



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:02 PM UTC

PDB ID : 2VOK / pdb_00002vok
Title : Murine TRIM21
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Deposited on : 2008-02-19
Resolution : 1.30 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

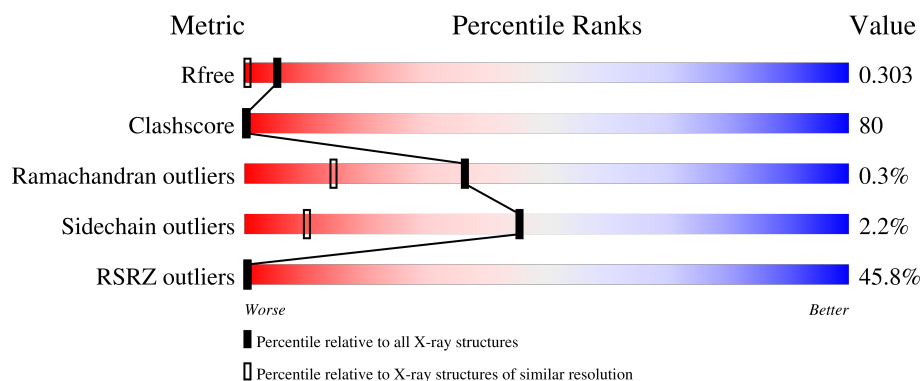
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	188	60% 53% 43% ..
1	B	188	30% 45% 53% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3476 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 52 KDA RO PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1499	956	265	270	8			
1	B	185	Total	C	N	O	S	0	0	0
			1496	953	264	271	8			

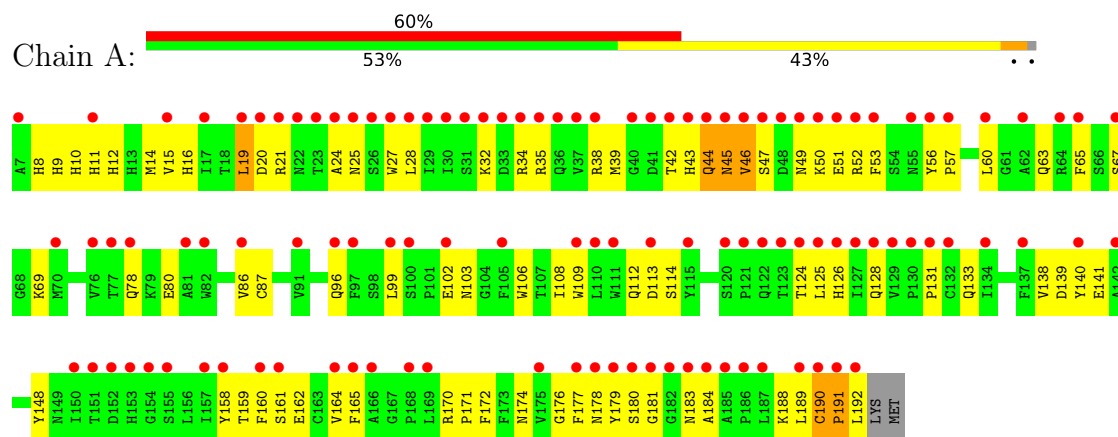
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	217	Total	O	0	0
			217	217		
2	B	264	Total	O	0	0
			264	264		

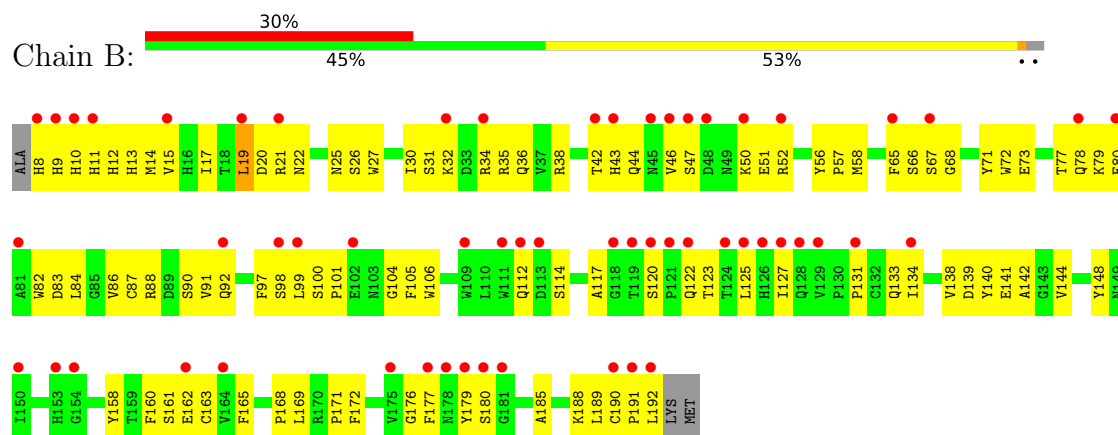
3 Residue-property plots

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: 52 KDA RO PROTEIN



• Molecule 1: 52 KDA RO PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.95Å 44.89Å 71.79Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	67.57 – 1.30 67.51 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (67.57-1.30) 99.6 (67.51-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.214 , 0.236 0.292 , 0.303	Depositor DCC
R_{free} test set	4636 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 28.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3476	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	A	0.53	0/1547	0.79	4/2104 (0.2%)
1	B	0.55	0/1544	0.72	0/2100
All	All	0.54	0/3091	0.76	4/4204 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	CYS	CA-C-N	9.40	131.59	119.84
1	A	190	CYS	C-N-CA	9.40	131.59	119.84
1	A	191	PRO	N-CA-C	6.60	126.06	112.47
1	A	45	ASN	N-CA-C	5.15	118.69	111.74

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	A	1499	0	1416	193	3
1	B	1496	0	1411	273	8
2	A	217	0	0	189	4
2	B	264	0	0	257	9
All	All	3476	0	2827	465	12

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 80.

