



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:41 AM UTC

PDB ID : 7CO3 / pdb_00007co3
Title : HtrA-type protease AlgWS227A with tripeptide
Authors : Li, T.; Song, Y.J.; Bao, R.
Deposited on : 2020-08-03
Resolution : 1.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

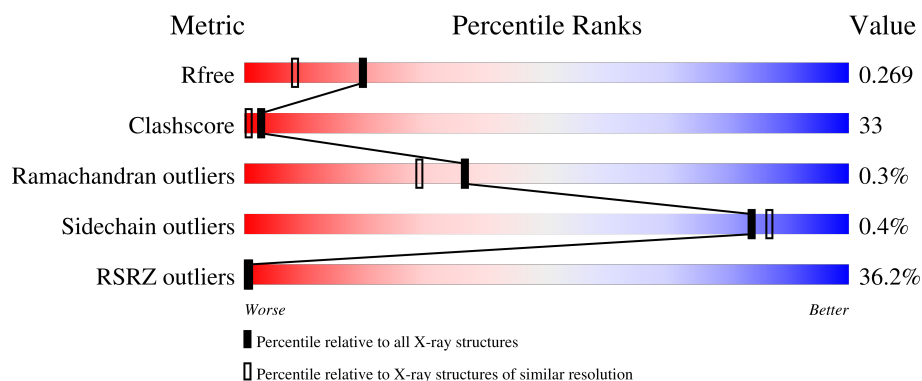
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	C	3	100% 100%
2	A	389	28% 51% 25% • 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2371 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 TRP-VAL-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	3	Total	C	N	O	0	0	0
			32	25	4	3			

- Molecule 2 is a protein called AlgW protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	301	Total	C	N	O	S	0	0	0
			2174	1352	387	428	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	ALA	SER	engineered mutation	UNP Q9H VX1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total	O	0	0
			165	165		

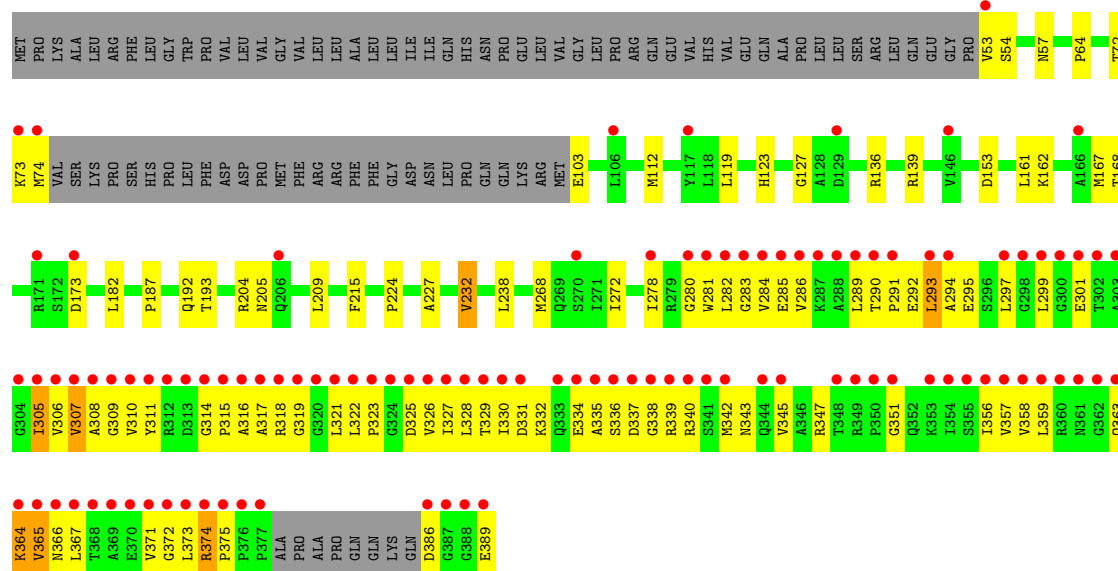
3 Residue-property plots

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 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: TRP-VAL-PHE



• Molecule 2: AlgW protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.61Å 96.61Å 119.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.49 – 1.90 39.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.49-1.90) 99.9 (39.49-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.234 , 0.270 0.234 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2371	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.37	0/34	0.79	0/46
2	A	0.55	2/2197 (0.1%)	0.85	5/2980 (0.2%)
All	All	0.55	2/2231 (0.1%)	0.85	5/3026 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	293	LEU	CG-CD2	-5.91	1.33	1.52
2	A	307	VAL	CB-CG2	-5.37	1.34	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	374	ARG	CG-CD-NE	6.47	126.23	112.00
2	A	293	LEU	CB-CG-CD2	-5.60	93.90	110.70
2	A	305	ILE	CA-CB-CG1	5.20	119.24	110.40
2	A	364	LYS	CA-C-N	5.11	131.18	121.97
2	A	364	LYS	C-N-CA	5.11	131.18	121.97

There are no chirality outliers.

