



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 4WVM / pdb_00004wvm
Title : Stonustoxin structure
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Deposited on : 2014-11-06
Resolution : 3.10 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

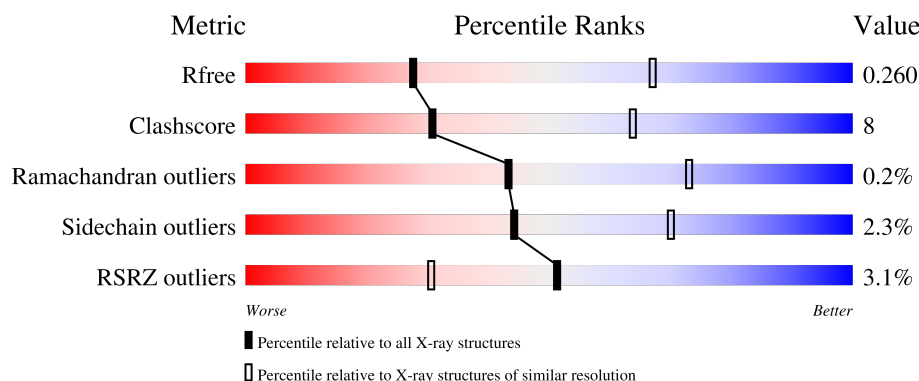
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	703	
2	B	700	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9691 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 Stonustoxin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4799	3074	803	905	17			

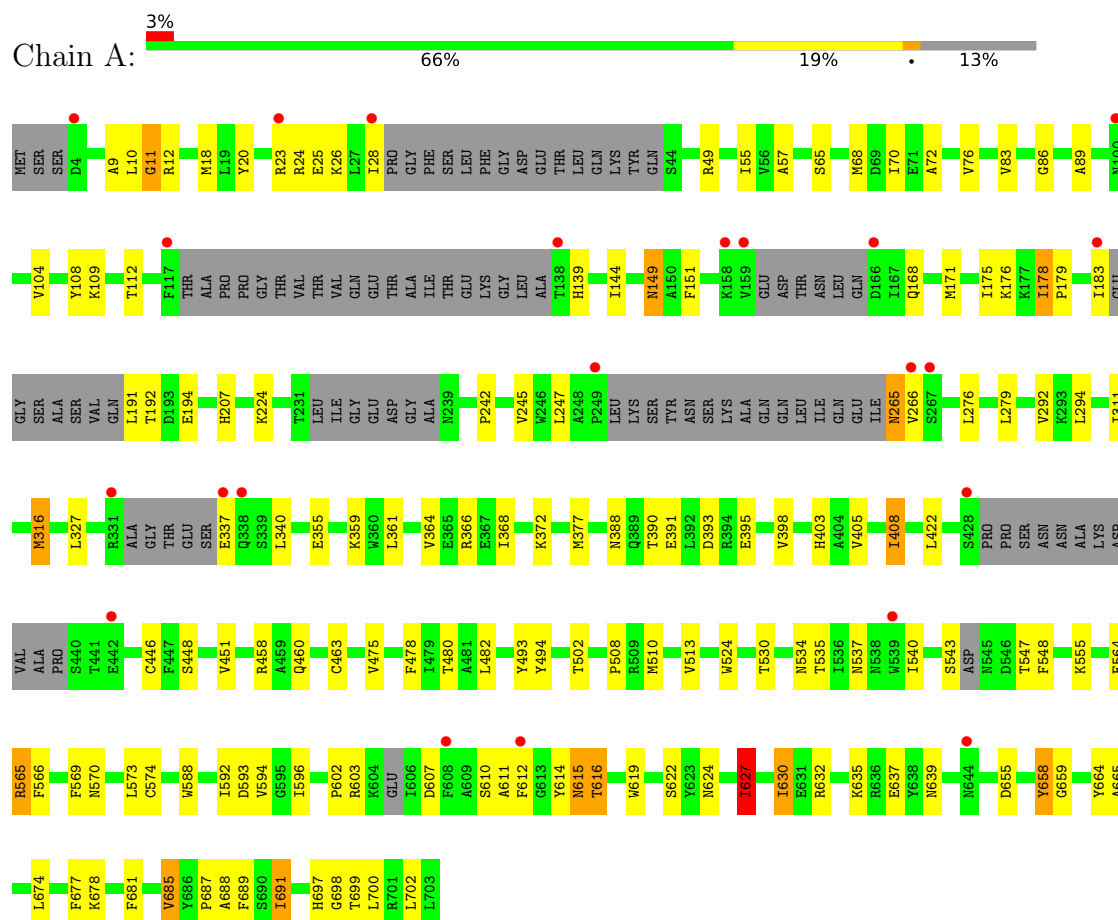
- Molecule 2 is a protein called Stonustoxin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	616	Total	C	N	O	S	0	0	0
			4892	3137	801	929	25			

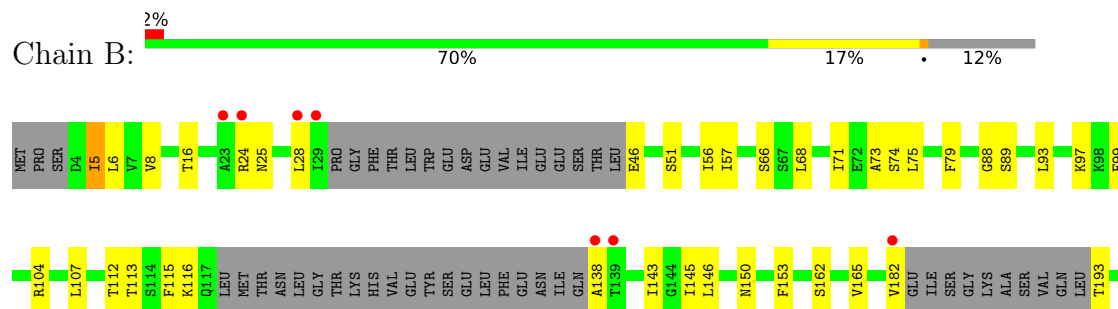
3 Residue-property plots [i](#)

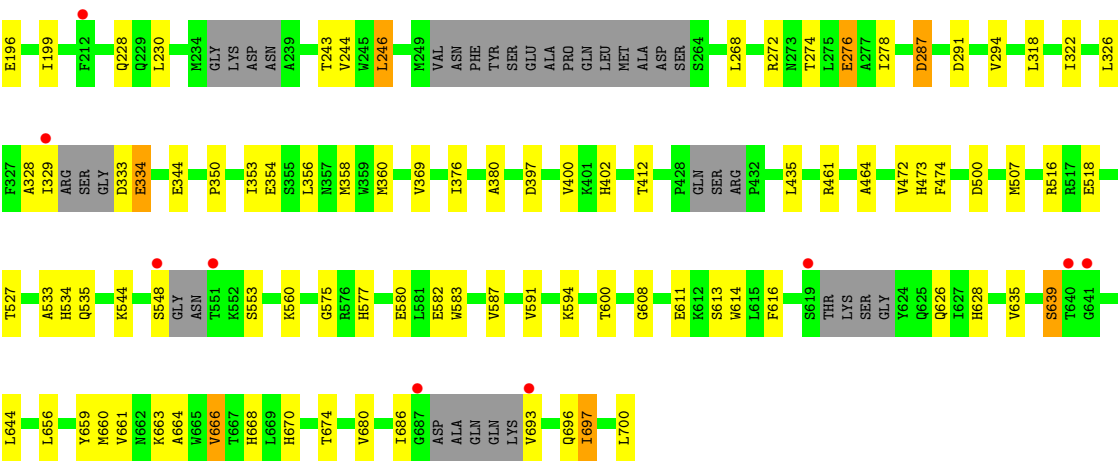
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Stonustoxin subunit alpha



• Molecule 2: Stonustoxin subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	107.91Å 107.91Å 244.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.15 – 3.10 38.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.15-3.10) 99.5 (38.15-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.236 0.231 , 0.260	Depositor DCC
