



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:37 PM UTC

PDB ID : 1Z52 / pdb_00001z52
Title : Proaerolysin Mutant W373L
Authors : Parker, M.W.; Feil, S.C.; Tang, J.W.
Deposited on : 2005-03-16
Resolution : 2.38 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

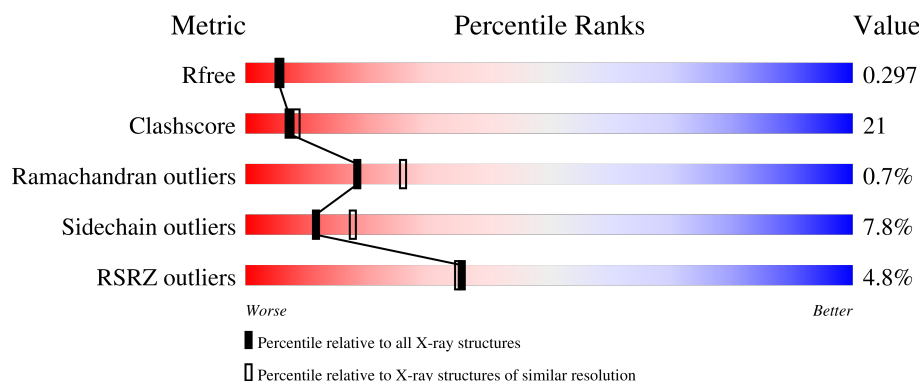
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	470	5% 62% 29% ...
1	B	470	4% 57% 33% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7179 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 Aerolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3525	2227	607	682	9			
1	B	450	Total	C	N	O	S	0	0	0
			3522	2226	605	682	9			

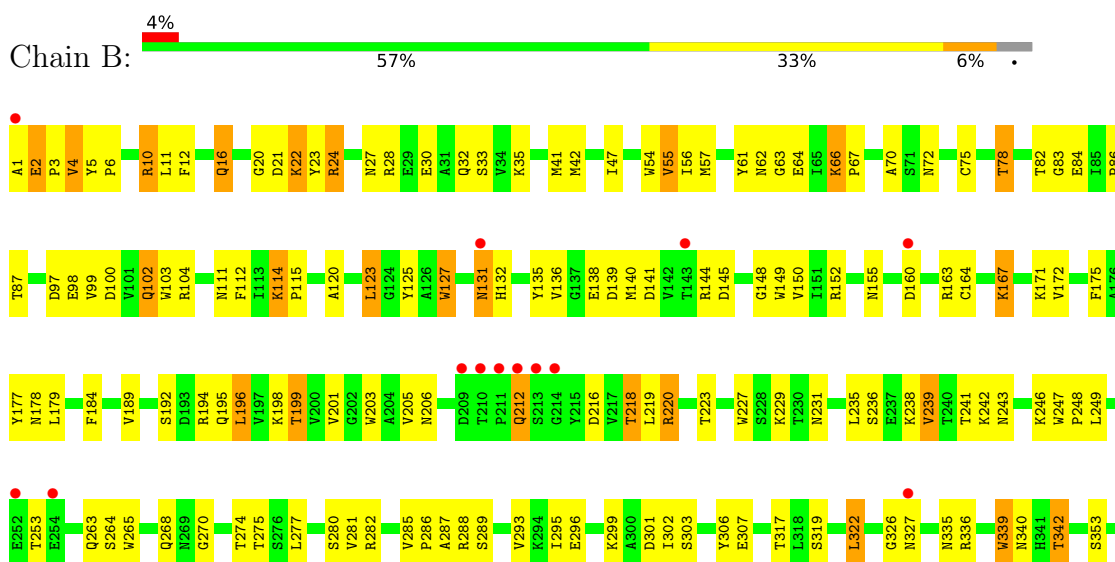
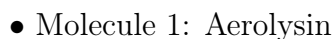
There are 2 discrepancies between the modelled and reference sequences:

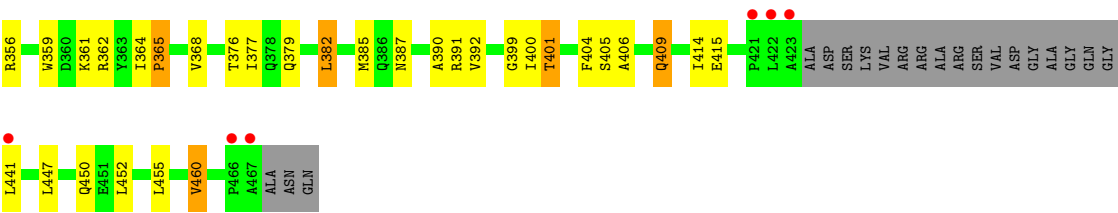
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	LEU	TRP	engineered mutation	UNP P09167
B	373	LEU	TRP	engineered mutation	UNP P09167