There are no planarity outliers.

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	C	32	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2174	0	2217	147	1
3	A	165	0	0	27	0
All	All	2371	0	2247	148	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 33.

All (148) 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)
2:A:322:LEU:HD23	2:A:325:ASP:OD1	1.38	1.24
2:A:282:LEU:HD12	2:A:284:VAL:HB	1.28	1.12
2:A:310:VAL:HG23	3:A:442:HOH:O	1.63	0.99
2:A:358:VAL:HG12	3:A:499:HOH:O	1.65	0.97
2:A:373:LEU:HD12	3:A:536:HOH:O	1.69	0.91
2:A:282:LEU:HD12	2:A:284:VAL:CB	2.03	0.88
2:A:293:LEU:HD23	2:A:293:LEU:H	1.37	0.88
2:A:289:LEU:HD11	2:A:294:ALA:HB2	1.57	0.87
2:A:366:ASN:OD1	3:A:401:HOH:O	1.94	0.86
2:A:53:VAL:O	3:A:402:HOH:O	1.94	0.85
2:A:322:LEU:CD2	2:A:325:ASP:OD1	2.23	0.85
2:A:305:ILE:HG21	2:A:335:ALA:O	1.76	0.85
2:A:293:LEU:HD23	2:A:293:LEU:N	1.92	0.84
2:A:363:GLN:NE2	3:A:408:HOH:O	2.13	0.82
2:A:326:VAL:HB	2:A:359:LEU:HB2	1.63	0.78
2:A:290:THR:HB	2:A:293:LEU:HD21	1.65	0.78
2:A:357:VAL:HG13	2:A:365:VAL:H	1.52	0.73
2:A:297:LEU:HG	2:A:299:LEU:CD2	2.19	0.73
2:A:307:VAL:HG11	2:A:327:ILE:HD13	1.69	0.72
2:A:334:GLU:O	3:A:406:HOH:O	2.08	0.72
2:A:327:ILE:O	3:A:404:HOH:O	2.06	0.71
2:A:205:ASN:O	3:A:405:HOH:O	2.07	0.71
2:A:307:VAL:HG12	3:A:520:HOH:O	1.90	0.71
2:A:289:LEU:HD13	2:A:306:VAL:HG23	1.74	0.69
2:A:305:ILE:HB	2:A:336:SER:O	1.92	0.69
2:A:325:ASP:OD2	2:A:358:VAL:CG1	2.40	0.68
2:A:282:LEU:CD1	2:A:284:VAL:CG2	2.72	0.67
2:A:57:ASN:OD1	3:A:407:HOH:O	2.12	0.66
2:A:224:PRO:HA	2:A:386:ASP:HB3	1.77	0.65
2:A:290:THR:HG22	2:A:292:GLU:OE1	1.96	0.65
2:A:305:ILE:HD13	2:A:335:ALA:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:VAL:O	2:A:359:LEU:N	2.29	0.64
2:A:285:GLU:OE2	2:A:309:GLY:HA3	1.97	0.64
2:A:366:ASN:ND2	3:A:409:HOH:O	2.18	0.64
2:A:347:ARG:NH1	3:A:415:HOH:O	2.31	0.63
2:A:289:LEU:CD1	2:A:306:VAL:HG23	2.29	0.63
2:A:290:THR:HB	2:A:293:LEU:CD2	2.28	0.62
2:A:307:VAL:CG2	2:A:327:ILE:H	2.12	0.62
2:A:123:HIS:HD2	2:A:153:ASP:OD2	1.83	0.62
2:A:292:GLU:OE1	2:A:292:GLU:N	2.30	0.61
2:A:278:ILE:HG23	3:A:536:HOH:O	2.00	0.61
2:A:343:ASN:O	2:A:347:ARG:HG2	2.01	0.60
2:A:282:LEU:CD1	2:A:284:VAL:HB	2.17	0.60
2:A:297:LEU:HG	2:A:299:LEU:HD22	1.84	0.60
2:A:317:ALA:N	3:A:417:HOH:O	2.35	0.60
