



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:25 PM GMT

PDB ID : 1OY5
Title : Crystal structure of tRNA (m1G37) methyltransferase from Aquifex aeolicus
Authors : Liu, J.; Wang, W.; Shin, D.H.; Yokota, H.; Kim, R.; Kim, S.H.; Berkeley
Structural Genomics Center (BSGC)
Deposited on : 2003-04-03
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

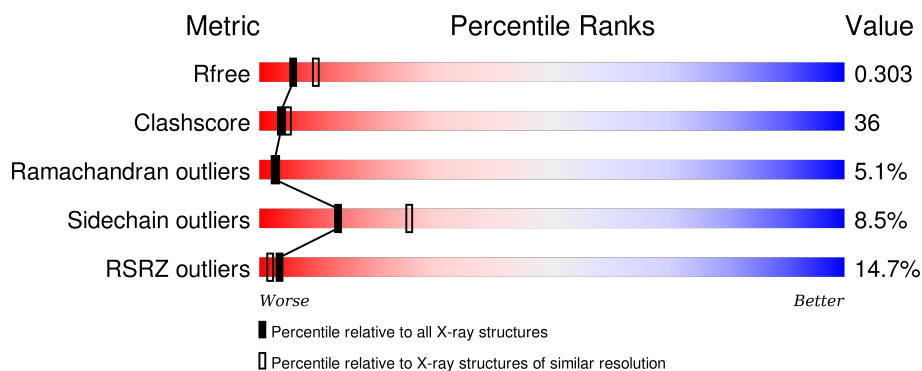
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	257	<div> <div>14%</div> <div>39%</div> <div>36%</div> <div>8%</div> <div>•</div> <div>15%</div> </div>
1	B	257	<div> <div>10%</div> <div>47%</div> <div>29%</div> <div>7%</div> <div>•</div> <div>15%</div> </div>
1	C	257	<div> <div>13%</div> <div>44%</div> <div>30%</div> <div>8%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5379 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 tRNA (Guanine-N(1)-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1768	1155	290	317	6			
1	B	218	Total	C	N	O	S	0	0	0
			1767	1155	289	317	6			
1	C	218	Total	C	N	O	S	0	0	0
			1768	1155	290	317	6			

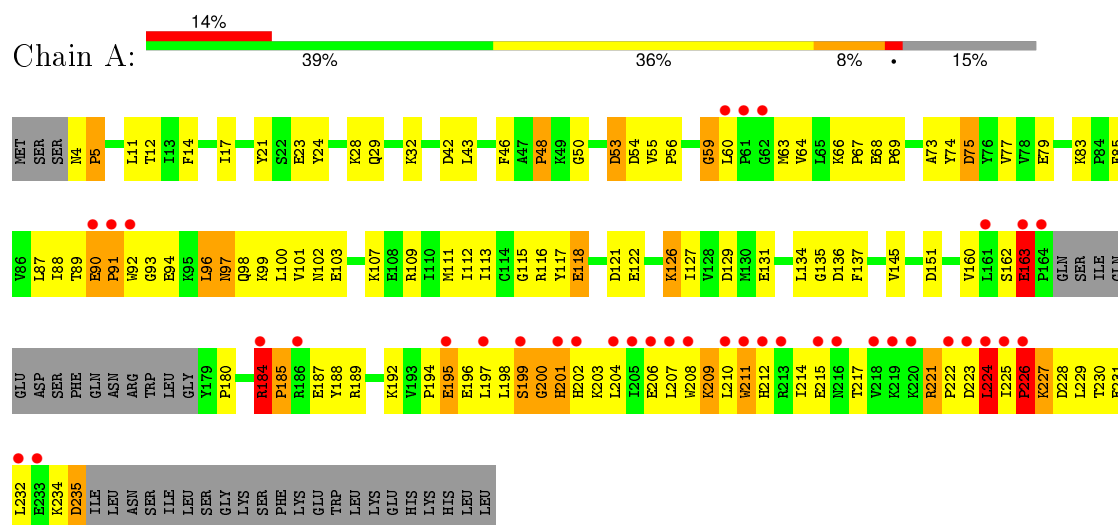
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	21	Total	O	0	0
			21	21		
2	C	32	Total	O	0	0
			32	32		

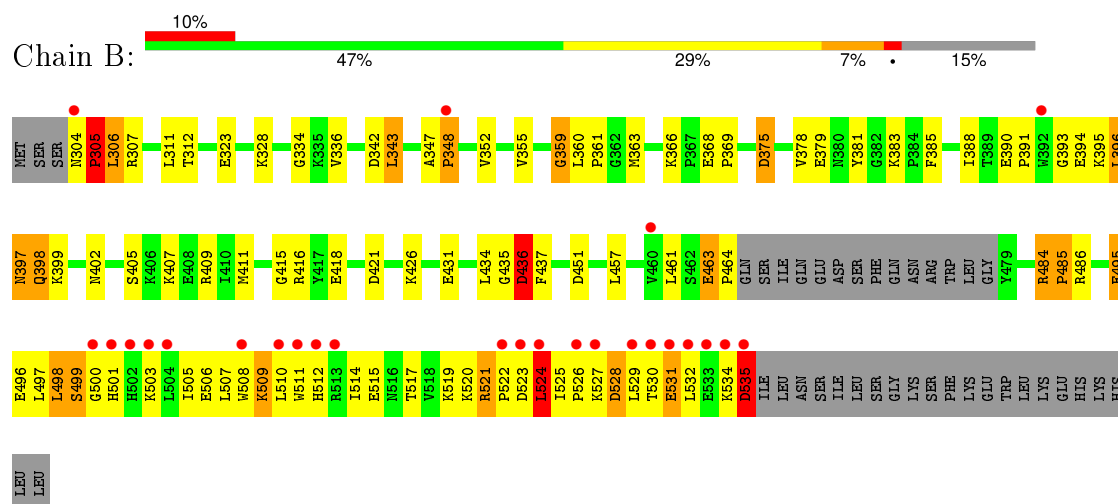
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

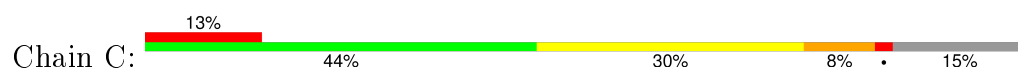
- Molecule 1: tRNA (Guanine-N(1)-)-methyltransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.35Å 96.14Å 57.43Å 90.00° 96.24° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.60) 98.8 (19.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.279 , 0.300 0.278 , 0.303	Depositor DCC
R_{free} test set	1313 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 32020 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5379	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.75	0/1811	1.07	16/2452 (0.7%)