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	82	Total	O	0	0
			82	82		

- Molecule 1: Aerolysin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.71Å 91.14Å 168.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.38 25.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.38) 86.6 (25.00-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.301 0.246 , 0.297	Depositor DCC
R_{free} test set	1908 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7179	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	1.00	12/3621 (0.3%)	1.10	19/4941 (0.4%)
1	B	0.71	8/3618 (0.2%)	1.04	12/4938 (0.2%)
All	All	0.87	20/7239 (0.3%)	1.07	31/9879 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	ASP	C-N	38.87	1.86	1.33
1	B	102	GLN	C-N	15.17	1.53	1.33
1	A	189	VAL	C-N	15.04	1.54	1.33
1	A	370	TRP	C-N	-14.25	1.12	1.33
1	A	413	ASN	C-N	-10.24	1.22	1.33
1	A	203	TRP	C-N	-9.96	1.19	1.33
1	A	421	PRO	C-N	8.46	1.44	1.33
1	B	195	GLN	C-N	-7.05	1.23	1.33
1	B	203	TRP	C-N	-6.67	1.24	1.33
1	B	289	SER	C-N	-6.42	1.25	1.33
1	A	266	ALA	C-N	6.09	1.41	1.33
1	A	271	GLY	C-N	-5.85	1.25	1.33
1	A	216	ASP	C-N	-5.55	1.26	1.33
1	B	286	PRO	C-N	-5.52	1.26	1.33
1	A	103	TRP	NE1-CE2	-5.50	1.31	1.37
1	B	149	TRP	NE1-CE2	-5.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	TRP	NE1-CE2	-5.42	1.31	1.37
1	B	127	TRP	NE1-CE2	-5.32	1.31	1.37
1	A	371	TRP	NE1-CE2	-5.22	1.31	1.37
1	A	149	TRP	NE1-CE2	-5.17	1.31	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	O-C-N	20.35	149.66	122.59
1	A	82	THR	N-CA-C	6.69	119.59	110.55
1	A	216	ASP	O-C-N	-6.58	115.56	123.13
1	B	339	TRP	N-CA-C	6.22	119.33	109.50
1	A	370	TRP	CA-C-N	6.04	131.03	122.09
1	A	370	TRP	C-N-CA	6.04	131.03	122.09
1	A	192	SER	O-C-N	5.95	130.50	122.59
1	A	189	VAL	O-C-N	5.88	129.91	122.57
1	A	73	THR	N-CA-C	5.83	118.26	109.23
1	A	412	GLY	N-CA-C	-5.82	103.69	112.60
1	B	286	PRO	CA-C-N	5.80	129.07	120.90
1	B	286	PRO	C-N-CA	5.80	129.07	120.90
1	B	5	TYR	CA-C-N	5.72	126.99	119.84
1	B	5	TYR	C-N-CA	5.72	126.99	119.84
1	A	203	TRP	CA-C-N	5.53	130.13	122.77
1	A	203	TRP	C-N-CA	5.53	130.13	122.77
1	A	104	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	78	THR	N-CA-C	-5.48	105.39	111.36
1	A	442	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	B	218	THR	N-CA-C	5.40	117.21	108.41
1	A	220	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	163	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	144	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	364	ILE	CA-C-N	5.36	126.53	119.84
1	A	364	ILE	C-N-CA	5.36	126.53	119.84
1	B	152	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	104	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	194	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	278	SER	N-CA-C	5.08	116.46	107.61
1	B	78	THR	N-CA-C	-5.08	106.34	112.54
1	B	401	THR	N-CA-C	5.04	116.34	109.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	LEU	Mainchain
1	B	172	VAL	Mainchain
1	B	196	LEU	Mainchain

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	3525	0	3363	139	1
1	B	3522	0	3365	153	1
2	A	50	0	0	14	2
2	B	82	0	0	27	2
All	All	7179	0	6728	288	3

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 21.