All (465) 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:124:THR:CG2	2:A:2146:HOH:O	1.67	1.37
1:A:178:ASN:ND2	2:A:2196:HOH:O	1.60	1.33
1:B:52:ARG:NH1	2:B:2090:HOH:O	1.61	1.32
1:A:80:GLU:HB2	2:A:2098:HOH:O	1.26	1.31
1:A:42:THR:HG23	2:A:2054:HOH:O	1.26	1.30
1:B:158:TYR:HE2	2:B:2219:HOH:O	1.05	1.30
1:B:97:PHE:CA	2:B:2160:HOH:O	1.65	1.29
1:B:11:HIS:CB	2:B:2013:HOH:O	1.74	1.29
1:A:12:HIS:NE2	2:A:2012:HOH:O	1.56	1.29
1:B:32:LYS:HE2	2:B:2057:HOH:O	1.26	1.29
1:B:15:VAL:HB	2:B:2029:HOH:O	1.24	1.28
1:A:49:ASN:CB	2:A:2066:HOH:O	1.72	1.28
1:B:87:CYS:HB2	2:B:2168:HOH:O	1.34	1.28
1:B:142:ALA:HB2	2:B:2206:HOH:O	1.20	1.28
1:A:131:PRO:HB2	2:A:2164:HOH:O	1.16	1.28
1:B:20:ASP:C	2:B:2039:HOH:O	1.76	1.27
1:B:27:TRP:CD2	2:B:2073:HOH:O	1.83	1.27
1:B:106:TRP:CE3	2:B:2172:HOH:O	1.73	1.26
1:B:21:ARG:HG3	2:B:2036:HOH:O	1.17	1.26
1:A:113:ASP:HB3	2:A:2140:HOH:O	1.31	1.25
1:B:165:PHE:CB	2:B:2204:HOH:O	1.73	1.25
1:B:8:HIS:NE2	2:B:2003:HOH:O	1.61	1.24
1:B:104:GLY:HA3	2:B:2169:HOH:O	1.07	1.24
1:B:11:HIS:HB2	2:B:2013:HOH:O	1.34	1.24
1:A:28:LEU:N	2:A:2035:HOH:O	1.66	1.24
1:A:192:LEU:HD11	2:A:2015:HOH:O	1.34	1.24
1:A:140:TYR:CZ	2:A:2167:HOH:O	1.90	1.23
1:B:97:PHE:HD2	2:B:2159:HOH:O	1.19	1.23
1:B:144:VAL:HG23	2:B:2208:HOH:O	1.38	1.23
1:A:114:SER:CB	2:A:2145:HOH:O	1.83	1.23
1:B:11:HIS:CG	2:B:2013:HOH:O	1.82	1.22
1:B:117:ALA:O	2:B:2188:HOH:O	1.54	1.22
1:A:34:ARG:HD2	2:A:2024:HOH:O	1.37	1.22
1:B:106:TRP:N	2:B:2172:HOH:O	1.69	1.21
1:B:8:HIS:CD2	2:B:2003:HOH:O	1.87	1.21
1:B:158:TYR:CE1	2:B:2215:HOH:O	1.89	1.21
1:B:160:PHE:HA	2:B:2221:HOH:O	1.10	1.21
1:B:34:ARG:HG2	2:B:2042:HOH:O	1.05	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:HG23	2:A:2146:HOH:O	1.29	1.19
1:B:47:SER:N	2:B:2078:HOH:O	1.74	1.18
1:B:122:GLN:OE1	2:B:2195:HOH:O	1.58	1.18
1:B:133:GLN:CD	2:B:2200:HOH:O	1.82	1.18
1:B:162:GLU:O	2:B:2230:HOH:O	1.60	1.18
1:A:46:VAL:HG12	2:A:2058:HOH:O	1.37	1.18
1:B:161:SER:N	2:B:2221:HOH:O	1.74	1.18
1:B:165:PHE:HB2	2:B:2204:HOH:O	1.28	1.17
1:A:102:GLU:OE2	2:A:2120:HOH:O	1.64	1.16
1:A:49:ASN:HA	2:A:2066:HOH:O	1.36	1.16
1:B:142:ALA:C	2:B:2208:HOH:O	1.86	1.16
1:B:158:TYR:CZ	2:B:2215:HOH:O	1.97	1.16
1:A:16:HIS:NE2	2:A:2018:HOH:O	1.76	1.15
1:B:13:HIS:HE1	2:B:2024:HOH:O	1.26	1.15
1:B:140:TYR:CD2	2:B:2110:HOH:O	2.00	1.15
1:A:114:SER:CA	2:A:2145:HOH:O	1.91	1.14
1:B:158:TYR:OH	2:B:2215:HOH:O	1.63	1.14
1:A:140:TYR:N	2:A:2166:HOH:O	1.80	1.14
1:B:91:VAL:HG11	2:B:2168:HOH:O	1.47	1.14
1:B:158:TYR:CE2	2:B:2219:HOH:O	1.80	1.14
1:A:138:VAL:HG12	2:A:2166:HOH:O	1.47	1.14
1:B:169:LEU:HA	2:B:2236:HOH:O	0.95	1.13
1:B:30:ILE:C	2:B:2052:HOH:O	1.92	1.12
1:A:179:TYR:CE2	2:A:2206:HOH:O	2.02	1.12
1:B:43:HIS:HA	2:B:2047:HOH:O	0.95	1.12
1:B:97:PHE:CB	2:B:2160:HOH:O	1.75	1.11
1:A:177:PHE:CD1	2:A:2200:HOH:O	2.03	1.11
1:A:162:GLU:HB2	2:A:2181:HOH:O	1.48	1.11
1:B:117:ALA:O	2:B:2192:HOH:O	1.66	1.11
1:B:105:PHE:O	2:B:2170:HOH:O	1.67	1.10
1:B:30:ILE:O	2:B:2052:HOH:O	1.70	1.09
1:A:192:LEU:N	2:A:2216:HOH:O	1.70	1.09
1:B:9:HIS:N	2:B:2010:HOH:O	1.85	1.09
1:B:142:ALA:O	2:B:2208:HOH:O	1.65	1.09
1:A:177:PHE:CB	2:A:2200:HOH:O	2.01	1.08
1:B:72:TRP:CD1	2:B:2120:HOH:O	2.02	1.08
1:B:177:PHE:N	2:B:2244:HOH:O	1.84	1.07
1:B:46:VAL:HA	2:B:2078:HOH:O	1.52	1.07
1:A:109:TRP:CZ3	2:A:2129:HOH:O	2.05	1.06
1:A:192:LEU:HD12	2:A:2216:HOH:O	1.55	1.06
1:B:122:GLN:CD	2:B:2195:HOH:O	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:O	2:A:2048:HOH:O	1.74	1.06
1:A:49:ASN:CA	2:A:2066:HOH:O	1.80	1.06