1	B	0.89	1/1810 (0.1%)	0.99	9/2450 (0.4%)
1	C	0.72	0/1811	0.92	11/2452 (0.4%)
All	All	0.79	1/5432 (0.0%)	1.00	36/7354 (0.5%)

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	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	MET	SD-CE	-5.16	1.49	1.77

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ASN	C-N-CD	-20.77	74.92	120.60
1	C	675	ASP	CB-CG-OD2	8.24	125.72	118.30
1	A	4	ASN	C-N-CA	7.77	154.63	122.00
1	B	501	HIS	N-CA-C	-7.47	90.83	111.00
1	B	436	ASP	CB-CG-OD2	7.42	124.98	118.30
1	B	535	ASP	N-CA-CB	7.30	123.74	110.60
1	A	201	HIS	N-CA-C	-6.96	92.22	111.00
1	B	528	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	721	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	435	GLY	N-CA-C	-6.33	97.26	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	751	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	342	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	42	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	226	PRO	N-CA-C	5.99	127.66	112.10
1	A	163	GLU	N-CA-C	5.92	127.00	111.00
1	A	151	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	129	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	121	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	5	PRO	CA-N-CD	-5.53	103.76	111.50
1	B	375	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	799	SER	N-CA-C	-5.51	96.12	111.00
1	A	53	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	729	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	736	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	800	GLY	N-CA-C	5.38	126.55	113.10
1	A	199	SER	N-CA-C	-5.38	96.48	111.00
1	B	421	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	451	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	824	LEU	N-CA-C	5.18	125.00	111.00
1	C	823	ASP	CB-CA-C	-5.16	100.07	110.40
1	A	75	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	184	ARG	N-CA-C	5.09	124.74	111.00