All (288) 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:193:ASP:C	1:A:194:ARG:N	1.86	1.34
1:A:193:ASP:CA	1:A:194:ARG:N	1.92	1.33
1:A:193:ASP:HA	1:A:194:ARG:N	1.50	1.26
1:A:442:ARG:HH11	1:A:442:ARG:CG	1.53	1.21
1:B:353:SER:HB3	2:B:535:HOH:O	1.41	1.18
1:B:131:ASN:HD21	1:B:167:LYS:NZ	1.43	1.16
1:A:442:ARG:HH11	1:A:442:ARG:HG3	1.20	1.05
1:B:155:ASN:OD1	1:B:167:LYS:HE3	1.55	1.04
1:B:249:LEU:HD13	2:B:530:HOH:O	1.58	1.00
1:A:41:MET:HE3	1:A:74:TRP:CH2	1.99	0.97
1:A:324:TRP:HE3	1:A:336:ARG:HE	1.03	0.97
1:B:131:ASN:ND2	1:B:167:LYS:NZ	2.12	0.96
1:B:249:LEU:HB2	2:B:530:HOH:O	1.67	0.94
1:A:442:ARG:HG3	1:A:442:ARG:NH1	1.76	0.94
1:B:155:ASN:OD1	1:B:167:LYS:CE	2.17	0.93
1:B:361:LYS:HD3	2:B:544:HOH:O	1.69	0.92
1:A:442:ARG:CG	1:A:442:ARG:NH1	2.24	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HH11	1:A:442:ARG:HG2	1.33	0.91
1:B:22:LYS:HE2	1:B:22:LYS:HA	1.53	0.89
1:A:144:ARG:CD	2:A:485:HOH:O	2.20	0.89
1:B:131:ASN:HD21	1:B:167:LYS:HZ1	1.10	0.87
1:A:190:THR:HG22	1:A:190:THR:O	1.73	0.86
1:B:148:GLY:HA3	2:B:526:HOH:O	1.76	0.84
1:A:152:ARG:HE	1:A:167:LYS:HB2	1.44	0.82
1:B:189:VAL:HG11	1:B:192:SER:HB2	1.63	0.80
1:A:324:TRP:CD1	1:A:325:GLY:H	1.99	0.79
1:A:368:VAL:HG21	1:A:372:ASP:HB2	1.65	0.79
1:B:178:ASN:HD21	1:B:242:LYS:H	1.29	0.77
1:A:144:ARG:HD3	2:A:485:HOH:O	1.80	0.76
1:B:452:LEU:HD13	1:B:460:VAL:HG11	1.68	0.76
1:A:142:VAL:HG12	1:A:151:ILE:HG12	1.67	0.76
1:A:292:PRO:HG2	1:A:417:GLY:HA3	1.68	0.76
1:A:144:ARG:HD2	2:A:485:HOH:O	1.85	0.75
1:B:132:HIS:HB2	1:B:139:ASP:CG	2.12	0.75
1:A:236:SER:HA	1:A:239:VAL:HG12	1.67	0.75
1:A:192:SER:O	1:A:193:ASP:HB2	1.87	0.74
1:B:206:ASN:OD1	1:B:212:GLN:HB2	1.87	0.74
1:B:317:THR:OG1	1:B:342:THR:HB	1.87	0.74
1:B:220:ARG:HG2	2:B:484:HOH:O	1.87	0.74
2:A:473:HOH:O	1:B:356:ARG:HD3	1.88	0.73
1:B:322:LEU:HB3	1:B:327:ASN:ND2	2.03	0.73
1:B:155:ASN:CG	1:B:167:LYS:HE3	2.13	0.73
1:A:341:HIS:CD2	1:A:371:TRP:HE1	2.06	0.72
1:A:465:THR:HG23	1:A:469:ASN:ND2	2.04	0.71
1:B:447:LEU:HA	2:B:518:HOH:O	1.91	0.71
2:A:473:HOH:O	1:B:356:ARG:CG	2.40	0.70
1:A:361:LYS:C	2:A:498:HOH:O	2.34	0.69
1:A:202:GLY:HA3	1:A:445:ILE:HG12	1.74	0.69
1:B:231:ASN:HA	2:B:549:HOH:O	1.93	0.69
1:A:344:VAL:HG23	1:A:353:SER:HB2	1.75	0.69
1:B:249:LEU:CD1	2:B:530:HOH:O	2.28	0.68
1:B:212:GLN:HG2	1:B:441:LEU:HB2	1.75	0.68
1:A:107:HIS:NE2	1:A:142:VAL:HG21	2.09	0.68
1:A:279:GLN:NE2	1:A:413:ASN:HA	2.09	0.67
1:A:465:THR:HG23	1:A:469:ASN:HD22	1.60	0.67
1:B:28:ARG:HD2	1:B:54:TRP:CE2	2.29	0.67
1:A:87:THR:O	1:A:87:THR:HG23	1.95	0.66
1:B:194:ARG:O	1:B:194:ARG:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:O	1:A:63:GLY:HA2	1.95	0.65
1:B:220:ARG:CG	2:B:484:HOH:O	2.43	0.65
1:B:229:LYS:NZ	1:B:231:ASN:HD21	1.94	0.65
1:A:324:TRP:HE3	1:A:336:ARG:NE	1.86	0.65
1:A:219:LEU:HD22	1:A:295:ILE:HG21	1.79	0.64
1:A:41:MET:HE3	1:A:74:TRP:HH2	1.56	0.64
1:B:229:LYS:HZ2	1:B:231:ASN:HD21	1.42	0.64
1:B:189:VAL:CG1	1:B:192:SER:HB2	2.27	0.64
1:A:324:TRP:HD1	1:A:325:GLY:H	1.45	0.64
1:A:372:ASP:HA	2:A:494:HOH:O	1.97	0.64
1:A:229:LYS:HA	1:A:403:ASP:O	1.98	0.63
1:A:142:VAL:HA	1:A:150:VAL:O	1.97	0.63
2:A:473:HOH:O	1:B:356:ARG:HG2	1.97	0.63