1:B:98:SER:O	2:B:2159:HOH:O	1.72	1.06
1:A:28:LEU:O	2:A:2034:HOH:O	1.74	1.05
1:B:176:GLY:C	2:B:2244:HOH:O	2.00	1.05
1:A:165:PHE:HA	2:A:2185:HOH:O	1.55	1.05
1:A:170:ARG:HB2	2:A:2192:HOH:O	1.57	1.04
2:A:2207:HOH:O	1:B:56:TYR:CD2	2.09	1.04
1:B:142:ALA:HB1	2:B:2207:HOH:O	1.57	1.04
1:B:191:PRO:O	2:B:2264:HOH:O	1.76	1.04
1:B:105:PHE:C	2:B:2172:HOH:O	1.96	1.03
1:B:8:HIS:HD2	2:B:2010:HOH:O	1.41	1.03
1:B:104:GLY:CA	2:B:2169:HOH:O	1.72	1.03
1:A:113:ASP:CG	2:A:2143:HOH:O	2.00	1.03
1:A:165:PHE:CA	2:A:2185:HOH:O	2.07	1.03
1:B:104:GLY:O	2:B:2168:HOH:O	1.77	1.03
1:B:106:TRP:CD2	2:B:2172:HOH:O	1.98	1.03
1:B:80:GLU:O	2:B:2129:HOH:O	1.75	1.03
1:A:165:PHE:O	2:A:2185:HOH:O	1.76	1.02
1:A:9:HIS:CD2	2:A:2006:HOH:O	2.12	1.02
1:A:28:LEU:HB2	2:A:2032:HOH:O	1.60	1.01
1:A:63:GLN:HB2	2:A:2078:HOH:O	1.59	1.01
1:B:168:PRO:O	2:B:2236:HOH:O	1.77	1.01
1:B:66:SER:O	2:B:2113:HOH:O	1.79	1.01
1:A:114:SER:HA	2:A:2145:HOH:O	1.52	1.01
1:A:46:VAL:CG1	2:A:2058:HOH:O	2.00	1.00
1:A:86:VAL:HB	2:A:2189:HOH:O	0.82	1.00
1:A:47:SER:N	2:A:2060:HOH:O	1.95	1.00
1:B:51:GLU:N	2:B:2089:HOH:O	1.93	1.00
1:B:9:HIS:CB	2:B:2009:HOH:O	1.99	1.00
1:A:158:TYR:CE1	2:A:2175:HOH:O	2.14	0.99
1:B:44:GLN:HB2	2:B:2051:HOH:O	1.62	0.99
1:B:97:PHE:HB2	2:B:2160:HOH:O	1.47	0.99
1:B:160:PHE:CA	2:B:2221:HOH:O	1.66	0.98
1:B:158:TYR:CZ	2:B:2216:HOH:O	2.00	0.98
1:B:20:ASP:HA	2:B:2035:HOH:O	1.61	0.98
1:A:172:PHE:HB2	2:A:2190:HOH:O	1.63	0.98
1:B:78:GLN:CG	2:B:2126:HOH:O	2.09	0.98
1:B:9:HIS:CG	2:B:2006:HOH:O	2.16	0.98
1:B:140:TYR:C	2:B:2202:HOH:O	1.72	0.97
1:A:180:SER:O	2:A:2209:HOH:O	1.81	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD12	2:A:2032:HOH:O	1.61	0.97
1:A:60:LEU:HD22	2:A:2192:HOH:O	1.65	0.97
1:A:158:TYR:CZ	2:A:2175:HOH:O	2.18	0.96
1:A:165:PHE:HB2	2:A:2167:HOH:O	1.65	0.96
1:B:30:ILE:CB	2:B:2052:HOH:O	2.13	0.95
1:B:142:ALA:CA	2:B:2206:HOH:O	2.08	0.95
1:B:10:HIS:HB2	2:B:2001:HOH:O	1.65	0.95
1:B:31:SER:OG	2:B:2054:HOH:O	1.84	0.95
1:B:73:GLU:OE2	2:B:2122:HOH:O	1.83	0.95
1:B:51:GLU:CA	2:B:2089:HOH:O	2.14	0.95
1:B:78:GLN:CD	2:B:2126:HOH:O	2.10	0.94
1:B:140:TYR:CE2	2:B:2204:HOH:O	2.20	0.94
1:B:12:HIS:CE1	2:B:2018:HOH:O	2.21	0.94
1:B:30:ILE:HG22	2:B:2052:HOH:O	1.65	0.94
1:B:100:SER:HB2	2:B:2162:HOH:O	1.67	0.94
1:B:133:GLN:NE2	2:B:2200:HOH:O	1.96	0.94
1:B:51:GLU:CG	2:B:2089:HOH:O	2.14	0.94
1:B:8:HIS:CD2	2:B:2010:HOH:O	2.16	0.93
1:A:12:HIS:CD2	2:A:2012:HOH:O	2.06	0.93
1:B:142:ALA:CB	2:B:2206:HOH:O	1.85	0.93
1:A:139:ASP:C	2:A:2166:HOH:O	2.06	0.92
1:B:140:TYR:CZ	2:B:2204:HOH:O	2.21	0.92
1:A:160:PHE:HE1	2:A:2127:HOH:O	1.51	0.92
1:B:34:ARG:CG	2:B:2042:HOH:O	1.75	0.91
1:B:78:GLN:OE1	2:B:2126:HOH:O	1.87	0.91
1:A:44:GLN:HB2	2:A:2053:HOH:O	1.69	0.91
1:B:190:CYS:SG	2:B:2200:HOH:O	2.21	0.91
1:A:49:ASN:HB2	2:A:2066:HOH:O	1.43	0.91
1:A:177:PHE:HD1	2:A:2200:HOH:O	1.41	0.91
1:B:133:GLN:CG	2:B:2200:HOH:O	2.07	0.91
1:B:68:GLY:CA	2:B:2116:HOH:O	2.11	0.90
1:A:24:ALA:HB1	2:A:2032:HOH:O	1.72	0.90
1:B:12:HIS:HE1	2:B:2020:HOH:O	1.55	0.90
1:B:65:PHE:O	2:B:2110:HOH:O	1.91	0.89
1:A:8:HIS:HD2	1:A:10:HIS:H	1.12	0.89
1:B:176:GLY:CA	2:B:2244:HOH:O	2.19	0.89
1:B:98:SER:C	2:B:2159:HOH:O	2.13	0.88
1:B:114:SER:HB2	2:B:2183:HOH:O	1.72	0.88
1:B:27:TRP:CG	2:B:2073:HOH:O	2.12	0.88
1:A:160:PHE:CE1	2:A:2127:HOH:O	2.26	0.88
1:A:124:THR:O	2:A:2156:HOH:O	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PHE:HA	2:B:2160:HOH:O	1.35	0.88
1:B:99:LEU:HD11	2:B:2131:HOH:O	1.71	0.88