R_{free} test set	2549 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9691	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

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	0.90	4/4896 (0.1%)	1.33	23/6614 (0.3%)
2	B	0.86	1/4996 (0.0%)	1.33	20/6753 (0.3%)
All	All	0.88	5/9892 (0.1%)	1.33	43/13367 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	ILE	CG1-CD1	5.66	1.73	1.51
1	A	316	MET	SD-CE	-5.50	1.65	1.79
2	B	113	THR	CA-C	5.32	1.57	1.52
1	A	691	ILE	CA-C	5.10	1.59	1.53
1	A	178	ILE	CA-CB	5.01	1.56	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	ARG	CA-C-N	11.36	138.78	122.08
2	B	24	ARG	C-N-CA	11.36	138.78	122.08
1	A	615	ASN	CA-CB-CG	7.20	119.80	112.60
1	A	149	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	616	THR	N-CA-C	-6.70	105.11	113.28
1	A	266	VAL	CA-C-N	6.35	128.79	120.28
1	A	266	VAL	C-N-CA	6.35	128.79	120.28
1	A	23	ARG	CA-C-N	6.03	132.51	123.05
1	A	23	ARG	C-N-CA	6.03	132.51	123.05
1	A	191	LEU	CA-C-N	6.01	129.65	120.82
1	A	191	LEU	C-N-CA	6.01	129.65	120.82
1	A	658	TYR	N-CA-C	-5.73	101.97	110.46
2	B	150	ASN	CA-CB-CG	5.73	118.33	112.60
2	B	360	MET	CA-C-N	5.67	127.87	120.28
2	B	360	MET	C-N-CA	5.67	127.87	120.28
1	A	681	PHE	CA-C-N	5.57	128.20	120.29