1:B:223:THR:HB	1:B:409:GLN:HB2	1.80	0.63
1:B:131:ASN:HD21	1:B:167:LYS:HZ3	1.43	0.62
1:A:190:THR:O	1:A:191:GLN:HB2	2.00	0.62
1:A:177:TYR:HD2	1:A:312:VAL:HG22	1.65	0.62
1:B:131:ASN:ND2	1:B:167:LYS:HZ3	1.97	0.61
1:A:28:ARG:HD3	1:A:54:TRP:CE3	2.37	0.60
1:B:319:SER:HA	1:B:339:TRP:O	2.02	0.60
1:A:48:SER:O	1:A:55:VAL:HG22	2.02	0.60
1:B:327:ASN:HB3	2:B:499:HOH:O	2.01	0.59
1:A:190:THR:O	1:A:190:THR:CG2	2.45	0.59
1:B:164:CYS:HB2	2:B:519:HOH:O	2.02	0.59
1:A:205:VAL:HG13	1:A:422:LEU:HD21	1.85	0.58
1:A:236:SER:HA	1:A:239:VAL:CG1	2.31	0.58
1:A:377:ILE:HD13	1:A:382:LEU:CD1	2.34	0.58
1:B:216:ASP:OD1	1:B:282:ARG:HD3	2.04	0.58
1:B:280:SER:HA	1:B:414:ILE:HD12	1.84	0.58
1:A:359:TRP:HA	1:A:373:LEU:HD12	1.85	0.58
1:B:66:LYS:HD2	1:B:67:PRO:O	2.04	0.58
1:A:253:THR:HG23	1:A:300:ALA:HB3	1.85	0.58
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.68	0.58
1:A:44:GLN:NE2	1:B:356:ARG:HD3	2.19	0.57
1:A:451:GLU:O	1:A:455:LEU:HD12	2.03	0.57
1:A:107:HIS:CD2	1:A:142:VAL:HG21	2.39	0.57
1:A:101:VAL:HG11	1:A:235:LEU:HD22	1.87	0.57
1:A:324:TRP:HB3	1:A:336:ARG:NH2	2.20	0.56
1:A:359:TRP:CA	1:A:373:LEU:HD12	2.35	0.56
1:A:193:ASP:CB	1:A:194:ARG:N	2.66	0.56
1:B:184:PHE:CG	1:B:248:PRO:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:HA	2:B:476:HOH:O	2.06	0.56
1:B:115:PRO:HB2	1:B:392:VAL:HG12	1.88	0.56
1:A:229:LYS:HE2	1:A:265:TRP:CZ2	2.40	0.56
1:A:368:VAL:O	1:A:368:VAL:HG13	2.04	0.56
1:B:319:SER:HB3	1:B:340:ASN:ND2	2.20	0.56
1:B:132:HIS:HB2	1:B:139:ASP:OD2	2.04	0.56
1:B:24:ARG:HG2	1:B:24:ARG:HH11	1.71	0.56
1:A:253:THR:O	1:A:255:LEU:HD13	2.07	0.55
1:B:1:ALA:C	1:B:3:PRO:HD2	2.32	0.54
1:B:98:GLU:OE1	1:B:238:LYS:HD2	2.06	0.54
1:A:114:LYS:HB2	1:A:115:PRO:HD3	1.89	0.54
1:A:41:MET:CE	1:A:74:TRP:CH2	2.82	0.54
1:A:331:THR:OG1	1:A:333:PRO:HD3	2.08	0.54
1:A:189:VAL:HA	1:A:304:TYR:HB3	1.89	0.54
1:A:208:SER:O	1:A:288:ARG:HD2	2.08	0.54
1:B:57:MET:O	1:B:63:GLY:HA2	2.08	0.54
1:A:253:THR:HG23	1:A:300:ALA:CB	2.38	0.54
1:B:179:LEU:O	1:B:241:THR:HG22	2.07	0.54
1:A:291:ILE:HD12	1:A:416:ILE:HG23	1.91	0.53
1:B:452:LEU:CD1	1:B:460:VAL:HG11	2.37	0.53
1:A:229:LYS:HE2	1:A:265:TRP:CE2	2.43	0.53
1:A:317:THR:OG1	1:A:342:THR:HB	2.09	0.53
1:B:171:LYS:HE3	2:B:510:HOH:O	2.08	0.53
1:B:42:MET:HE1	1:B:56:ILE:O	2.09	0.53
1:B:218:THR:HG22	1:B:220:ARG:HD2	1.91	0.53
1:A:361:LYS:HA	2:A:498:HOH:O	2.09	0.53
1:B:227:TRP:CE2	1:B:270:GLY:HA2	2.43	0.53
1:A:194:ARG:HG2	1:A:195:GLN:N	2.23	0.52
1:A:294:LYS:HE3	1:B:135:TYR:CE2	2.44	0.52
1:A:324:TRP:HB3	1:A:336:ARG:HH21	1.73	0.52
1:B:450:GLN:NE2	2:B:550:HOH:O	2.41	0.52
1:B:127:TRP:CE2	1:B:164:CYS:HA	2.45	0.52
1:B:179:LEU:HB3	1:B:241:THR:CG2	2.40	0.52
1:B:86:PRO:HD2	1:B:390:ALA:HB2	1.92	0.52
1:A:375:TRP:HA	1:A:378:GLN:CD	2.35	0.51
1:B:178:ASN:ND2	1:B:242:LYS:H	2.05	0.51
1:B:206:ASN:HB2	1:B:285:VAL:CG1	2.40	0.51
1:A:10:ARG:HD3	2:A:520:HOH:O	2.09	0.51
1:B:10:ARG:NH2	2:B:491:HOH:O	2.26	0.51
1:B:306:TYR:CD1	1:B:306:TYR:C	2.89	0.51
1:B:377:ILE:HD13	1:B:382:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HG2	2:A:504:HOH:O	2.10	0.51
1:B:47:ILE:HG23	1:B:55:VAL:HG11	1.92	0.50