1	A	235	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	42	ASP	CB-CG-OD1	-5.01	113.80	118.30
1	C	835	ASP	CB-CG-OD2	5.00	122.80	118.30
1	C	735	GLY	N-CA-C	-5.00	100.59	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	535	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLU	Peptide

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	1768	0	1818	145	2
1	B	1767	0	1816	108	0
1	C	1768	0	1818	155	2
2	A	23	0	0	1	0
2	B	21	0	0	0	0
2	C	32	0	0	0	0
All	All	5379	0	5452	384	2

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 36.

All (384) 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:C:824:LEU:HD12	1:C:826:PRO:CD	1.57	1.34
1:A:199:SER:O	1:A:203:LYS:HD2	1.42	1.17
1:C:799:SER:OG	1:C:803:LYS:NZ	1.78	1.16
1:B:304:ASN:HB3	1:B:305:PRO:CD	1.77	1.14
1:B:304:ASN:HB3	1:B:305:PRO:HD3	1.22	1.14
1:A:180:PRO:HB3	1:C:722:GLU:HG3	1.32	1.11
1:C:696:LEU:H	1:C:696:LEU:HD23	1.14	1.11
1:C:800:GLY:HA2	1:C:803:LYS:HB2	1.11	1.09
1:A:64:VAL:CG1	1:C:783:THR:HB	1.83	1.08
1:A:200:GLY:CA	1:A:203:LYS:HB2	1.84	1.07
1:A:122:GLU:HG3	1:C:780:PRO:HB3	1.31	1.07
1:A:200:GLY:HA3	1:A:203:LYS:HB2	1.34	1.05
1:C:800:GLY:CA	1:C:803:LYS:HB2	1.86	1.05
1:C:761:LEU:HD22	1:C:764:PRO:HG2	1.37	1.04
1:C:824:LEU:CD1	1:C:826:PRO:HD2	1.86	1.04
1:C:824:LEU:HD12	1:C:826:PRO:CG	1.88	1.03
1:B:500:GLY:HA3	1:B:503:LYS:HB2	1.35	1.02
1:C:824:LEU:HD12	1:C:826:PRO:HD2	1.06	1.02
1:A:96:LEU:HD23	1:A:96:LEU:H	1.20	1.02
1:C:800:GLY:HA2	1:C:803:LYS:CB	1.92	0.99
1:A:211:TRP:O	1:A:215:GLU:HB2	1.64	0.98
1:C:763:GLU:HG3	1:C:763:GLU:O	1.61	0.98
1:B:396:LEU:HD23	1:B:396:LEU:H	1.24	0.98
1:C:811:TRP:O	1:C:815:GLU:HB2	1.66	0.95
1:C:648:PRO:O	1:C:650:GLY:N	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASP:OD1	1:B:436:ASP:N	2.00	0.92
1:A:163:GLU:O	1:A:163:GLU:OE1	1.88	0.91
1:A:98:GLN:O	1:A:102:ASN:ND2	2.03	0.91
1:A:64:VAL:HG11	1:C:783:THR:HB	1.48	0.91
1:A:223:ASP:C	1:A:224:LEU:HD23	1.92	0.90
1:A:135:GLY:O	1:A:136:ASP:HB2	1.72	0.89
