	PHE	N-CA-C	7.68	122.37	112.92
1	A	191	PRO	CA-N-CD	-7.49	101.02	111.50
1	A	525	SER	N-CA-C	-7.37	102.83	112.41
1	A	125	ASP	N-CA-C	-6.94	100.53	110.59
1	A	169	LYS	N-CA-C	-6.81	100.23	110.24
1	A	209	VAL	N-CA-C	-6.80	97.83	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	THR	N-CA-C	-6.72	106.02	114.56
1	A	210	ARG	N-CA-C	6.68	121.59	113.38
1	A	516	ASP	N-CA-C	-6.59	97.99	108.73
1	A	191	PRO	N-CA-CB	6.58	109.83	102.60
1	A	564	ASN	N-CA-C	6.23	120.08	110.42
1	A	192	PRO	CA-N-CD	-6.10	103.46	112.00
1	A	101	SER	N-CA-C	-6.08	105.12	112.54
1	A	572	ARG	CA-C-N	6.01	127.35	119.84
1	A	572	ARG	C-N-CA	6.01	127.35	119.84
1	A	132	CYS	N-CA-C	-5.97	98.80	108.52
1	A	406	GLY	N-CA-C	-5.72	107.57	114.66
1	A	392	ASP	N-CA-C	-5.71	106.53	112.93
1	A	160	SER	N-CA-C	-5.71	106.66	113.97
1	A	116	ALA	N-CA-C	-5.37	105.51	111.36
1	A	528	ALA	N-CA-C	5.19	117.86	110.24
1	A	369	GLN	N-CA-C	-5.16	104.25	110.44
1	A	371	HIS	N-CA-C	-5.14	103.61	110.55
1	A	102	ASN	N-CA-C	-5.14	104.33	111.52
1	A	73	SER	N-CA-C	-5.02	102.91	110.24

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	4675	0	4572	209	1
2	A	1	0	0	0	1
3	A	132	0	0	3	0
All	All	4808	0	4572	209	1

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 23.

All (209) 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:190:GLY:CA	1:A:190:GLY:N	1.72	1.50
1:A:189:GLN:C	1:A:190:GLY:CA	1.95	1.39
1:A:191:PRO:N	1:A:191:PRO:CD	1.73	1.34
1:A:190:GLY:C	1:A:191:PRO:CD	2.00	1.34
1:A:301:GLN:NE2	1:A:314:SER:OG	1.66	1.28
1:A:190:GLY:O	1:A:191:PRO:CD	1.86	1.24
1:A:189:GLN:O	1:A:190:GLY:CA	1.83	1.22
1:A:174:MET:HB2	1:A:191:PRO:HD3	1.35	1.08
1:A:189:GLN:O	1:A:190:GLY:HA3	1.55	1.03
1:A:179:VAL:HG21	1:A:209:VAL:CG1	1.93	0.98
1:A:301:GLN:HE21	1:A:314:SER:HG	0.99	0.95
1:A:179:VAL:HG22	1:A:209:VAL:HB	1.51	0.93
1:A:190:GLY:O	1:A:191:PRO:HD2	1.71	0.91
1:A:45:CYS:SG	1:A:47:ASP:HB2	2.12	0.90
1:A:179:VAL:CG2	1:A:209:VAL:CG1	2.50	0.89
1:A:594:THR:HG22	1:A:596:SER:H	1.38	0.89
1:A:519:SER:O	1:A:520:ARG:HG2	1.73	0.89
1:A:16:THR:CG2	1:A:317:LEU:HD12	2.04	0.87
1:A:594:THR:HB	1:A:597:THR:OG1	1.75	0.86
1:A:190:GLY:O	1:A:191:PRO:HD3	1.77	0.84
1:A:179:VAL:HG21	1:A:209:VAL:HG11	1.58	0.84
1:A:220:GLU:HG3	1:A:221:PHE:CD2	2.13	0.83
1:A:262:LEU:HD11	1:A:312:ILE:HD11	1.62	0.81
1:A:16:THR:HG21	1:A:317:LEU:O	1.82	0.80
1:A:270:VAL:HG13	1:A:301:GLN:CB	2.12	0.80
1:A:16:THR:HG21	1:A:317:LEU:HD12	1.63	0.79