1:B:47:ILE:HG23	1:B:55:VAL:CG1	2.42	0.50
1:B:35:LYS:HE3	1:B:63:GLY:O	2.12	0.50
1:B:16:GLN:HE21	1:B:16:GLN:C	2.20	0.50
1:A:224:ALA:HA	1:A:273:THR:O	2.11	0.50
1:A:190:THR:O	1:A:191:GLN:CB	2.59	0.49
1:A:420:VAL:HG23	1:A:420:VAL:O	2.11	0.49
1:B:229:LYS:HE3	1:B:268:GLN:O	2.12	0.49
1:B:127:TRP:NE1	1:B:164:CYS:HA	2.28	0.49
1:A:142:VAL:HG23	1:A:142:VAL:O	2.13	0.49
1:B:198:LYS:HG3	1:B:199:THR:N	2.27	0.49
1:B:415:GLU:HG3	2:B:531:HOH:O	2.13	0.49
1:B:16:GLN:HG2	1:B:70:ALA:O	2.13	0.49
1:B:23:TYR:HB3	1:B:75:CYS:HB3	1.95	0.49
1:B:102:GLN:NE2	1:B:175:PHE:CD2	2.81	0.48
1:B:219:LEU:HD22	1:B:295:ILE:HD13	1.94	0.48
1:B:120:ALA:O	1:B:125:TYR:HB2	2.14	0.48
1:A:57:MET:SD	1:A:66:LYS:HE2	2.52	0.48
1:B:30:GLU:O	1:B:33:SER:HB3	2.13	0.48
1:A:328:ALA:HB3	1:A:371:TRP:CE3	2.49	0.48
1:B:22:LYS:HG3	1:B:78:THR:OG1	2.14	0.48
1:B:145:ASP:HB2	1:B:150:VAL:HG23	1.94	0.48
1:A:90:ALA:C	1:A:394:ARG:HH12	2.22	0.48
1:A:227:TRP:CE2	1:A:270:GLY:HA2	2.48	0.48
1:A:443:LEU:HD13	1:A:464:VAL:HG22	1.95	0.47
1:A:377:ILE:HG23	1:A:382:LEU:HA	1.96	0.47
1:A:299:LYS:HE3	1:A:407:GLU:OE2	2.14	0.47
1:A:394:ARG:HD2	2:A:478:HOH:O	2.14	0.47
1:B:301:ASP:HA	1:B:406:ALA:O	2.14	0.47
1:A:223:THR:O	1:A:274:THR:HA	2.15	0.47
1:A:359:TRP:CH2	1:A:377:ILE:HD11	2.50	0.47
1:B:359:TRP:NE1	1:B:362:ARG:NH2	2.62	0.47
1:A:375:TRP:O	1:A:378:GLN:HG2	2.14	0.47
1:B:387:ASN:O	1:B:391:ARG:HG3	2.15	0.47
1:A:252:GLU:CD	1:B:111:ASN:HD21	2.23	0.47
1:B:206:ASN:O	1:B:288:ARG:HA	2.15	0.47
1:A:108:ASP:CG	1:A:111:ASN:HB2	2.40	0.46
1:A:162:TYR:HE2	1:A:336:ARG:CD	2.28	0.46
1:A:223:THR:HG21	1:A:409:GLN:O	2.15	0.46
1:A:219:LEU:HD22	1:A:295:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD11	1:B:72:ASN:HD22	1.80	0.46
1:B:206:ASN:HB2	1:B:285:VAL:HG13	1.97	0.46
1:A:82:THR:HG23	1:A:382:LEU:HD21	1.96	0.46
1:A:377:ILE:HD13	1:A:382:LEU:HD13	1.97	0.46
1:B:1:ALA:N	1:B:83:GLY:H	2.14	0.46
1:A:292:PRO:CG	1:A:417:GLY:HA3	2.44	0.46
1:B:12:PHE:CE1	1:B:20:GLY:HA3	2.51	0.46
1:B:299:LYS:HB2	1:B:409:GLN:HE22	1.80	0.46
1:B:239:VAL:HG22	1:B:265:TRP:CB	2.45	0.45
1:B:275:THR:O	1:B:277:LEU:HG	2.16	0.45
1:B:281:VAL:HG22	1:B:282:ARG:N	2.31	0.45
1:A:291:ILE:HD12	1:A:416:ILE:CG2	2.46	0.45
1:B:62:ASN:O	1:B:63:GLY:C	2.59	0.45
1:A:191:GLN:HA	1:A:191:GLN:NE2	2.32	0.45
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.32	0.45
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.78	0.45
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.81	0.45
1:B:112:PHE:C	1:B:115:PRO:HD2	2.42	0.45
1:B:322:LEU:HB3	1:B:327:ASN:HD22	1.82	0.45
1:A:204:ALA:HB3	1:A:291:ILE:HG13	1.98	0.45
1:B:220:ARG:CD	2:B:484:HOH:O	2.64	0.45
1:B:231:ASN:CB	2:B:549:HOH:O	2.65	0.45
1:A:217:VAL:HA	1:A:463:SER:O	2.17	0.44
1:A:442:ARG:NH1	1:A:442:ARG:HG2	2.12	0.44
1:B:155:ASN:OD1	1:B:167:LYS:NZ	2.49	0.44
1:B:98:GLU:CD	1:B:238:LYS:HD2	2.42	0.44
1:B:231:ASN:HB3	2:B:549:HOH:O	2.17	0.44
1:A:217:VAL:HG13	1:A:443:LEU:HD21	1.99	0.44
1:B:263:GLN:NE2	1:B:268:GLN:HG2	2.32	0.44
1:B:307:GLU:HB2	1:B:401:THR:HG22	2.00	0.44
1:B:194:ARG:O	1:B:194:ARG:CG	2.65	0.44
1:A:87:THR:O	1:A:87:THR:CG2	2.66	0.44
1:A:363:TYR:N	2:A:498:HOH:O	2.51	0.44
1:A:95:ASP:CG	1:A:399:GLY:O	2.61	0.43