1	A	681	PHE	C-N-CA	5.57	128.20	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	376	ILE	CA-C-N	5.56	128.05	120.54
2	B	376	ILE	C-N-CA	5.56	128.05	120.54
1	A	265	ASN	CA-CB-CG	5.56	118.16	112.60
2	B	611	GLU	N-CA-C	-5.55	106.10	112.92
2	B	639	SER	CA-C-N	5.47	129.03	120.82
2	B	639	SER	C-N-CA	5.47	129.03	120.82
1	A	405	VAL	N-CA-CB	5.40	118.26	111.46
1	A	393	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	537	ASN	CA-C-N	5.37	128.23	120.38
1	A	537	ASN	C-N-CA	5.37	128.23	120.38
2	B	344	GLU	CA-C-N	5.35	127.45	120.28
2	B	344	GLU	C-N-CA	5.35	127.45	120.28
2	B	333	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	555	LYS	CA-C-N	5.29	128.38	120.87
1	A	555	LYS	C-N-CA	5.29	128.38	120.87
1	A	607	ASP	CA-C-N	5.14	127.17	120.28
1	A	607	ASP	C-N-CA	5.14	127.17	120.28
2	B	16	THR	CA-C-N	5.14	131.36	121.54
2	B	16	THR	C-N-CA	5.14	131.36	121.54
2	B	287	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	611	GLU	CA-C-N	5.10	130.24	122.29
2	B	611	GLU	C-N-CA	5.10	130.24	122.29
1	A	398	VAL	CA-C-N	5.08	125.74	119.99
1	A	398	VAL	C-N-CA	5.08	125.74	119.99
2	B	369	VAL	N-CA-CB	5.05	118.16	110.58
2	B	500	ASP	CA-CB-CG	5.03	117.63	112.60

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	4799	0	4656	90	0
2	B	4892	0	4766	75	0
All	All	9691	0	9422	159	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 8.