2:A:310:VAL:HG21	2:A:322:LEU:N	2.17	0.59
2:A:74:MET:HG2	3:A:422:HOH:O	2.02	0.58
2:A:305:ILE:HD12	2:A:337:ASP:C	2.28	0.58
2:A:321:LEU:HD12	2:A:322:LEU:H	1.68	0.57
2:A:281:TRP:HB3	2:A:372:GLY:O	2.04	0.57
2:A:284:VAL:HG21	2:A:321:LEU:HD23	1.85	0.57
2:A:307:VAL:HB	2:A:326:VAL:HA	1.87	0.57
2:A:167:MET:HG2	2:A:238:LEU:HB2	1.87	0.56
2:A:301:GLU:O	2:A:301:GLU:HG3	2.04	0.56
2:A:307:VAL:HG21	2:A:327:ILE:N	2.21	0.56
2:A:307:VAL:HG21	2:A:327:ILE:HD13	1.87	0.56
2:A:268:MET:O	2:A:272:ILE:HG13	2.04	0.56
2:A:293:LEU:CD1	2:A:306:VAL:HG21	2.35	0.56
2:A:285:GLU:HB2	2:A:309:GLY:O	2.07	0.54
2:A:290:THR:CB	2:A:293:LEU:HD21	2.36	0.54
2:A:286:VAL:HG23	2:A:307:VAL:HA	1.88	0.54
2:A:330:ILE:HB	2:A:356:ILE:CD1	2.37	0.53
2:A:227:ALA:HB2	2:A:386:ASP:HA	1.91	0.53
2:A:314:GLY:O	2:A:317:ALA:HB3	2.09	0.53
2:A:337:ASP:OD1	2:A:338:GLY:N	2.41	0.53
2:A:332:LYS:HD3	3:A:403:HOH:O	2.09	0.53
2:A:295:GLU:OE2	2:A:295:GLU:HA	2.08	0.53
2:A:307:VAL:HG21	2:A:327:ILE:H	1.74	0.53
2:A:358:VAL:HG22	2:A:365:VAL:CG1	2.40	0.52
2:A:209:LEU:HD11	2:A:389:GLU:OE1	2.10	0.52
2:A:328:LEU:HB3	3:A:473:HOH:O	2.09	0.52
2:A:373:LEU:CD1	3:A:536:HOH:O	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:73:LYS:HG2	2:A:74:MET:N	2.25	0.51
2:A:329:THR:HG22	3:A:439:HOH:O	2.10	0.51
1:C:3:PHE:C	2:A:283:GLY:H	2.18	0.51
1:C:2:VAL:O	2:A:374:ARG:NH2	2.43	0.51
2:A:292:GLU:HA	2:A:295:GLU:HB2	1.92	0.51
2:A:328:LEU:HG	3:A:515:HOH:O	2.11	0.51
2:A:73:LYS:HG3	2:A:127:GLY:O	2.11	0.51
2:A:331:ASP:O	3:A:410:HOH:O	2.20	0.50
2:A:316:ALA:HB1	2:A:321:LEU:HB3	1.92	0.50
2:A:307:VAL:H	2:A:326:VAL:HG13	1.76	0.50
2:A:139:ARG:HH21	2:A:161:LEU:HB3	1.75	0.50
1:C:1:TRP:CE3	2:A:338:GLY:HA3	2.47	0.50
2:A:73:LYS:HG2	2:A:74:MET:H	1.75	0.50
2:A:282:LEU:HD12	2:A:284:VAL:CG2	2.37	0.50
2:A:293:LEU:H	2:A:293:LEU:CD2	2.17	0.49
2:A:307:VAL:HG23	2:A:327:ILE:H	1.78	0.48
2:A:358:VAL:HG22	2:A:365:VAL:HB	1.95	0.48
2:A:363:GLN:OE1	2:A:363:GLN:HA	2.14	0.48
2:A:328:LEU:O	2:A:334:GLU:HG2	2.14	0.47
2:A:53:VAL:HG22	2:A:54:SER:H	1.79	0.47
2:A:305:ILE:O	3:A:411:HOH:O	2.20	0.47
2:A:339:ARG:HG2	2:A:340:ARG:N	2.29	0.47
2:A:321:LEU:HD12	2:A:322:LEU:N	2.30	0.46
2:A:325:ASP:OD2	2:A:358:VAL:HG12	2.14	0.46
2:A:325:ASP:OD2	2:A:358:VAL:HB	2.16	0.46
2:A:281:TRP:HB2	2:A:374:ARG:N	2.30	0.46