1:B:167:LYS:H	1:B:167:LYS:HG2	1.52	0.43
1:A:152:ARG:NE	1:A:167:LYS:HB2	2.24	0.43
1:B:223:THR:CB	1:B:409:GLN:HB2	2.48	0.43
1:B:206:ASN:ND2	1:B:287:ALA:HA	2.33	0.43
1:B:236:SER:N	2:B:496:HOH:O	2.43	0.43
1:A:107:HIS:NE2	1:A:142:VAL:CG2	2.79	0.43
1:B:205:VAL:O	1:B:441:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HD3	2:B:484:HOH:O	2.18	0.43
1:B:359:TRP:CD1	1:B:362:ARG:HH21	2.36	0.43
1:A:95:ASP:OD2	1:A:233:TYR:HB2	2.19	0.43
1:B:263:GLN:O	1:B:264:SER:C	2.62	0.43
1:B:319:SER:HB3	1:B:340:ASN:CG	2.44	0.43
1:A:422:LEU:O	1:A:423:ALA:C	2.61	0.43
1:A:44:GLN:HE21	1:B:356:ARG:HD3	1.83	0.42
1:B:4:VAL:O	1:B:6:PRO:HD3	2.20	0.42
1:B:84:GLU:OE2	2:B:492:HOH:O	2.22	0.42
1:A:42:MET:HG2	1:A:46:GLN:NE2	2.34	0.42
1:A:162:TYR:HE2	1:A:336:ARG:HD2	1.84	0.42
1:B:177:TYR:CD1	1:B:177:TYR:N	2.87	0.42
1:B:235:LEU:N	2:B:496:HOH:O	2.52	0.42
1:B:27:ASN:OD1	1:B:30:GLU:HG3	2.19	0.42
1:A:204:ALA:O	1:A:290:LYS:HA	2.20	0.42
1:A:253:THR:O	1:A:255:LEU:CD1	2.67	0.42
1:B:61:TYR:O	1:B:62:ASN:HB2	2.19	0.42
1:B:177:TYR:CE2	1:B:235:LEU:HD11	2.54	0.42
1:B:239:VAL:HG22	1:B:265:TRP:HB2	2.01	0.42
1:B:376:THR:CB	1:B:385:MET:HE2	2.49	0.42
1:B:97:ASP:O	1:B:98:GLU:C	2.63	0.42
1:B:141:ASP:HA	2:B:502:HOH:O	2.19	0.42
1:B:223:THR:O	1:B:274:THR:HA	2.19	0.42
1:A:179:LEU:HA	1:A:310:ALA:HA	2.01	0.42
1:B:364:ILE:HA	1:B:365:PRO:HD2	1.77	0.42
1:A:220:ARG:NH1	1:A:463:SER:OG	2.53	0.42
1:A:93:ILE:HA	1:A:94:PRO:HD3	1.90	0.42
1:A:292:PRO:HG2	1:A:417:GLY:CA	2.44	0.42
1:B:99:VAL:HG13	1:B:100:ASP:N	2.34	0.42
1:B:359:TRP:NE1	1:B:362:ARG:HH21	2.18	0.42
1:A:321:PHE:CD1	1:A:321:PHE:C	2.97	0.42
1:B:303:SER:HA	1:B:404:PHE:O	2.20	0.42
1:B:399:GLY:O	1:B:400:ILE:HD13	2.20	0.42
1:A:206:ASN:OD1	1:A:208:SER:HB3	2.20	0.41
1:A:205:VAL:HG22	1:A:290:LYS:CB	2.51	0.41
1:A:329:TRP:CE2	1:A:339:TRP:CZ2	3.08	0.41
2:A:473:HOH:O	1:B:356:ARG:CD	2.50	0.41
1:B:11:LEU:HD21	1:B:72:ASN:HD22	1.85	0.41
1:A:23:TYR:CE1	1:A:77:PRO:HG3	2.54	0.41
1:A:205:VAL:HG22	1:A:290:LYS:HB3	2.02	0.41
1:B:132:HIS:ND1	1:B:139:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PRO:O	1:A:368:VAL:HG12	2.20	0.41
1:A:306:TYR:CD2	1:A:306:TYR:C	2.98	0.41
1:B:379:GLN:NE2	2:B:528:HOH:O	2.53	0.41
1:A:253:THR:HG22	1:A:255:LEU:CD1	2.51	0.41
1:A:303:SER:O	1:A:304:TYR:HB3	2.20	0.41
1:A:329:TRP:CE2	1:A:339:TRP:HZ2	2.37	0.41
1:B:246:LYS:O	1:B:247:TRP:C	2.63	0.41
1:A:105:LEU:HD13	1:A:396:VAL:HG11	2.02	0.41
1:B:179:LEU:HB3	1:B:241:THR:HG22	2.03	0.41
1:A:321:PHE:HA	1:A:337:PRO:O	2.21	0.41
1:B:1:ALA:HA	1:B:82:THR:HB	2.03	0.41
1:B:55:VAL:CG1	1:B:56:ILE:N	2.84	0.41
1:B:302:ILE:O	1:B:405:SER:HA	2.21	0.41
1:A:27:ASN:OD1	1:A:27:ASN:C	2.64	0.40
1:A:301:ASP:OD2	1:A:407:GLU:OE1	2.39	0.40
1:B:177:TYR:CD2	1:B:235:LEU:HD11	2.57	0.40
1:B:64:GLU:OE2	1:B:66:LYS:HB3	2.21	0.40
1:B:114:LYS:HE3	1:B:138:GLU:HG3	2.03	0.40
1:B:179:LEU:HD13	1:B:265:TRP:CE3	2.56	0.40
1:B:361:LYS:CD	2:B:544:HOH:O	2.48	0.40
1:A:91:LEU:HB2	1:A:394:ARG:NH1	2.36	0.40
1:A:344:VAL:HG11	1:A:349:LYS:HG3	2.03	0.40
1:B:196:LEU:CD1	1:B:296:GLU:HB3	2.51	0.40
1:B:198:LYS:CG	1:B:199:THR:N	2.83	0.40
1:B:335:ASN:O	1:B:336:ARG:C	2.63	0.40