All (159) 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:28:ILE:HG13	2:B:143:ILE:HD12	1.44	0.99
2:B:51:SER:HB3	2:B:112:THR:HG22	1.48	0.93
1:A:588:TRP:HB2	1:A:592:ILE:HD11	1.55	0.85
1:A:588:TRP:HB2	1:A:592:ILE:CD1	2.06	0.84
2:B:51:SER:HB3	2:B:112:THR:CG2	2.17	0.75
2:B:328:ALA:HB1	2:B:334:GLU:HB3	1.70	0.73
1:A:697:HIS:ND1	2:B:594:LYS:HG3	2.05	0.72
1:A:28:ILE:CG1	2:B:143:ILE:HD12	2.20	0.71
1:A:612:PHE:CZ	1:A:688:ALA:HB1	2.25	0.71
2:B:535:GLN:HB3	2:B:553:SER:H	1.56	0.70
1:A:279:LEU:HB3	1:A:316:MET:HE3	1.74	0.69
2:B:400:VAL:HG22	2:B:473:HIS:ND1	2.08	0.67
2:B:616:PHE:HE1	2:B:635:VAL:HG21	1.59	0.67
2:B:380:ALA:HB2	2:B:461:ARG:HG3	1.77	0.67
1:A:543:SER:HB2	1:A:548:PHE:HB3	1.77	0.67
1:A:535:THR:HG21	1:A:573:LEU:HB2	1.77	0.65
1:A:20:TYR:HD1	1:A:26:LYS:HB3	1.62	0.65
1:A:592:ILE:HG22	1:A:691:ILE:HA	1.79	0.65
1:A:535:THR:HA	1:A:565:ARG:HA	1.79	0.64
1:A:72:ALA:O	1:A:76:VAL:HG23	1.97	0.64
1:A:144:ILE:HG12	1:A:245:VAL:HG12	1.80	0.64
2:B:644:LEU:HG	2:B:661:VAL:HB	1.79	0.64
1:A:68:MET:HE1	1:A:89:ALA:HA	1.81	0.62
1:A:592:ILE:HG23	1:A:698:GLY:HA3	1.82	0.62
1:A:183:ILE:HD11	1:A:224:LYS:HB3	1.80	0.62
2:B:244:VAL:HG12	2:B:246:LEU:HD23	1.82	0.62
1:A:49:ARG:H	1:A:112:THR:HA	1.63	0.61
1:A:624:ASN:HB2	1:A:627:ILE:HG22	1.82	0.61
1:A:659:GLY:O	1:A:678:LYS:HA	2.01	0.60
2:B:162:SER:O	2:B:165:VAL:HG12	2.00	0.60
2:B:322:ILE:O	2:B:326:LEU:HB2	2.02	0.59
2:B:6:LEU:HD11	2:B:246:LEU:HD11	1.86	0.58
2:B:575:GLY:H	2:B:577:HIS:HE1	1.51	0.57
2:B:274:THR:O	2:B:278:ILE:HD12	2.04	0.57
1:A:20:TYR:CD1	1:A:26:LYS:HB3	2.38	0.57
2:B:193:THR:HG22	2:B:196:GLU:HB2	1.87	0.57
2:B:639:SER:HB2	2:B:660:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:TRP:HB2	1:A:592:ILE:HD12	1.87	0.57
1:A:65:SER:HA	1:A:70:ILE:HD12	1.86	0.56
1:A:18:MET:HG3	1:A:28:ILE:HG22	1.88	0.56
1:A:108:TYR:O	1:A:149:ASN:HB2	2.06	0.56
2:B:326:LEU:O	2:B:329:ILE:HG12	2.06	0.55
1:A:624:ASN:HB2	1:A:627:ILE:CG2	2.36	0.55
2:B:318:LEU:O	2:B:322:ILE:HG12	2.06	0.55
2:B:534:HIS:HD2	2:B:535:GLN:H	1.53	0.55
1:A:614:TYR:HD1	1:A:635:LYS:HA	1.72	0.55
1:A:619:TRP:HB3	1:A:677:PHE:CZ	2.43	0.53
1:A:361:LEU:HA	1:A:364:VAL:HG12	1.91	0.53
2:B:608:GLY:H	2:B:613:SER:HB3	1.72	0.53
1:A:655:ASP:O	1:A:658:TYR:O	2.27	0.52
1:A:377:MET:HE1	1:A:460:GLN:HA	1.91	0.52