1:B:21:ARG:O	1:B:52:ARG:NH2	2.07	0.87
1:B:140:TYR:CE2	2:B:2110:HOH:O	2.21	0.87
1:B:142:ALA:N	2:B:2206:HOH:O	2.08	0.87
1:A:27:TRP:C	2:A:2035:HOH:O	2.04	0.87
1:B:9:HIS:NE2	2:B:2008:HOH:O	2.01	0.87
1:B:34:ARG:CD	2:B:2042:HOH:O	2.07	0.86
1:A:63:GLN:OE1	2:A:2078:HOH:O	1.90	0.86
1:B:46:VAL:CA	2:B:2078:HOH:O	2.12	0.86
1:A:15:VAL:C	2:A:2015:HOH:O	2.18	0.86
1:A:113:ASP:CB	2:A:2140:HOH:O	1.99	0.86
1:B:12:HIS:CE1	2:B:2020:HOH:O	2.27	0.86
1:A:165:PHE:C	2:A:2185:HOH:O	2.15	0.85
1:B:133:GLN:HG2	2:B:2200:HOH:O	1.73	0.85
1:B:9:HIS:ND1	2:B:2006:HOH:O	2.10	0.85
1:B:106:TRP:NE1	2:B:2171:HOH:O	2.09	0.85
1:A:42:THR:CG2	2:A:2054:HOH:O	1.98	0.84
1:B:163:CYS:HB3	2:B:2171:HOH:O	1.77	0.84
1:B:160:PHE:CG	2:B:2219:HOH:O	2.29	0.84
1:B:162:GLU:HB2	2:B:2222:HOH:O	1.78	0.84
1:B:176:GLY:HA2	2:B:2244:HOH:O	1.75	0.84
1:B:158:TYR:CE2	2:B:2216:HOH:O	2.24	0.83
1:A:172:PHE:N	2:A:2190:HOH:O	2.12	0.83
1:A:99:LEU:CD1	2:A:2129:HOH:O	2.27	0.83
1:A:65:PHE:O	2:A:2188:HOH:O	1.97	0.83
1:B:20:ASP:N	2:B:2039:HOH:O	2.11	0.83
1:A:20:ASP:OD2	2:A:2026:HOH:O	1.97	0.82
1:A:177:PHE:HA	2:A:2200:HOH:O	1.77	0.82
1:B:78:GLN:HG2	2:B:2126:HOH:O	1.73	0.82
1:B:36:GLN:HG3	2:B:2053:HOH:O	1.78	0.82
1:A:190:CYS:O	2:A:2216:HOH:O	1.97	0.82
1:A:140:TYR:CA	2:A:2166:HOH:O	2.25	0.81
1:A:177:PHE:HB3	2:A:2200:HOH:O	1.72	0.81
1:B:139:ASP:O	2:B:2210:HOH:O	1.98	0.81
1:A:57:PRO:HD2	2:A:2193:HOH:O	1.80	0.81
1:A:177:PHE:CA	2:A:2200:HOH:O	2.21	0.81
1:B:15:VAL:CG1	2:B:2029:HOH:O	2.20	0.81
1:A:172:PHE:CB	2:A:2190:HOH:O	2.24	0.81
1:A:192:LEU:N	2:A:2217:HOH:O	2.12	0.81
1:B:11:HIS:ND1	2:B:2003:HOH:O	2.05	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PHE:O	2:B:2226:HOH:O	1.96	0.81
1:B:163:CYS:CB	2:B:2171:HOH:O	2.28	0.80
1:A:35:ARG:NE	2:A:2018:HOH:O	2.15	0.80
1:A:114:SER:HB2	2:A:2145:HOH:O	1.61	0.80
1:B:27:TRP:CE3	2:B:2073:HOH:O	2.20	0.80
1:B:57:PRO:HG2	2:B:2244:HOH:O	1.80	0.80
1:A:159:THR:C	2:A:2177:HOH:O	2.14	0.80
1:B:91:VAL:O	2:B:2148:HOH:O	1.99	0.80
1:B:192:LEU:HA	2:B:2264:HOH:O	1.81	0.80
1:A:15:VAL:O	2:A:2015:HOH:O	2.00	0.80
1:B:169:LEU:HD23	2:B:2236:HOH:O	1.81	0.79
1:B:42:THR:C	2:B:2073:HOH:O	2.25	0.79
1:A:99:LEU:HD12	2:A:2129:HOH:O	1.83	0.78
1:A:188:LYS:HG2	2:A:2044:HOH:O	1.81	0.78
1:A:170:ARG:O	2:A:2190:HOH:O	2.00	0.78
1:A:170:ARG:CB	2:A:2192:HOH:O	2.21	0.78
1:B:57:PRO:O	2:B:2098:HOH:O	2.01	0.78
1:A:32:LYS:HE2	2:A:2039:HOH:O	1.82	0.78
1:B:46:VAL:C	2:B:2078:HOH:O	2.14	0.78
1:B:91:VAL:CG1	2:B:2168:HOH:O	2.15	0.78
1:B:122:GLN:HB2	2:B:2188:HOH:O	1.84	0.77
1:B:72:TRP:HD1	2:B:2120:HOH:O	1.51	0.77
1:B:165:PHE:CD2	2:B:2204:HOH:O	2.30	0.77
1:B:101:PRO:HG3	2:B:2170:HOH:O	1.83	0.77
1:B:8:HIS:HD2	1:B:10:HIS:H	1.32	0.77
1:A:87:CYS:O	2:A:2191:HOH:O	2.03	0.76
1:A:171:PRO:C	2:A:2190:HOH:O	2.27	0.76
1:B:46:VAL:HB	2:B:2090:HOH:O	1.84	0.76
1:B:13:HIS:CE1	2:B:2024:HOH:O	2.12	0.76
1:A:28:LEU:C	2:A:2034:HOH:O	2.24	0.75
1:A:141:GLU:OE1	2:A:2168:HOH:O	2.03	0.75
1:B:191:PRO:C	2:B:2264:HOH:O	2.21	0.75
1:B:8:HIS:C	2:B:2010:HOH:O	2.25	0.75
1:B:12:HIS:ND1	2:B:2022:HOH:O	1.91	0.74
1:B:11:HIS:ND1	2:B:2013:HOH:O	1.99	0.74
1:A:179:TYR:CZ	2:A:2206:HOH:O	2.25	0.74
1:B:50:LYS:NZ	2:B:2083:HOH:O	2.20	0.74
1:A:184:ALA:HA	2:A:2196:HOH:O	1.89	0.73
1:B:91:VAL:HB	2:B:2144:HOH:O	1.88	0.73
1:B:26:SER:O	2:B:2047:HOH:O	2.07	0.73
1:B:66:SER:HB3	2:B:2113:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HB3	2:B:2262:HOH:O	1.87	0.72
1:B:71:TYR:HE1	2:B:2122:HOH:O	1.70	0.72
1:B:98:SER:N	2:B:2160:HOH:O	2.19	0.72