1:A:220:GLU:HG3	1:A:221:PHE:CE2	2.20	0.77
1:A:179:VAL:CG2	1:A:209:VAL:HG11	2.13	0.77
1:A:179:VAL:HG21	1:A:209:VAL:HG12	1.67	0.76
1:A:189:GLN:O	1:A:190:GLY:HA2	1.86	0.75
1:A:114:VAL:HG21	1:A:133:VAL:HG11	1.70	0.74
1:A:220:GLU:CG	1:A:221:PHE:CE2	2.70	0.74
1:A:199:ASP:OD2	1:A:202:HIS:HD2	1.70	0.74
1:A:519:SER:C	1:A:520:ARG:HG2	2.14	0.72
1:A:4:ILE:HG13	1:A:577:ILE:HG22	1.73	0.71
1:A:270:VAL:HG13	1:A:301:GLN:HB3	1.73	0.71
1:A:60:THR:HB	1:A:584:LYS:HD2	1.73	0.70
1:A:220:GLU:CD	1:A:221:PHE:CE2	2.70	0.70
1:A:6:LEU:HD21	1:A:9:ILE:HD11	1.73	0.69
1:A:510:GLY:HA2	1:A:534:ILE:CD1	2.23	0.69
1:A:423:LEU:CD1	1:A:452:VAL:HG22	2.24	0.68
1:A:186:VAL:HG12	1:A:188:TYR:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ARG:NH2	1:A:566:PHE:HB2	2.08	0.67
1:A:270:VAL:CG1	1:A:301:GLN:HB3	2.24	0.67
1:A:530:ARG:HD3	1:A:566:PHE:CE2	2.29	0.67
1:A:179:VAL:CG2	1:A:209:VAL:HB	2.24	0.66
1:A:79:GLN:HG2	1:A:95:TRP:CZ2	2.30	0.66
1:A:237:LYS:HB3	1:A:237:LYS:NZ	2.11	0.66
1:A:510:GLY:HA2	1:A:534:ILE:HD11	1.77	0.66
1:A:190:GLY:C	1:A:191:PRO:HD3	2.17	0.65
1:A:371:HIS:CE1	1:A:396:LYS:HD2	2.32	0.65
1:A:270:VAL:HG13	1:A:301:GLN:HB2	1.79	0.65
1:A:220:GLU:CG	1:A:221:PHE:CD2	2.80	0.64
1:A:530:ARG:HH21	1:A:566:PHE:HB2	1.63	0.64
1:A:179:VAL:HG22	1:A:209:VAL:CB	2.26	0.64
1:A:190:GLY:N	1:A:190:GLY:C	2.55	0.64
1:A:59:PHE:HD1	1:A:106:VAL:HG11	1.61	0.63
1:A:551:ILE:HG22	1:A:551:ILE:O	1.98	0.62
1:A:162:ARG:HD3	1:A:164:ASN:OD1	1.98	0.62
1:A:498:PRO:HG2	1:A:553:GLU:OE1	1.99	0.62
1:A:59:PHE:CD1	1:A:106:VAL:HG11	2.34	0.62
1:A:90:VAL:HG22	1:A:119:ILE:HD13	1.82	0.62
1:A:179:VAL:CG2	1:A:209:VAL:CB	2.79	0.61
1:A:382:LYS:HE2	1:A:385:GLU:OE2	1.99	0.61
1:A:463:LEU:O	1:A:467:ASN:HA	2.01	0.61
1:A:4:ILE:HG13	1:A:577:ILE:CG2	2.30	0.61
1:A:155:GLU:OE2	1:A:194:LYS:HE2	2.00	0.60
1:A:177:MET:HG3	1:A:222:VAL:HG11	1.81	0.60
1:A:59:PHE:CZ	1:A:61:GLY:HA3	2.37	0.60
1:A:483:LEU:HA	1:A:520:ARG:HB2	1.83	0.60
1:A:161:GLN:HB3	1:A:181:ASP:HB2	1.84	0.59
1:A:594:THR:HG23	1:A:595:PRO:HD2	1.83	0.59
1:A:174:MET:HB2	1:A:191:PRO:CD	2.22	0.59
1:A:355:TYR:HA	1:A:374:LEU:HA	1.85	0.59
1:A:347:VAL:HG11	1:A:593:GLU:HA	1.84	0.59
1:A:502:TYR:HB3	1:A:514:LEU:HD21	1.85	0.58
1:A:562:ASP:O	1:A:563:THR:OG1	2.13	0.57
1:A:141:PHE:HB3	1:A:163:ILE:HG13	1.86	0.57
1:A:265:GLN:O	1:A:281:VAL:HG22	2.05	0.57
1:A:270:VAL:CG2	1:A:276:ILE:HG13	2.35	0.57