1:B:498:LEU:O	1:B:499:SER:HB2	1.69	0.89
1:C:799:SER:OG	1:C:803:LYS:CE	2.21	0.89
1:A:163:GLU:OE1	1:A:163:GLU:C	2.12	0.88
1:C:696:LEU:N	1:C:696:LEU:HD23	1.89	0.87
1:C:832:LEU:HD23	1:C:832:LEU:O	1.74	0.87
1:A:195:GLU:O	1:A:198:LEU:HB2	1.76	0.86
1:B:511:TRP:O	1:B:515:GLU:HB2	1.74	0.85
1:C:823:ASP:O	1:C:824:LEU:HG	1.76	0.84
1:A:122:GLU:CG	1:C:780:PRO:HB3	2.06	0.84
1:A:227:LYS:HG2	1:A:231:GLU:HG2	1.59	0.84
1:C:761:LEU:HD22	1:C:764:PRO:CG	2.07	0.84
1:A:199:SER:OG	1:A:203:LYS:NZ	2.11	0.84
1:C:824:LEU:HD12	1:C:826:PRO:HG2	1.58	0.83
1:C:722:GLU:OE2	1:C:725:LYS:NZ	2.11	0.83
1:B:525:ILE:O	1:B:529:LEU:HG	1.79	0.82
1:A:196:GLU:O	1:A:203:LYS:HD3	1.80	0.81
1:B:434:LEU:H	1:B:434:LEU:HD12	1.45	0.81
1:C:824:LEU:CD1	1:C:826:PRO:CD	2.51	0.80
1:A:97:ASN:HD22	1:A:99:LYS:HB3	1.47	0.79
1:C:824:LEU:CD1	1:C:826:PRO:HG2	2.13	0.79
1:A:97:ASN:ND2	1:A:99:LYS:HB3	1.96	0.78
1:A:197:LEU:HA	1:A:207:LEU:HD22	1.64	0.78
1:A:184:ARG:NH2	1:C:657:TYR:CD2	2.50	0.78
1:A:197:LEU:HA	1:A:207:LEU:CD2	2.14	0.78
1:A:200:GLY:HA2	1:A:203:LYS:HB2	1.65	0.77
1:C:761:LEU:CD2	1:C:764:PRO:HG2	2.12	0.77
1:C:697:ASN:ND2	1:C:699:LYS:HB3	1.99	0.77
1:A:225:ILE:N	1:A:226:PRO:HD2	1.99	0.77
1:C:649:LYS:O	1:C:651:GLN:N	2.18	0.76
1:A:64:VAL:HG13	1:C:783:THR:HB	1.67	0.76
1:A:94:GLU:HG3	1:A:137:PHE:CE1	2.20	0.76
1:B:388:ILE:HG23	1:B:431:GLU:HG3	1.67	0.75
1:A:200:GLY:HA2	1:A:203:LYS:CB	2.16	0.74
1:A:96:LEU:N	1:A:96:LEU:HD23	2.01	0.74
1:A:99:LYS:NZ	1:C:827:LYS:HB3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:LEU:O	1:C:833:GLU:HB2	1.87	0.74
1:B:500:GLY:CA	1:B:503:LYS:HB2	2.15	0.73
1:B:532:LEU:HD23	1:B:532:LEU:O	1.88	0.73
1:A:200:GLY:CA	1:A:203:LYS:CB	2.66	0.73
1:C:763:GLU:HA	1:C:763:GLU:OE1	1.87	0.73
1:A:210:LEU:HG	1:A:214:ILE:HD12	1.71	0.73
1:C:604:ASN:N	1:C:605:PRO:CD	2.52	0.72
1:A:96:LEU:CD2	1:A:96:LEU:H	2.01	0.72
1:A:209:LYS:NZ	1:A:209:LYS:HA	2.05	0.72
1:B:385:PHE:CD2	1:B:407:LYS:HE2	2.24	0.71