2:A:325:ASP:HB2	2:A:358:VAL:HB	1.98	0.45
2:A:281:TRP:CD2	2:A:374:ARG:HA	2.51	0.45
2:A:72:THR:HA	2:A:103:GLU:O	2.16	0.45
2:A:167:MET:HG3	2:A:168:THR:O	2.16	0.45
2:A:305:ILE:HG23	3:A:411:HOH:O	2.17	0.45
2:A:139:ARG:NH2	2:A:162:LYS:O	2.49	0.45
2:A:290:THR:C	2:A:293:LEU:HD21	2.42	0.45
2:A:309:GLY:H	2:A:323:PRO:HA	1.82	0.44
2:A:325:ASP:OD2	2:A:358:VAL:HG11	2.17	0.44
2:A:342:MET:HB3	2:A:342:MET:HE2	1.61	0.44
2:A:351:GLY:N	2:A:371:VAL:O	2.32	0.44
2:A:334:GLU:OE1	2:A:336:SER:HB3	2.18	0.44
2:A:293:LEU:HD12	2:A:306:VAL:HG21	1.99	0.44
2:A:182:LEU:HB2	2:A:232:VAL:HG12	2.00	0.44
2:A:112:MET:HE2	2:A:119:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:305:ILE:O	2:A:305:ILE:HG23	2.18	0.43
2:A:167:MET:CG	2:A:238:LEU:HB2	2.47	0.43
2:A:293:LEU:HD11	2:A:306:VAL:HG21	2.00	0.43
2:A:329:THR:O	2:A:356:ILE:HD12	2.18	0.43
2:A:301:GLU:O	2:A:301:GLU:CG	2.67	0.43
2:A:356:ILE:CG2	2:A:367:LEU:HB2	2.49	0.43
2:A:374:ARG:HG3	2:A:375:PRO:HD2	2.00	0.43
2:A:187:PRO:HD2	2:A:193:THR:HB	2.01	0.43
2:A:282:LEU:HD11	2:A:284:VAL:HG21	1.99	0.43
2:A:307:VAL:CG2	2:A:326:VAL:HA	2.48	0.43
2:A:281:TRP:HD1	2:A:372:GLY:HA3	1.83	0.43
2:A:282:LEU:CD1	2:A:284:VAL:CB	2.80	0.43
2:A:315:PRO:O	2:A:319:GLY:N	2.51	0.43
2:A:204:ARG:HB2	2:A:215:PHE:HB2	2.01	0.42
2:A:314:GLY:O	2:A:318:ARG:HG2	2.19	0.42
2:A:310:VAL:HG21	2:A:322:LEU:CA	2.50	0.42
1:C:3:PHE:CE1	2:A:342:MET:HG2	2.54	0.42
2:A:364:LYS:NZ	3:A:401:HOH:O	2.52	0.42
2:A:64:PRO:HG3	2:A:136:ARG:NH2	2.35	0.42
2:A:328:LEU:HD22	2:A:363:GLN:O	2.19	0.42
2:A:192:GLN:HG3	3:A:475:HOH:O	2.20	0.42
2:A:281:TRP:HB3	2:A:372:GLY:C	2.45	0.42
1:C:3:PHE:N	1:C:3:PHE:CD1	2.88	0.41
2:A:268:MET:HE2	2:A:268:MET:HB3	1.88	0.41
2:A:291:PRO:O	2:A:295:GLU:N	2.52	0.41
2:A:310:VAL:HG13	3:A:417:HOH:O	2.19	0.41
2:A:173:ASP:O	2:A:173:ASP:OD2	2.38	0.41
2:A:283:GLY:O	2:A:311:TYR:HB2	2.20	0.41
2:A:307:VAL:HG12	2:A:308:ALA:N	2.35	0.41
2:A:282:LEU:CD1	2:A:284:VAL:HG21	2.50	0.41
2:A:280:GLY:HA3	2:A:345:VAL:O	2.21	0.41
2:A:305:ILE:HB	2:A:336:SER:C	2.45	0.41
2:A:357:VAL:HG11	2:A:364:LYS:HA	2.03	0.41
2:A:227:ALA:HB2	2:A:386:ASP:CA	2.51	0.41
2:A:310:VAL:HB	2:A:323:PRO:HD3	2.03	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)
2:A:322:LEU:CB	2:A:322:LEU:CD1[10_445]	2.03	0.17