1:A:564:GLU:HG3	1:A:603:ARG:NH1	2.25	0.52
1:A:565:ARG:O	1:A:603:ARG:HB3	2.09	0.52
1:A:593:ASP:HB3	1:A:622:SER:HA	1.92	0.52
1:A:619:TRP:HB3	1:A:677:PHE:HZ	1.75	0.52
2:B:548:SER:HB2	2:B:686:ILE:HG22	1.91	0.52
1:A:311:ILE:HG21	1:A:422:LEU:HB3	1.91	0.52
1:A:508:PRO:HB2	1:A:510:MET:HE2	1.92	0.51
1:A:596:ILE:HB	1:A:685:VAL:HG13	1.92	0.51
1:A:18:MET:HE2	1:A:28:ILE:HG21	1.92	0.50
1:A:602:PRO:HB2	1:A:610:SER:HB2	1.93	0.50
1:A:24:ARG:HB3	1:A:83:VAL:CG1	2.42	0.49
1:A:151:PHE:HB2	1:A:207:HIS:HB2	1.94	0.49
1:A:10:LEU:O	1:A:12:ARG:N	2.46	0.49
2:B:153:PHE:CZ	2:B:230:LEU:HD11	2.48	0.48
2:B:464:ALA:HA	2:B:474:PHE:CZ	2.48	0.48
1:A:55:ILE:HD11	1:A:176:LYS:HA	1.95	0.48
2:B:66:SER:HA	2:B:71:ILE:HD12	1.96	0.48
2:B:527:THR:HG22	2:B:544:LYS:HD3	1.94	0.48
2:B:146:LEU:HB3	2:B:243:THR:HB	1.96	0.47
2:B:516:ARG:NH1	2:B:580:GLU:OE2	2.47	0.47
2:B:614:TRP:HE1	2:B:674:THR:HG21	1.78	0.47
1:A:408:ILE:HA	1:A:480:THR:O	2.14	0.47
2:B:350:PRO:HB3	2:B:435:LEU:HA	1.96	0.47
1:A:408:ILE:HD11	1:A:482:LEU:HB2	1.96	0.47
2:B:587:VAL:HG11	2:B:697:ILE:CG2	2.45	0.47
1:A:547:THR:HG23	1:A:702:LEU:HB2	1.98	0.46
2:B:575:GLY:H	2:B:577:HIS:CE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:CD1	2:B:115:PHE:HZ	2.28	0.46
1:A:408:ILE:HD13	1:A:493:TYR:CZ	2.50	0.46
2:B:28:LEU:HD12	2:B:138:ALA:HB2	1.96	0.46
2:B:5:ILE:HD13	2:B:143:ILE:HD11	1.97	0.46
1:A:408:ILE:HG21	1:A:493:TYR:CD1	2.50	0.46
2:B:587:VAL:HG11	2:B:697:ILE:HG21	1.97	0.46
2:B:88:GLY:O	2:B:89:SER:HB3	2.15	0.46
1:A:368:ILE:O	1:A:372:LYS:HB2	2.16	0.45
1:A:510:MET:HE1	1:A:524:TRP:CD1	2.52	0.45
1:A:691:ILE:HG22	1:A:691:ILE:O	2.16	0.45
2:B:591:VAL:HB	2:B:680:VAL:HB	1.97	0.45
1:A:388:ASN:OD1	1:A:390:THR:HB	2.16	0.45
2:B:507:MET:HE1	2:B:518:GLU:O	2.16	0.45
1:A:11:GLY:HA3	1:A:86:GLY:CA	2.47	0.45
2:B:145:ILE:HG22	2:B:244:VAL:HG22	1.99	0.45
2:B:582:GLU:HG3	2:B:700:LEU:HD11	1.99	0.45
1:A:292:VAL:HG12	1:A:294:LEU:H	1.81	0.44
1:A:395:GLU:HB3	1:A:478:PHE:CE1	2.51	0.44
1:A:569:PHE:CZ	1:A:611:ALA:HB2	2.52	0.44
1:A:104:VAL:CG1	1:A:175:ILE:HG13	2.47	0.44
2:B:659:TYR:HB3	2:B:666:VAL:HG13	1.99	0.44
1:A:57:ALA:O	1:A:168:GLN:NE2	2.50	0.44
1:A:535:THR:CG2	1:A:573:LEU:H	2.31	0.44
1:A:86:GLY:H	1:A:89:ALA:HB3	1.82	0.44
1:A:144:ILE:CG2	1:A:242:PRO:HB3	2.48	0.44