1:C:697:ASN:HD21	1:C:699:LYS:HE2	1.56	0.71
1:A:225:ILE:H	1:A:226:PRO:HD2	1.55	0.71
1:A:230:THR:OG1	2:A:265:HOH:O	2.08	0.71
1:C:649:LYS:C	1:C:651:GLN:H	1.94	0.71
1:C:763:GLU:CG	1:C:763:GLU:O	2.36	0.70
1:C:811:TRP:O	1:C:815:GLU:CB	2.39	0.70
1:B:463:GLU:OE1	1:B:463:GLU:O	2.10	0.70
1:C:799:SER:HB2	1:C:802:HIS:HE1	1.56	0.70
1:B:500:GLY:HA2	1:B:503:LYS:HG3	1.73	0.69
1:B:359:GLY:C	1:B:360:LEU:HD22	2.13	0.69
1:C:821:ARG:HB2	1:C:821:ARG:CZ	2.23	0.69
1:B:304:ASN:CB	1:B:305:PRO:CD	2.62	0.68
1:B:521:ARG:N	1:B:522:PRO:CD	2.57	0.68
1:A:68:GLU:HB2	1:A:69:PRO:HD3	1.74	0.68
1:A:75:ASP:O	1:A:79:GLU:HG3	1.94	0.68
1:A:77:VAL:HG21	1:A:111:MET:CE	2.24	0.68
1:B:499:SER:O	1:B:503:LYS:NZ	2.26	0.67
1:A:90:GLU:OE1	1:A:92:TRP:NE1	2.28	0.67
1:B:305:PRO:HG3	1:B:334:GLY:O	1.95	0.67
1:C:824:LEU:HB2	1:C:826:PRO:HD2	1.78	0.66
1:B:388:ILE:CG2	1:B:431:GLU:HG3	2.26	0.65
1:B:532:LEU:HD23	1:B:532:LEU:C	2.16	0.65
1:A:224:LEU:HD23	1:A:224:LEU:N	2.12	0.65
1:C:803:LYS:HB3	1:C:807:LEU:HG	1.79	0.65
1:C:697:ASN:HD22	1:C:699:LYS:HB3	1.61	0.65
1:A:228:ASP:HB3	1:A:232:LEU:HD12	1.78	0.64
1:A:94:GLU:HG3	1:A:137:PHE:CZ	2.32	0.64
1:C:815:GLU:O	1:C:819:LYS:HG3	1.97	0.64
1:B:402:ASN:O	1:B:405:SER:OG	2.11	0.64
1:B:396:LEU:HD23	1:B:396:LEU:N	2.06	0.64
1:B:523:ASP:OD2	1:B:527:LYS:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:CG1	1:C:783:THR:CB	2.71	0.64
1:C:797:LEU:HD21	1:C:810:LEU:HD13	1.80	0.64
1:A:185:PRO:O	1:C:723:ARG:NH1	2.31	0.63
1:A:223:ASP:C	1:A:224:LEU:CD2	2.66	0.63
1:C:784:ARG:O	1:C:785:PRO:C	2.36	0.63
1:A:135:GLY:O	1:A:136:ASP:CB	2.43	0.62
1:A:11:LEU:HD22	1:A:113:ILE:HG12	1.81	0.62
1:B:524:LEU:HD22	1:B:525:ILE:H	1.63	0.62
1:C:784:ARG:O	1:C:786:ARG:N	2.32	0.62
1:C:784:ARG:HE	1:C:784:ARG:HA	1.65	0.61
1:C:788:TYR:CE1	1:C:789:ARG:HG2	2.34	0.61
1:C:647:ALA:O	1:C:648:PRO:O	2.18	0.61
1:A:224:LEU:HG	1:A:226:PRO:HD2	1.82	0.61
1:C:823:ASP:C	1:C:824:LEU:HG	2.20	0.61