1:B:114:SER:CB	2:B:2183:HOH:O	2.32	0.72
1:A:126:HIS:NE2	2:A:2156:HOH:O	2.22	0.72
1:B:158:TYR:HE1	2:B:2215:HOH:O	1.45	0.72
1:A:160:PHE:N	2:A:2179:HOH:O	2.22	0.72
1:A:35:ARG:CZ	2:A:2018:HOH:O	2.37	0.71
1:B:22:ASN:OD1	2:B:2045:HOH:O	2.07	0.71
1:B:30:ILE:HB	2:B:2052:HOH:O	1.83	0.71
1:B:106:TRP:CE2	2:B:2171:HOH:O	2.43	0.71
1:B:168:PRO:C	2:B:2236:HOH:O	2.22	0.71
1:B:163:CYS:SG	2:B:2231:HOH:O	2.28	0.71
1:A:21:ARG:N	2:A:2030:HOH:O	2.25	0.70
1:A:164:VAL:O	2:A:2103:HOH:O	2.08	0.70
1:A:174:ASN:ND2	2:A:2193:HOH:O	2.17	0.70
1:A:109:TRP:HZ3	2:A:2129:HOH:O	1.52	0.70
1:A:112:GLN:HB3	2:A:2134:HOH:O	1.90	0.70
1:A:140:TYR:HA	2:A:2166:HOH:O	1.88	0.70
1:B:179:TYR:OH	2:B:2251:HOH:O	2.04	0.70
1:B:30:ILE:CG2	2:B:2052:HOH:O	2.20	0.69
1:B:21:ARG:CG	2:B:2036:HOH:O	1.95	0.69
1:A:46:VAL:C	2:A:2060:HOH:O	2.31	0.69
1:A:131:PRO:CB	2:A:2164:HOH:O	1.95	0.68
1:B:141:GLU:OE2	2:B:2205:HOH:O	2.11	0.68
1:A:43:HIS:CE1	2:A:2052:HOH:O	2.46	0.68
1:A:178:ASN:HB3	2:A:2199:HOH:O	1.94	0.68
1:B:117:ALA:C	2:B:2192:HOH:O	2.22	0.68
1:A:106:TRP:HH2	2:A:2103:HOH:O	1.77	0.68
1:B:21:ARG:CZ	2:B:2042:HOH:O	2.42	0.68
1:B:21:ARG:N	2:B:2039:HOH:O	2.08	0.68
1:B:38:ARG:NH2	2:B:2067:HOH:O	2.06	0.67
1:B:142:ALA:CB	2:B:2208:HOH:O	2.38	0.67
1:A:50:LYS:HG3	2:A:2064:HOH:O	1.93	0.67
1:A:19:LEU:O	2:A:2024:HOH:O	2.12	0.67
1:A:34:ARG:CD	2:A:2024:HOH:O	2.11	0.67
1:A:69:LYS:HD3	2:A:2014:HOH:O	1.94	0.67
1:A:99:LEU:CB	2:A:2129:HOH:O	2.43	0.67
1:A:44:GLN:CD	2:A:2054:HOH:O	2.28	0.66
1:B:19:LEU:C	2:B:2039:HOH:O	2.39	0.66
1:B:176:GLY:HA2	2:B:2240:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:HIS:N	2:A:2007:HOH:O	1.77	0.66
1:A:28:LEU:CD1	2:A:2032:HOH:O	2.31	0.66
1:B:163:CYS:CA	2:B:2171:HOH:O	2.43	0.65
1:A:28:LEU:CA	2:A:2035:HOH:O	2.29	0.65
1:A:8:HIS:HE1	2:A:2091:HOH:O	1.78	0.65
1:B:17:ILE:HD11	2:B:2029:HOH:O	1.96	0.65
1:B:46:VAL:N	2:B:2076:HOH:O	2.21	0.65
1:B:51:GLU:HG2	2:B:2089:HOH:O	1.88	0.65
1:A:28:LEU:CG	2:A:2032:HOH:O	2.43	0.64
1:A:67:SER:O	2:A:2089:HOH:O	0.65	0.64
1:B:112:GLN:CB	2:B:2177:HOH:O	2.42	0.64
2:A:2207:HOH:O	1:B:56:TYR:CE2	2.41	0.64
1:A:28:LEU:HG	2:A:2035:HOH:O	1.96	0.64
1:A:108:ILE:CG2	2:A:2127:HOH:O	2.45	0.64
1:A:174:ASN:OD1	2:A:2193:HOH:O	2.15	0.64
1:B:32:LYS:O	2:B:2058:HOH:O	2.15	0.64
1:A:183:ASN:HB2	2:A:2098:HOH:O	1.98	0.64
1:B:10:HIS:HE1	1:B:148:TYR:OH	1.80	0.64
1:B:71:TYR:CD2	2:B:2001:HOH:O	2.51	0.63
1:B:9:HIS:HB2	2:B:2009:HOH:O	1.81	0.63
1:A:80:GLU:N	2:A:2098:HOH:O	2.25	0.63
1:B:11:HIS:CE1	2:B:2003:HOH:O	2.13	0.63
1:B:15:VAL:HG23	2:B:2027:HOH:O	1.98	0.63
1:A:103:ASN:CG	2:A:2125:HOH:O	2.41	0.63
1:A:108:ILE:HG23	2:A:2127:HOH:O	1.99	0.62
1:B:142:ALA:HB1	2:B:2208:HOH:O	1.95	0.62
1:A:9:HIS:NE2	2:A:2006:HOH:O	2.24	0.62
1:B:160:PHE:CA	2:B:2219:HOH:O	2.47	0.62
1:A:38:ARG:HD2	2:A:2046:HOH:O	1.98	0.62
1:A:10:HIS:HE1	1:A:148:TYR:OH	1.82	0.62
1:A:99:LEU:HB2	2:A:2129:HOH:O	2.00	0.61
1:A:183:ASN:CB	2:A:2098:HOH:O	2.47	0.61
1:A:28:LEU:CB	2:A:2032:HOH:O	2.31	0.61
1:A:8:HIS:CD2	1:A:10:HIS:H	2.05	0.61
1:B:58:MET:HA	2:B:2098:HOH:O	2.00	0.61
1:B:38:ARG:NE	2:B:2067:HOH:O	2.30	0.61
1:A:126:HIS:CE1	2:A:2156:HOH:O	2.54	0.61
1:A:80:GLU:CB	2:A:2098:HOH:O	2.04	0.61
1:A:109:TRP:CE3	2:A:2129:HOH:O	2.45	0.61
1:B:169:LEU:CA	2:B:2236:HOH:O	1.76	0.61
1:A:28:LEU:CG	2:A:2035:HOH:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:HB3	2:A:2194:HOH:O	2.00	0.60
1:B:8:HIS:NE2	2:B:2001:HOH:O	2.31	0.60
1:B:9:HIS:CD2	2:B:2008:HOH:O	2.50	0.60
1:B:68:GLY:HA3	2:B:2116:HOH:O	1.85	0.60