1:A:155:GLU:HB2	1:A:194:LYS:NZ	2.19	0.57
1:A:49:GLY:O	1:A:50:ASP:C	2.48	0.56
1:A:130:ARG:HG2	1:A:153:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HD2	1:A:611:ASN:OD1	2.05	0.56
1:A:360:MET:HE1	1:A:367:MET:HB3	1.88	0.56
1:A:530:ARG:HD3	1:A:566:PHE:CD2	2.41	0.55
1:A:276:ILE:HD12	1:A:276:ILE:N	2.21	0.55
1:A:367:MET:O	1:A:367:MET:HG3	2.05	0.55
1:A:347:VAL:HG13	1:A:348:ASN:ND2	2.21	0.55
1:A:332:LEU:HD21	3:A:667:HOH:O	2.06	0.55
1:A:283:THR:HB	1:A:285:LYS:HE2	1.88	0.54
1:A:54:PRO:HB3	1:A:97:PHE:CD1	2.42	0.54
1:A:459:VAL:HB	1:A:472:PHE:HB2	1.88	0.54
1:A:301:GLN:NE2	1:A:314:SER:HG	1.79	0.54
1:A:360:MET:HG2	1:A:362:TRP:CZ2	2.43	0.54
1:A:530:ARG:NE	1:A:566:PHE:CD2	2.75	0.54
1:A:550:GLU:C	1:A:551:ILE:HD12	2.33	0.54
1:A:395:LEU:C	1:A:395:LEU:HD23	2.33	0.54
1:A:175:ARG:CZ	1:A:189:GLN:HG2	2.39	0.53
1:A:534:ILE:CD1	1:A:534:ILE:N	2.72	0.53
1:A:530:ARG:NH1	1:A:560:SER:OG	2.41	0.53
1:A:75:ILE:HB	1:A:78:SER:HB3	1.91	0.53
1:A:49:GLY:O	1:A:50:ASP:O	2.27	0.53
1:A:169:LYS:NZ	1:A:171:SER:OG	2.37	0.53
1:A:469:ILE:HD12	1:A:494:ILE:HD11	1.92	0.52
1:A:90:VAL:CG2	1:A:119:ILE:HD13	2.39	0.52
1:A:90:VAL:CG2	1:A:119:ILE:CD1	2.88	0.52
1:A:262:LEU:N	1:A:262:LEU:HD23	2.25	0.52
1:A:395:LEU:HB3	1:A:403:HIS:HB3	1.91	0.51
1:A:411:VAL:HG23	1:A:452:VAL:HG23	1.92	0.51
1:A:66:VAL:HB	1:A:86:GLU:CD	2.35	0.51
1:A:134:VAL:HG22	1:A:163:ILE:HD12	1.92	0.51
1:A:212:VAL:HG23	1:A:224:THR:HG22	1.93	0.51
1:A:540:LYS:HB2	1:A:592:TRP:CZ2	2.45	0.51
1:A:95:TRP:HZ3	1:A:97:PHE:HB2	1.75	0.51
1:A:261:TRP:HH2	1:A:281:VAL:HG11	1.76	0.50
1:A:302:VAL:HG13	1:A:302:VAL:O	2.11	0.50
1:A:506:GLY:HA2	1:A:511:LYS:O	2.11	0.50
1:A:189:GLN:C	1:A:190:GLY:HA2	2.19	0.49
1:A:74:PRO:HG2	1:A:125:ASP:O	2.13	0.49
1:A:79:GLN:HA	3:A:683:HOH:O	2.12	0.49
1:A:262:LEU:HD22	1:A:306:ALA:CB	2.42	0.48
1:A:214:PHE:CD2	1:A:222:VAL:HG22	2.48	0.48
1:A:495:SER:HG	1:A:539:TRP:CD1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TRP:CE3	1:A:556:VAL:HG22	2.48	0.48
1:A:214:PHE:CE2	1:A:222:VAL:HG22	2.48	0.48
1:A:469:ILE:HB	1:A:483:LEU:HD12	1.95	0.48
1:A:248:ASP:HB2	1:A:249:GLN:HE21	1.79	0.48
1:A:594:THR:HG22	1:A:596:SER:N	2.19	0.48
1:A:195:PHE:C	1:A:195:PHE:CD2	2.91	0.48
1:A:423:LEU:HD12	1:A:452:VAL:HG22	1.96	0.48
1:A:347:VAL:HG21	1:A:593:GLU:HB3	1.96	0.47
1:A:262:LEU:HD22	1:A:306:ALA:HB2	1.95	0.47
1:A:98:ASP:O	1:A:102:ASN:N	2.42	0.47
1:A:502:TYR:HB3	1:A:514:LEU:CD2	2.45	0.47