1:A:171:MET:O	1:A:175:ILE:HG12	2.17	0.44
1:A:377:MET:HB3	1:A:463:CYS:SG	2.58	0.44
2:B:182:VAL:HG13	2:B:228:GLN:HG3	2.00	0.44
1:A:9:ALA:HB2	1:A:245:VAL:HG13	1.99	0.44
2:B:99:PHE:HB3	2:B:287:ASP:OD1	2.18	0.44
2:B:196:GLU:HA	2:B:199:ILE:HD12	2.00	0.44
1:A:614:TYR:HA	1:A:635:LYS:H	1.84	0.43
1:A:355:GLU:O	1:A:359:LYS:HB2	2.18	0.43
1:A:25:GLU:HG2	2:B:5:ILE:HG23	2.01	0.43
2:B:272:ARG:O	2:B:276:GLU:HB2	2.19	0.43
2:B:326:LEU:HD12	2:B:326:LEU:HA	1.91	0.43
2:B:73:ALA:HB1	2:B:268:LEU:HD13	2.00	0.43
1:A:540:ILE:HD11	1:A:570:ASN:C	2.44	0.43
2:B:397:ASP:HB3	2:B:400:VAL:HG23	2.00	0.43
2:B:663:LYS:HG2	2:B:664:ALA:H	1.84	0.42
1:A:632:ARG:HG2	1:A:637:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ASP:HB3	2:B:294:VAL:HG23	2.01	0.42
1:A:192:THR:HG22	1:A:194:GLU:H	1.84	0.42
1:A:513:VAL:O	1:A:664:TYR:OH	2.26	0.42
1:A:566:PHE:HE2	1:A:573:LEU:HD13	1.83	0.42
2:B:97:LYS:HG3	2:B:104:ARG:HH11	1.85	0.42
2:B:97:LYS:HA	2:B:104:ARG:NH1	2.34	0.42
1:A:178:ILE:HB	1:A:179:PRO:HD3	2.01	0.42
1:A:534:ASN:O	1:A:564:GLU:O	2.37	0.42
2:B:626:GLN:OE1	2:B:670:HIS:CE1	2.72	0.42
2:B:582:GLU:O	2:B:697:ILE:HA	2.20	0.42
2:B:659:TYR:CD1	2:B:668:HIS:HA	2.54	0.42
1:A:265:ASN:HB3	1:A:337:GLU:OE1	2.19	0.42
1:A:448:SER:HB3	1:A:451:VAL:HB	2.01	0.42
1:A:566:PHE:HA	1:A:603:ARG:O	2.20	0.42
1:A:665:ALA:HB2	1:A:674:LEU:HD21	2.02	0.41
2:B:583:TRP:HE3	2:B:587:VAL:HB	1.85	0.41
2:B:591:VAL:HG22	2:B:656:LEU:HD22	2.01	0.41
1:A:104:VAL:HG13	1:A:175:ILE:HG13	2.01	0.41
1:A:594:VAL:HG13	1:A:689:PHE:CE1	2.56	0.41
1:A:391:GLU:OE2	2:B:162:SER:OG	2.33	0.41
2:B:193:THR:CG2	2:B:196:GLU:HB2	2.50	0.41
1:A:139:HIS:HB3	1:A:247:LEU:HD12	2.02	0.41
2:B:25:ASN:ND2	2:B:75:LEU:HA	2.35	0.41
2:B:57:ILE:HG21	2:B:68:LEU:HD11	2.03	0.41
2:B:79:PHE:CZ	2:B:93:LEU:HB3	2.56	0.41
1:A:630:ILE:HG22	1:A:639:ASN:HA	2.02	0.41
2:B:693:VAL:O	2:B:693:VAL:HG22	2.21	0.41
2:B:402:HIS:HB2	2:B:472:VAL:HG22	2.03	0.41
1:A:574:CYS:HB2	1:A:687:PRO:HD2	2.02	0.41
2:B:46:GLU:HA	2:B:116:LYS:HG2	2.03	0.41
2:B:533:ALA:O	2:B:560:LYS:HE3	2.21	0.41
1:A:403:HIS:HB2	1:A:475:VAL:HG22	2.03	0.41
1:A:494:TYR:HB3	1:A:502:THR:HG22	2.02	0.40
1:A:366:ARG:HG3	1:A:446:CYS:HB2	2.03	0.40
2:B:56:ILE:HG12	2:B:107:LEU:HD13	2.03	0.40
2:B:353:ILE:HD12	2:B:356:LEU:HD12	2.02	0.40