1:B:83:ASP:HB2	2:B:2131:HOH:O	2.01	0.60
1:A:184:ALA:CA	2:A:2196:HOH:O	2.47	0.60
1:A:57:PRO:HD2	2:A:2194:HOH:O	2.02	0.59
1:B:177:PHE:O	2:B:2245:HOH:O	2.11	0.59
1:B:163:CYS:HA	2:B:2171:HOH:O	2.02	0.59
1:A:32:LYS:CE	2:A:2039:HOH:O	2.46	0.59
1:A:112:GLN:HA	2:A:2138:HOH:O	2.02	0.59
1:A:38:ARG:CD	2:A:2046:HOH:O	2.51	0.58
1:A:38:ARG:NH2	2:A:2047:HOH:O	2.36	0.58
1:A:53:PHE:CD1	2:A:2072:HOH:O	2.56	0.58
1:B:189:LEU:HD21	2:B:2120:HOH:O	2.04	0.58
1:B:160:PHE:HA	2:B:2219:HOH:O	2.04	0.58
1:B:11:HIS:CG	2:B:2003:HOH:O	2.55	0.57
1:B:46:VAL:CG2	2:B:2090:HOH:O	2.53	0.57
1:A:21:ARG:CA	2:A:2030:HOH:O	2.53	0.56
1:A:131:PRO:HG2	2:A:2164:HOH:O	2.01	0.56
1:A:174:ASN:CG	2:A:2193:HOH:O	2.45	0.56
1:B:88:ARG:HA	2:B:2236:HOH:O	2.05	0.56
1:B:51:GLU:HG3	2:B:2089:HOH:O	1.93	0.56
1:B:9:HIS:CE1	2:B:2006:HOH:O	2.53	0.56
1:B:80:GLU:CA	2:B:2129:HOH:O	2.53	0.56
1:B:163:CYS:HA	2:B:2231:HOH:O	2.06	0.56
1:B:9:HIS:HB3	2:B:2009:HOH:O	1.87	0.55
1:B:112:GLN:CB	2:B:2176:HOH:O	2.53	0.55
1:B:19:LEU:O	2:B:2035:HOH:O	2.13	0.55
1:B:120:SER:HB3	2:B:2162:HOH:O	2.06	0.55
1:B:163:CYS:CA	2:B:2231:HOH:O	2.54	0.55
1:B:172:PHE:CE2	2:B:2131:HOH:O	2.53	0.55
1:B:144:VAL:N	2:B:2210:HOH:O	2.40	0.55
1:A:10:HIS:N	2:A:2007:HOH:O	2.40	0.54
1:A:140:TYR:CE1	2:A:2167:HOH:O	2.34	0.54
1:A:179:TYR:HE2	2:A:2206:HOH:O	1.58	0.54
1:B:188:LYS:CE	2:B:2260:HOH:O	2.54	0.54
1:B:36:GLN:CD	2:B:2066:HOH:O	2.51	0.54
1:B:15:VAL:CB	2:B:2029:HOH:O	1.97	0.54
1:A:188:LYS:CB	2:A:2044:HOH:O	2.55	0.54
1:B:22:ASN:CG	2:B:2045:HOH:O	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:HIS:HA	2:A:2015:HOH:O	2.07	0.54
1:A:181:GLY:HA3	2:A:2210:HOH:O	2.09	0.53
1:B:106:TRP:CZ2	2:B:2171:HOH:O	2.62	0.53
1:B:86:VAL:HG11	1:B:138:VAL:HG21	1.90	0.53
1:B:84:LEU:HD12	1:B:134:ILE:HD13	1.90	0.53
1:B:189:LEU:CD2	2:B:2120:HOH:O	2.56	0.53
1:A:21:ARG:HA	2:A:2030:HOH:O	2.09	0.53
1:A:86:VAL:CB	2:A:2189:HOH:O	1.69	0.53
1:B:92:GLN:HG2	2:B:2145:HOH:O	2.09	0.52
1:A:172:PHE:CA	2:A:2190:HOH:O	2.45	0.52
1:B:165:PHE:CG	2:B:2204:HOH:O	2.25	0.52
1:A:16:HIS:CA	2:A:2015:HOH:O	2.58	0.52
1:B:112:GLN:HB3	2:B:2177:HOH:O	2.08	0.52
1:A:128:GLN:CD	2:A:2162:HOH:O	2.53	0.51
1:A:96:GLN:NE2	1:B:25:ASN:HD21	2.09	0.51
1:B:8:HIS:N	2:B:2004:HOH:O	2.43	0.51
1:B:172:PHE:HE2	2:B:2131:HOH:O	1.91	0.51
1:B:14:MET:HE1	2:B:2264:HOH:O	2.08	0.51
1:B:68:GLY:C	2:B:2116:HOH:O	2.49	0.50
1:A:16:HIS:CD2	2:A:2018:HOH:O	2.46	0.50
1:A:53:PHE:CG	2:A:2072:HOH:O	2.33	0.50
1:B:112:GLN:HB2	2:B:2176:HOH:O	2.11	0.50
1:A:86:VAL:HG11	1:A:138:VAL:HG21	1.93	0.50
1:B:67:SER:HB3	2:B:2115:HOH:O	2.11	0.50
1:B:43:HIS:CG	2:B:2047:HOH:O	2.62	0.50
1:A:113:ASP:CG	2:A:2140:HOH:O	2.45	0.50
1:B:112:GLN:HB3	2:B:2176:HOH:O	2.12	0.50
1:B:12:HIS:CE1	2:B:2022:HOH:O	2.50	0.49
1:B:43:HIS:CA	2:B:2047:HOH:O	1.82	0.49
1:B:72:TRP:CH2	1:B:86:VAL:HG12	2.48	0.49
1:B:122:GLN:CG	2:B:2195:HOH:O	2.48	0.49
1:B:171:PRO:HB3	2:B:2121:HOH:O	2.12	0.49
1:B:127:ILE:HG21	1:B:131:PRO:HD3	1.94	0.49
1:A:161:SER:O	2:A:2181:HOH:O	2.19	0.49
1:B:161:SER:CB	2:B:2223:HOH:O	2.38	0.49
1:A:25:ASN:O	2:A:2032:HOH:O	2.20	0.48
1:A:47:SER:OG	2:A:2061:HOH:O	2.02	0.48
1:A:160:PHE:HZ	2:A:2130:HOH:O	1.95	0.48
1:B:77:THR:O	1:B:78:GLN:HB2	2.13	0.48
1:B:52:ARG:NH1	2:B:2091:HOH:O	0.64	0.48
1:B:46:VAL:HG23	2:B:2090:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:HIS:HB3	2:A:2005:HOH:O	2.13	0.47
1:A:78:GLN:NE2	2:A:2095:HOH:O	2.02	0.47
1:B:71:TYR:CE2	2:B:2001:HOH:O	2.66	0.47
1:B:32:LYS:NZ	2:B:2055:HOH:O	2.46	0.47