1:A:225:ILE:N	1:A:226:PRO:CD	2.63	0.61
1:C:606:LEU:HD12	1:C:607:ARG:N	2.16	0.61
1:B:323:GLU:O	1:B:328:LYS:HD2	2.00	0.61
1:C:761:LEU:HD22	1:C:764:PRO:CD	2.31	0.60
1:A:134:LEU:H	1:A:134:LEU:HD12	1.66	0.60
1:B:497:LEU:HA	1:B:507:LEU:HD22	1.83	0.60
1:B:383:LYS:O	1:B:409:ARG:NH1	2.35	0.60
1:B:509:LYS:HA	1:B:509:LYS:NZ	2.17	0.60
1:A:99:LYS:HZ3	1:C:827:LYS:HB3	1.65	0.60
1:A:185:PRO:HG2	1:C:668:GLU:OE2	2.02	0.60
1:B:503:LYS:HA	1:B:506:GLU:HB3	1.83	0.60
1:C:647:ALA:C	1:C:648:PRO:O	2.35	0.59
1:A:225:ILE:HG23	1:A:229:LEU:HD11	1.84	0.59
1:B:397:ASN:HD22	1:B:399:LYS:HB3	1.67	0.59
1:B:521:ARG:HB2	1:B:521:ARG:CZ	2.33	0.59
1:C:726:LYS:HE3	1:C:726:LYS:HA	1.85	0.59
1:C:696:LEU:H	1:C:696:LEU:CD2	1.95	0.58
1:A:223:ASP:CA	1:A:224:LEU:HD23	2.32	0.58
1:C:832:LEU:CD2	1:C:832:LEU:C	2.72	0.58
1:A:200:GLY:HA2	1:A:203:LYS:HG3	1.84	0.58
1:A:63:MET:O	1:A:117:TYR:HB3	2.04	0.58
1:B:393:GLY:C	1:B:394:GLU:OE1	2.42	0.58
1:A:200:GLY:HA2	1:A:203:LYS:CG	2.34	0.58
1:C:696:LEU:N	1:C:696:LEU:CD2	2.62	0.58
1:C:761:LEU:HD13	1:C:764:PRO:HB2	1.85	0.58
1:B:306:LEU:HD23	1:B:307:ARG:N	2.19	0.58
1:B:534:LYS:O	1:B:535:ASP:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASN:ND2	1:B:399:LYS:HB3	2.19	0.57
1:A:195:GLU:O	1:A:198:LEU:N	2.37	0.57
1:B:375:ASP:O	1:B:379:GLU:HG3	2.03	0.57
1:B:434:LEU:CD1	1:B:434:LEU:H	2.16	0.57
1:C:824:LEU:CG	1:C:826:PRO:HD2	2.35	0.57
1:B:528:ASP:O	1:B:532:LEU:HB3	2.05	0.57
1:A:91:PRO:HD3	1:A:115:GLY:HA3	1.86	0.57
1:B:498:LEU:O	1:B:499:SER:CB	2.47	0.57
1:C:649:LYS:C	1:C:651:GLN:N	2.57	0.57
1:C:823:ASP:C	1:C:824:LEU:CG	2.73	0.56
1:B:500:GLY:HA3	1:B:503:LYS:CB	2.24	0.56
1:A:223:ASP:HB3	1:A:224:LEU:HD23	1.86	0.56
1:A:201:HIS:HA	1:A:204:LEU:HG	1.85	0.56
1:B:499:SER:O	1:B:503:LYS:CD	2.53	0.56
1:C:824:LEU:CD1	1:C:826:PRO:CG	2.69	0.56
1:C:809:LYS:HA	1:C:809:LYS:NZ	2.21	0.56
1:A:208:TRP:HA	1:A:211:TRP:HB2	1.87	0.56
1:C:698:GLN:O	1:C:702:ASN:ND2	2.38	0.56
1:C:832:LEU:C	1:C:832:LEU:HD23	2.26	0.56