2:B:354:GLU:O	2:B:358:MET:HB2	2.20	0.40
2:B:613:SER:O	2:B:628:HIS:HD2	2.04	0.40
1:A:109:LYS:HA	1:A:149:ASN:HB3	2.03	0.40
2:B:534:HIS:HD2	2:B:535:GLN:N	2.18	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	590/703 (84%)	559 (95%)	29 (5%)	2 (0%)	36	67
2	B	594/700 (85%)	570 (96%)	24 (4%)	0	100	100
All	All	1184/1403 (84%)	1129 (95%)	53 (4%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	A	565	ARG

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	510/617 (83%)	497 (98%)	13 (2%)	42	69
2	B	536/625 (86%)	525 (98%)	11 (2%)	47	71
All	All	1046/1242 (84%)	1022 (98%)	24 (2%)	44	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	LEU
1	A	327	LEU
1	A	340	LEU
1	A	408	ILE

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Mol	Chain	Res	Type
1	A	458	ARG
1	A	530	THR
1	A	615	ASN
1	A	616	THR
1	A	627	ILE
1	A	630	ILE
1	A	685	VAL
1	A	699	THR
1	A	700	LEU
2	B	5	ILE
2	B	8	VAL
2	B	74	SER
2	B	246	LEU
2	B	276	GLU
2	B	334	GLU
2	B	412	THR
2	B	600	THR
2	B	666	VAL
2	B	696	GLN
2	B	697	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	201	ASN
1	A	273	HIS
2	B	25	ASN
2	B	96	GLN
2	B	388	GLN
2	B	422	ASN
2	B	484	GLN
2	B	534	HIS
2	B	543	ASN
2	B	563	HIS
2	B	577	HIS
2	B	610	ASN
2	B	628	HIS
2	B	670	HIS
2	B	673	HIS

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	A	612/703 (87%)	0.21	22 (3%) 46 26	10, 48, 89, 162	0
2	B	616/700 (88%)	0.07	16 (2%) 57 36	9, 48, 87, 124	0
All	All	1228/1403 (87%)	0.14	38 (3%) 51 30	9, 48, 88, 162	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	6.4
2	B	182	VAL	5.4
1	A	266	VAL	5.4
2	B	329	ILE	4.8
2	B	687	GLY	4.8
2	B	138	ALA	4.2
1	A	539	TRP	4.1
2	B	619	SER	3.7
1	A	428	SER	3.6
1	A	159	VAL	3.6
1	A	28	ILE	3.4
2	B	29	ILE	3.2
2	B	24	ARG	3.2
2	B	640	THR	3.2
1	A	183	ILE	3.0
1	A	23	ARG	3.0
1	A	267	SER	2.8
1	A	331	ARG	2.6
1	A	158	LYS	2.5
1	A	337	GLU	2.5
1	A	138	THR	2.5
1	A	100	ASN	2.5
2	B	693	VAL	2.4
2	B	139	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	641	GLY	2.3
1	A	4	ASP	2.3
2	B	212	PHE	2.2
1	A	117	PHE	2.2
1	A	612	PHE	2.2
2	B	548	SER	2.1
1	A	644	ASN	2.1
1	A	442	GLU	2.1
2	B	28	LEU	2.1
1	A	166	ASP	2.1
1	A	338	GLN	2.1
2	B	23	ALA	2.0
2	B	551	THR	2.0
1	A	608	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.