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	C	1/3 (33%)	1 (100%)	0	0	100	100
2	A	295/389 (76%)	278 (94%)	16 (5%)	1 (0%)	36	29
All	All	296/392 (76%)	279 (94%)	16 (5%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	365	VAL

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	C	3/3 (100%)	3 (100%)	0	100	100
2	A	227/305 (74%)	226 (100%)	1 (0%)	84	87
All	All	230/308 (75%)	229 (100%)	1 (0%)	84	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	57	ASN
2	A	123	HIS
2	A	269	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](#)

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

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, 95th 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	C	3/3 (100%)	4.67	3 (100%) 0 0	81, 81, 86, 104	0
2	A	301/389 (77%)	1.60	107 (35%) 1 0	15, 46, 130, 159	1 (0%)
All	All	304/392 (77%)	1.63	110 (36%) 1 0	15, 46, 130, 159	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	356	ILE	12.7
2	A	335	ALA	10.8
2	A	330	ILE	8.9
2	A	365	VAL	8.0
2	A	364	LYS	6.6
2	A	286	VAL	6.3
2	A	357	VAL	6.1
2	A	322	LEU	6.1
1	C	1	TRP	5.8
2	A	323	PRO	5.4
2	A	358	VAL	5.4
2	A	311	TYR	5.3
2	A	282	LEU	5.3
2	A	367	LEU	5.3
2	A	351	GLY	5.2
2	A	302	THR	5.2
2	A	386	ASP	5.2
2	A	326	VAL	5.1
2	A	328	LEU	5.1
2	A	359	LEU	5.1
2	A	284	VAL	4.9
2	A	310	VAL	4.9
2	A	319	GLY	4.8
2	A	303	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	A	327	ILE	4.7
2	A	348	THR	4.6
2	A	281	TRP	4.6
2	A	369	ALA	4.5
2	A	306	VAL	4.5
2	A	288	ALA	4.3
2	A	366	ASN	4.3
2	A	368	THR	4.2
2	A	354	ILE	4.2
2	A	373	LEU	4.1
2	A	324	GLY	4.1
1	C	3	PHE	4.1
1	C	2	VAL	4.1
2	A	299	LEU	4.0
2	A	307	VAL	4.0
2	A	316	ALA	4.0
2	A	305	ILE	4.0
2	A	362	GLY	3.9
2	A	371	VAL	3.9
2	A	293	LEU	3.9
2	A	289	LEU	3.8
2	A	308	ALA	3.8
2	A	345	VAL	3.8
2	A	313	ASP	3.7
2	A	321	LEU	3.7
2	A	341	SER	3.7
2	A	329	THR	3.7
2	A	283	GLY	3.6
2	A	320	GLY	3.5
2	A	349	ARG	3.5
2	A	331	ASP	3.5
2	A	337	ASP	3.5
2	A	377	PRO	3.4
2	A	317	ALA	3.4
2	A	376	PRO	3.4
2	A	363	GLN	3.3
2	A	309	GLY	3.3
2	A	297	LEU	3.3
2	A	291	PRO	3.3
2	A	361	ASN	3.2
2	A	334	GLU	3.2
2	A	336	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	338	GLY	3.1
2	A	312	ARG	3.1
2	A	355	SER	3.1
2	A	375	PRO	3.1
2	A	314	GLY	3.1
2	A	360	ARG	3.0
2	A	53	VAL	3.0
2	A	290	THR	3.0
2	A	294	ALA	3.0
2	A	285	GLU	2.9
2	A	106	LEU	2.9
2	A	387	GLY	2.9
2	A	350	PRO	2.9
2	A	270	SER	2.8
2	A	388	GLY	2.8
2	A	389	GLU	2.8
2	A	353	LYS	2.6
2	A	280	GLY	2.5
2	A	146	VAL	2.5
2	A	342	MET	2.5
2	A	171	ARG	2.4
2	A	340	ARG	2.4
2	A	333	GLN	2.4
2	A	339	ARG	2.4
2	A	374	ARG	2.4
2	A	206	GLN	2.4
2	A	304	GLY	2.4
2	A	74	MET	2.4
2	A	173	ASP	2.3
2	A	300	GLY	2.3
2	A	287	LYS	2.3
2	A	301	GLU	2.3
2	A	318	ARG	2.3
2	A	73	LYS	2.3
2	A	315	PRO	2.2
2	A	278	ILE	2.2
2	A	344	GLN	2.2
2	A	117	TYR	2.2
2	A	129	ASP	2.2
2	A	166	ALA	2.2
2	A	298	GLY	2.1
2	A	325	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	372	GLY	2.1
2	A	370	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.