1:B:10:HIS:CB	2:B:2001:HOH:O	2.41	0.47
1:B:99:LEU:CD1	2:B:2131:HOH:O	2.47	0.47
1:B:172:PHE:CZ	2:B:2131:HOH:O	2.66	0.47
1:A:24:ALA:O	1:A:52:ARG:NE	2.47	0.47
1:A:63:GLN:CB	2:A:2078:HOH:O	2.38	0.47
1:B:180:SER:C	2:B:2256:HOH:O	2.58	0.47
1:B:52:ARG:CZ	2:B:2090:HOH:O	2.33	0.46
1:B:34:ARG:HD3	2:B:2042:HOH:O	1.90	0.46
1:A:11:HIS:CB	2:A:2007:HOH:O	2.62	0.46
1:B:71:TYR:CG	2:B:2001:HOH:O	2.65	0.46
1:A:86:VAL:CA	2:A:2189:HOH:O	2.32	0.46
1:A:108:ILE:HG22	2:A:2127:HOH:O	2.12	0.46
1:B:46:VAL:CB	2:B:2090:HOH:O	2.50	0.46
1:A:161:SER:C	2:A:2181:HOH:O	2.58	0.45
1:B:50:LYS:C	2:B:2089:HOH:O	2.49	0.45
1:B:66:SER:HA	2:B:2110:HOH:O	2.16	0.45
1:B:57:PRO:CG	2:B:2244:HOH:O	2.53	0.45
1:A:9:HIS:C	2:A:2007:HOH:O	2.60	0.44
1:B:67:SER:CB	2:B:2115:HOH:O	2.50	0.44
1:A:46:VAL:HG13	2:A:2058:HOH:O	1.95	0.44
1:A:69:LYS:CD	2:A:2014:HOH:O	2.60	0.44
1:A:133:GLN:NE2	2:A:2165:HOH:O	2.51	0.44
1:A:188:LYS:NZ	2:A:2213:HOH:O	2.38	0.44
1:A:51:GLU:CG	2:A:2067:HOH:O	2.65	0.44
1:B:140:TYR:HD2	2:B:2110:HOH:O	1.61	0.44
1:B:35:ARG:N	2:B:2054:HOH:O	2.50	0.43
1:A:131:PRO:CG	2:A:2164:HOH:O	2.38	0.43
1:A:192:LEU:HD21	2:A:2015:HOH:O	2.18	0.43
1:B:72:TRP:CZ2	1:B:86:VAL:HG12	2.54	0.43
1:B:188:LYS:NZ	2:B:2260:HOH:O	2.06	0.43
1:B:86:VAL:HG11	1:B:138:VAL:CG2	2.48	0.42
1:B:105:PHE:CA	2:B:2172:HOH:O	2.56	0.42
1:B:82:TRP:CZ2	1:B:134:ILE:HD11	2.54	0.42
1:A:11:HIS:HB2	2:A:2007:HOH:O	2.17	0.42
1:B:57:PRO:CD	2:B:2244:HOH:O	2.68	0.42
1:B:80:GLU:HB3	2:B:2129:HOH:O	2.19	0.42
1:B:83:ASP:CB	2:B:2131:HOH:O	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:HG3	2:A:2067:HOH:O	2.19	0.42
1:B:51:GLU:HA	2:B:2089:HOH:O	1.95	0.42
1:A:188:LYS:CG	2:A:2044:HOH:O	2.49	0.42
1:A:51:GLU:HG3	2:A:2071:HOH:O	0.50	0.41
1:A:162:GLU:CB	2:A:2181:HOH:O	2.32	0.41
1:B:14:MET:CE	2:B:2264:HOH:O	2.67	0.41
1:B:46:VAL:HG22	2:B:2048:HOH:O	2.20	0.41
1:B:142:ALA:CB	2:B:2207:HOH:O	2.35	0.41
1:A:176:GLY:HA2	2:A:2193:HOH:O	2.21	0.41
1:B:34:ARG:NH1	2:B:2035:HOH:O	2.53	0.41
1:B:79:LYS:CG	1:B:185:ALA:HB3	2.50	0.41
1:B:160:PHE:CD2	2:B:2219:HOH:O	2.68	0.41
1:A:189:LEU:HD11	2:A:2025:HOH:O	2.21	0.40
1:B:42:THR:CA	2:B:2073:HOH:O	2.67	0.40
1:B:79:LYS:HG3	1:B:185:ALA:HB3	2.03	0.40
1:A:57:PRO:HD3	2:A:2077:HOH:O	0.53	0.40
1:A:80:GLU:CA	2:A:2098:HOH:O	2.50	0.40

All (12) 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:2009:HOH:O	2:B:2017:HOH:O[1_554]	1.35	0.85
1:B:180:SER:O	2:B:2055:HOH:O[2_554]	1.39	0.81
1:B:90:SER:CA	2:B:2220:HOH:O[2_444]	1.53	0.67
1:A:14:MET:SD	2:B:2021:HOH:O[1_554]	1.54	0.66
1:B:11:HIS:CD2	2:A:2012:HOH:O[1_556]	1.83	0.37
1:B:90:SER:CA	2:B:2223:HOH:O[2_444]	1.85	0.35
1:B:180:SER:C	2:B:2055:HOH:O[2_554]	1.95	0.25
1:B:11:HIS:CG	2:A:2012:HOH:O[1_556]	2.04	0.16
1:B:123:THR:CG2	2:B:2113:HOH:O[2_454]	2.06	0.14
1:A:192:LEU:O	2:B:2022:HOH:O[1_554]	2.11	0.09
1:B:11:HIS:CB	2:A:2012:HOH:O[1_556]	2.12	0.08
1:A:14:MET:CE	2:B:2021:HOH:O[1_554]	2.14	0.06

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	184/188 (98%)	178 (97%)	5 (3%)	1 (0%)	24	5
1	B	183/188 (97%)	178 (97%)	5 (3%)	0	100	100
All	All	367/376 (98%)	356 (97%)	10 (3%)	1 (0%)	36	15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	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	162/165 (98%)	157 (97%)	5 (3%)	35	5
1	B	163/165 (99%)	161 (99%)	2 (1%)	63	29
All	All	325/330 (98%)	318 (98%)	7 (2%)	45	10

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	44	GLN
1	A	45	ASN
1	A	46	VAL
1	A	125	LEU

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Mol	Chain	Res	Type