1:A:39:LYS:HB2	1:A:584:LYS:HE3	1.94	0.47
1:A:237:LYS:HB3	1:A:237:LYS:HZ2	1.79	0.47
1:A:283:THR:HB	1:A:285:LYS:CE	2.45	0.47
1:A:346:THR:HG22	1:A:351:ILE:H	1.80	0.47
1:A:391:TRP:C	1:A:393:ASP:H	2.23	0.47
1:A:566:PHE:CE1	1:A:578:LYS:HD3	2.50	0.47
1:A:534:ILE:N	1:A:534:ILE:HD12	2.29	0.47
1:A:16:THR:CG2	1:A:17:GLN:N	2.77	0.47
1:A:263:ASP:C	1:A:263:ASP:OD2	2.58	0.46
1:A:126:PHE:CE2	1:A:174:MET:HE2	2.50	0.46
1:A:562:ASP:C	1:A:563:THR:HG23	2.41	0.46
1:A:54:PRO:HB3	1:A:97:PHE:CE1	2.50	0.46
1:A:174:MET:CB	1:A:191:PRO:HD3	2.25	0.46
1:A:6:LEU:HD21	1:A:9:ILE:CD1	2.42	0.46
1:A:90:VAL:HG23	1:A:119:ILE:HD11	1.98	0.46
1:A:325:GLU:HB2	1:A:332:LEU:HD11	1.97	0.46
1:A:589:ASN:HB2	1:A:601:SER:OG	2.16	0.45
1:A:507:ASP:OD2	1:A:511:LYS:HB3	2.16	0.45
1:A:134:VAL:HG13	1:A:135:GLY:N	2.31	0.45
1:A:346:THR:HG22	1:A:351:ILE:N	2.31	0.45
1:A:551:ILE:O	1:A:551:ILE:CG2	2.63	0.45
1:A:599:VAL:HG22	1:A:609:ARG:HG2	1.98	0.45
1:A:79:GLN:HG2	1:A:95:TRP:CE2	2.52	0.45
1:A:462:GLY:HA2	1:A:469:ILE:HD13	1.98	0.45
1:A:208:PHE:O	1:A:226:GLY:HA3	2.17	0.45
1:A:360:MET:HE3	1:A:366:SER:O	2.17	0.45
1:A:536:ALA:C	1:A:537:ILE:HG13	2.43	0.44
1:A:584:LYS:HG2	1:A:585:ASP:OD2	2.17	0.44
1:A:98:ASP:C	1:A:100:GLU:N	2.75	0.44
1:A:427:ASP:OD1	1:A:448:PRO:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ILE:HD12	1:A:551:ILE:N	2.33	0.44
1:A:98:ASP:OD2	1:A:100:GLU:HB3	2.17	0.44
1:A:318:ASP:C	1:A:318:ASP:OD1	2.61	0.44
1:A:262:LEU:CD2	1:A:306:ALA:HB2	2.47	0.44
1:A:432:LEU:N	1:A:432:LEU:HD12	2.33	0.44
1:A:114:VAL:O	1:A:115:LEU:HD23	2.18	0.43
1:A:134:VAL:HG11	1:A:163:ILE:HG22	1.99	0.43
1:A:512:ILE:HD11	1:A:534:ILE:HG13	2.00	0.43
1:A:530:ARG:CD	1:A:566:PHE:CD2	3.01	0.43
1:A:100:GLU:HG3	1:A:101:SER:N	2.34	0.43
1:A:90:VAL:HG23	1:A:119:ILE:CD1	2.48	0.43
1:A:517:LEU:C	1:A:517:LEU:HD23	2.43	0.43
1:A:166:CYS:HA	1:A:177:MET:O	2.19	0.43
1:A:502:TYR:CB	1:A:514:LEU:HD21	2.48	0.43
1:A:344:ALA:CB	1:A:378:LEU:HD22	2.49	0.42
1:A:168:LEU:O	1:A:169:LYS:C	2.61	0.42
1:A:172:ARG:HA	1:A:173:PRO:C	2.45	0.42
1:A:584:LYS:O	1:A:585:ASP:HB2	2.20	0.42
1:A:247:ASP:OD2	1:A:247:ASP:C	2.61	0.42
1:A:98:ASP:O	1:A:100:GLU:N	2.53	0.42
1:A:182:ASP:OD1	1:A:200:ARG:NH1	2.53	0.42
1:A:314:SER:HB3	1:A:322:ASN:HB2	2.01	0.42
1:A:122:ILE:HG22	1:A:123:SER:N	2.34	0.42
1:A:583:HIS:HB3	1:A:602:GLY:HA3	2.01	0.42
1:A:411:VAL:HG23	1:A:452:VAL:CG2	2.49	0.41