All (3) 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:517:HOH:O	2:B:534:HOH:O[4_456]	1.94	0.26
1:A:210:THR:OG1	2:B:548:HOH:O[4_556]	2.14	0.06
1:B:1:ALA:CB	2:A:518:HOH:O[4_556]	2.16	0.04

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	447/470 (95%)	414 (93%)	30 (7%)	3 (1%)	18	26
1	B	446/470 (95%)	414 (93%)	29 (6%)	3 (1%)	18	26
All	All	893/940 (95%)	828 (93%)	59 (7%)	6 (1%)	18	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	145	ASP
1	A	193	ASP
1	B	365	PRO
1	B	2	GLU
1	B	326	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	379/392 (97%)	354 (93%)	25 (7%)	15	24
1	B	379/392 (97%)	345 (91%)	34 (9%)	9	13
All	All	758/784 (97%)	699 (92%)	59 (8%)	11	18

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	16	GLN
1	A	21	ASP
1	A	35	LYS
1	A	55	VAL
1	A	104	ARG

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Mol	Chain	Res	Type
1	A	106	VAL
1	A	134	GLN
1	A	177	TYR
1	A	193	ASP
1	A	201	VAL
1	A	208	SER
1	A	237	GLU
1	A	239	VAL
1	A	252	GLU
1	A	275	THR
1	A	337	PRO
1	A	342	THR
1	A	362	ARG
1	A	372	ASP
1	A	409	GLN
1	A	421	PRO
1	A	442	ARG
1	A	443	LEU
1	A	465	THR
1	B	2	GLU
1	B	4	VAL
1	B	10	ARG
1	B	16	GLN
1	B	21	ASP
1	B	22	LYS
1	B	24	ARG
1	B	32	GLN
1	B	41	MET
1	B	55	VAL
1	B	66	LYS
1	B	87	THR
1	B	114	LYS
1	B	123	LEU
1	B	131	ASN
1	B	136	VAL
1	B	140	MET
1	B	160	ASP
1	B	167	LYS
1	B	199	THR
1	B	201	VAL
1	B	212	GLN
1	B	220	ARG