1	B	19	LEU
1	B	125	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	10	HIS
1	A	11	HIS
1	A	43	HIS
1	A	63	GLN
1	A	96	GLN
1	A	122	GLN
1	A	133	GLN
1	B	8	HIS
1	B	10	HIS
1	B	13	HIS
1	B	44	GLN
1	B	133	GLN
1	B	153	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	186/188 (98%)	2.70	113 (60%) 0 0	13, 20, 30, 40	0
1	B	185/188 (98%)	1.71	57 (30%) 1 1	10, 15, 22, 26	0
All	All	371/376 (98%)	2.21	170 (45%) 0 0	10, 17, 27, 40	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	VAL	9.8
1	A	44	GLN	8.9
1	A	29	ILE	8.1
1	A	47	SER	7.6
1	A	191	PRO	6.5
1	A	179	TYR	6.4
1	A	192	LEU	6.1
1	A	120	SER	6.1
1	A	48	ASP	6.0
1	A	43	HIS	5.8
1	A	45	ASN	5.8
1	A	41	ASP	5.7
1	A	42	THR	5.7
1	A	15	VAL	5.6
1	B	120	SER	5.5
1	A	153	HIS	5.5
1	A	49	ASN	5.4
1	A	125	LEU	5.0
1	A	175	VAL	4.9
1	B	78	GLN	4.9
1	A	127	ILE	4.9
1	B	127	ILE	4.9
1	B	43	HIS	4.8
1	A	30	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	32	LYS	4.8
1	A	178	ASN	4.7
1	B	153	HIS	4.6
1	A	161	SER	4.6
1	A	181	GLY	4.6
1	B	9	HIS	4.5
1	A	180	SER	4.5
1	A	22	ASN	4.5
1	B	111	TRP	4.5
1	B	113	ASP	4.4
1	A	27	TRP	4.3
1	A	150	ILE	4.3
1	B	124	THR	4.3
1	A	184	ALA	4.3
1	A	177	PHE	4.2
1	A	62	ALA	4.2
1	A	40	GLY	4.1
1	A	189	LEU	4.0
1	B	46	VAL	4.0
1	A	65	PHE	4.0
1	B	48	ASP	4.0
1	A	78	GLN	3.9
1	A	182	GLY	3.9
1	A	53	PHE	3.9
1	B	179	TYR	3.9
1	B	129	VAL	3.9
1	A	17	ILE	3.9
1	A	56	TYR	3.9
1	A	134	ILE	3.8
1	B	126	HIS	3.7
1	A	31	SER	3.7
1	A	50	LYS	3.7
1	A	19	LEU	3.7
1	A	166	ALA	3.7
1	A	26	SER	3.6
1	B	177	PHE	3.5
1	A	121	PRO	3.5
1	B	102	GLU	3.5
1	A	132	CYS	3.5
1	A	23	THR	3.5
1	A	113	ASP	3.5
1	B	47	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	76	VAL	3.4
1	B	15	VAL	3.4
1	A	21	ARG	3.3
1	A	86	VAL	3.3
1	A	157	ILE	3.3
1	B	42	THR	3.3
1	B	128	GLN	3.3
1	B	162	GLU	3.3
1	A	129	VAL	3.3
1	B	180	SER	3.3
1	A	109	TRP	3.2
1	A	126	HIS	3.2
1	B	125	LEU	3.2
1	A	185	ALA	3.2
1	B	121	PRO	3.2
1	A	128	GLN	3.1
1	B	65	PHE	3.0
1	B	45	ASN	3.0
1	A	52	ARG	3.0
1	A	186	PRO	3.0
1	A	11	HIS	3.0
1	B	8	HIS	3.0
1	B	52	ARG	2.9
1	A	7	ALA	2.9
1	A	28	LEU	2.9
1	A	123	THR	2.9
1	A	140	TYR	2.9
1	A	34	ARG	2.9
1	A	131	PRO	2.9
1	B	164	VAL	2.9
1	A	165	PHE	2.9
1	B	134	ILE	2.9
1	B	181	GLY	2.9
1	A	169	LEU	2.8
1	B	19	LEU	2.8
1	B	150	ILE	2.8
1	B	118	GLY	2.8
1	B	175	VAL	2.8
1	A	77	THR	2.8
1	A	124	THR	2.8
1	A	151	THR	2.8
1	A	51	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	57	PRO	2.7
1	B	50	LYS	2.7
1	B	10	HIS	2.7
1	A	36	GLN	2.7
1	B	109	TRP	2.7
1	A	164	VAL	2.7
1	A	64	ARG	2.6
1	A	81	ALA	2.6
1	A	130	PRO	2.6
1	A	24	ALA	2.6
1	A	33	ASP	2.6
1	A	97	PHE	2.6
1	B	21	ARG	2.6
1	A	38	ARG	2.6
1	B	92	GLN	2.6
1	B	112	GLN	2.5
1	A	60	LEU	2.5
1	A	96	GLN	2.5
1	A	115	TYR	2.5
1	A	168	PRO	2.5
1	B	32	LYS	2.5
1	B	191	PRO	2.4
1	A	55	ASN	2.4
1	A	102	GLU	2.4
1	B	178	ASN	2.4
1	B	122	GLN	2.3
1	B	80	GLU	2.3
1	A	25	ASN	2.3
1	B	119	THR	2.3
1	B	192	LEU	2.3
1	A	183	ASN	2.3
1	A	37	VAL	2.3
1	A	91	VAL	2.3
1	B	190	CYS	2.3
1	B	34	ARG	2.2
1	A	142	ALA	2.2
1	A	111	TRP	2.2
1	B	154	GLY	2.2
1	A	187	LEU	2.2
1	A	100	SER	2.2
1	A	158	TYR	2.2
1	A	99	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	137	PHE	2.2
1	A	67	SER	2.2
1	B	98	SER	2.2
1	B	99	LEU	2.1
1	A	20	ASP	2.1
1	A	105	PHE	2.1
1	A	152	ASP	2.1
1	A	35	ARG	2.1
1	A	122	GLN	2.1
1	A	82	TRP	2.1
1	B	81	ALA	2.1
1	A	70	MET	2.1
1	A	154	GLY	2.1
1	A	155	SER	2.1
1	A	110	LEU	2.1
1	A	190	CYS	2.1
1	A	160	PHE	2.1
1	B	67	SER	2.0
1	B	11	HIS	2.0
1	B	131	PRO	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.