1:A:499:SER:O	1:A:500:GLU:HB2	2.20	0.41
1:A:56:VAL:HG12	1:A:57:VAL:N	2.35	0.41
1:A:453:SER:HB2	1:A:494:ILE:O	2.20	0.41
1:A:95:TRP:CZ3	1:A:97:PHE:HB2	2.54	0.41
1:A:39:LYS:CB	1:A:584:LYS:HE3	2.50	0.41
1:A:346:THR:HG22	1:A:351:ILE:HB	2.02	0.41
1:A:423:LEU:HD11	1:A:452:VAL:HG22	1.99	0.41
1:A:441:LYS:HE3	1:A:441:LYS:HB3	1.79	0.41
1:A:331:VAL:HG21	3:A:661:HOH:O	2.21	0.41
1:A:431:ILE:HB	1:A:441:LYS:HG2	2.02	0.41
1:A:347:VAL:CG2	1:A:593:GLU:HB3	2.51	0.41
1:A:60:THR:HB	1:A:584:LYS:CD	2.47	0.41
1:A:186:VAL:CG1	1:A:188:TYR:CE1	3.03	0.41
1:A:134:VAL:HG21	1:A:163:ILE:HG21	2.03	0.40
1:A:250:GLU:HG3	1:A:286:CYS:SG	2.61	0.40
1:A:346:THR:CG2	1:A:351:ILE:HB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:TYR:CD1	1:A:307:THR:HG22	2.57	0.40
1:A:194:LYS:HD2	1:A:194:LYS:HA	1.74	0.40
1:A:562:ASP:O	1:A:563:THR:CB	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:OE2	2:A:650:ZN:ZN[2_745]	1.26	0.94

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	602/615 (98%)	552 (92%)	43 (7%)	7 (1%)	10	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	192	PRO
1	A	551	ILE
1	A	99	LYS
1	A	374	LEU
1	A	524	THR
1	A	216	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	528/535 (99%)	477 (90%)	51 (10%)	8 17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	16	THR
1	A	18	ARG
1	A	51	SER
1	A	76	LYS
1	A	101	SER
1	A	109	LYS
1	A	110	SER
1	A	132	CYS
1	A	134	VAL
1	A	138	ARG
1	A	139	ASP
1	A	140	ASN
1	A	161	GLN
1	A	177	MET
1	A	191	PRO
1	A	194	LYS
1	A	201	THR
1	A	204	LYS
1	A	222	VAL
1	A	237	LYS
1	A	242	LEU
1	A	262	LEU
1	A	270	VAL
1	A	281	VAL
1	A	287	VAL
1	A	302	VAL
1	A	326	LEU
1	A	345	LEU
1	A	346	THR
1	A	347	VAL
1	A	367	MET
1	A	378	LEU
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	433	GLN
1	A	447	SER
1	A	452	VAL
1	A	459	VAL
1	A	464	GLU
1	A	468	THR
1	A	474	LEU
1	A	497	SER
1	A	511	LYS
1	A	514	LEU
1	A	520	ARG
1	A	526	ARG
1	A	534	ILE
1	A	550	GLU
1	A	555	LEU
1	A	578	LYS
1	A	594	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	17	GLN
1	A	19	ASN
1	A	202	HIS
1	A	205	GLN
1	A	249	GLN
1	A	301	GLN
1	A	309	ASN
1	A	348	ASN
1	A	433	GLN
1	A	446	ASN
1	A	457	ASN
1	A	589	ASN

5.3.3 RNA ⓘ

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 1 ligands modelled in this entry, 1 is 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3:SER	C	4:ILE	N	1.03

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.