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Mol	Chain	Res	Type
1	B	239	VAL
1	B	243	ASN
1	B	253	THR
1	B	293	VAL
1	B	322	LEU
1	B	342	THR
1	B	368	VAL
1	B	382	LEU
1	B	409	GLN
1	B	455	LEU
1	B	460	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	62	ASN
1	A	174	ASN
1	A	226	ASN
1	A	269	ASN
1	A	338	ASN
1	A	340	ASN
1	A	341	HIS
1	A	450	GLN
1	A	469	ASN
1	B	16	GLN
1	B	32	GLN
1	B	72	ASN
1	B	79	ASN
1	B	131	ASN
1	B	178	ASN
1	B	212	GLN
1	B	231	ASN
1	B	263	GLN
1	B	279	GLN
1	B	378	GLN
1	B	379	GLN
1	B	387	ASN
1	B	409	GLN
1	B	413	ASN
1	B	450	GLN
1	B	459	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	193:ASP	C	194:ARG	N	1.86
1	A	203:TRP	C	204:ALA	N	1.18
1	A	370:TRP	C	371:TRP	N	1.12

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	451/470 (95%)	0.34	24 (5%) 32 31	10, 26, 47, 66	0
1	B	450/470 (95%)	0.25	19 (4%) 40 40	9, 23, 49, 72	0
All	All	901/940 (95%)	0.29	43 (4%) 35 35	9, 25, 49, 72	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	GLN	4.2
1	A	423	ALA	4.1
1	A	422	LEU	4.0
1	A	190	THR	3.7
1	B	422	LEU	3.7
1	A	192	SER	3.6
1	B	213	SER	3.6
1	B	423	ALA	3.3
1	A	252	GLU	3.2
1	A	193	ASP	3.2
1	A	191	GLN	3.1
1	B	254	GLU	3.1
1	A	148	GLY	3.0
1	A	207	ASP	3.0
1	A	324	TRP	2.9
1	B	214	GLY	2.8
1	A	253	THR	2.7
1	B	466	PRO	2.6
1	A	94	PRO	2.6
1	B	211	PRO	2.5
1	B	131	ASN	2.4
1	A	249	LEU	2.4
1	B	421	PRO	2.4
1	A	3	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	421	PRO	2.3
1	B	467	ALA	2.3
1	A	146	GLY	2.3
1	A	147	ASP	2.2
1	B	441	LEU	2.2
1	A	194	ARG	2.2
1	A	363	TYR	2.1
1	B	327	ASN	2.1
1	A	447	LEU	2.1
1	B	160	ASP	2.1
1	B	1	ALA	2.1
1	A	334	ASP	2.1
1	B	210	THR	2.1
1	A	373	LEU	2.1
1	A	165	GLY	2.1
1	B	143	THR	2.0
1	B	252	GLU	2.0
1	A	195	GLN	2.0
1	B	209	ASP	2.0

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.