1:A:195:GLU:O	1:A:198:LEU:CB	2.53	0.56
1:A:198:LEU:HD21	1:C:657:TYR:CD2	2.41	0.56
1:B:503:LYS:O	1:B:507:LEU:HG	2.06	0.55
1:A:85:PHE:CD2	1:A:107:LYS:HE2	2.41	0.55
1:C:736:ASP:OD1	1:C:736:ASP:N	2.40	0.55
1:A:23:GLU:O	1:A:28:LYS:HD2	2.07	0.55
1:B:499:SER:O	1:B:503:LYS:HG3	2.07	0.55
1:A:99:LYS:HZ1	1:C:827:LYS:HB3	1.72	0.55
1:C:796:GLU:O	1:C:803:LYS:HD3	2.07	0.55
1:C:800:GLY:HA2	1:C:803:LYS:CG	2.36	0.54
1:C:799:SER:HG	1:C:803:LYS:CE	2.18	0.54
1:B:511:TRP:O	1:B:515:GLU:CB	2.53	0.54
1:A:221:ARG:HB2	1:A:221:ARG:CZ	2.37	0.54
1:B:495:GLU:HA	1:B:498:LEU:HD12	1.90	0.54
1:B:515:GLU:O	1:B:519:LYS:HG3	2.08	0.54
1:C:832:LEU:CD2	1:C:832:LEU:O	2.53	0.54
1:B:397:ASN:HD21	1:B:399:LYS:HE2	1.71	0.54
1:B:463:GLU:CD	1:B:463:GLU:O	2.46	0.53
1:A:221:ARG:N	1:A:222:PRO:CD	2.71	0.53
1:C:799:SER:HG	1:C:803:LYS:NZ	2.00	0.53
1:C:796:GLU:O	1:C:803:LYS:CD	2.56	0.53
1:B:394:GLU:HG3	1:B:437:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:LEU:CD2	1:C:810:LEU:HD13	2.38	0.53
1:A:225:ILE:O	1:A:229:LEU:HD13	2.08	0.53
1:C:833:GLU:O	1:C:834:LYS:HB2	2.08	0.53
1:B:484:ARG:O	1:B:486:ARG:N	2.42	0.53
1:B:390:GLU:HB3	1:B:391:PRO:HD2	1.91	0.52
1:C:821:ARG:N	1:C:822:PRO:CD	2.72	0.52
1:C:668:GLU:HB2	1:C:669:PRO:HD3	1.90	0.52
1:C:761:LEU:HD22	1:C:764:PRO:HD2	1.90	0.52
1:B:484:ARG:HA	1:B:484:ARG:HE	1.75	0.52
1:B:355:VAL:HG22	1:B:363:MET:CE	2.40	0.52
1:B:434:LEU:HD12	1:B:434:LEU:N	2.21	0.51
1:A:97:ASN:HD22	1:A:99:LYS:CB	2.19	0.51
1:C:799:SER:O	1:C:803:LYS:HD2	2.10	0.51
1:A:54:ASP:HB3	1:C:783:THR:OG1	2.11	0.51
1:C:688:ILE:HG23	1:C:731:GLU:HG3	1.92	0.51
1:A:46:PHE:O	1:A:48:PRO:HD3	2.10	0.51
1:C:799:SER:HG	1:C:803:LYS:HE2	1.75	0.51
1:C:784:ARG:HB3	1:C:785:PRO:HD3	1.92	0.51
1:A:63:MET:O	1:A:117:TYR:CB	2.59	0.51
1:B:530:THR:O	1:B:531:GLU:HB2	2.10	0.51
1:C:824:LEU:N	1:C:824:LEU:HD23	2.25	0.51
1:A:90:GLU:OE1	1:A:92:TRP:CE2	2.64	0.51
1:B:517:THR:HB	1:B:521:ARG:HH21	1.76	0.51
1:A:29:GLN:NE2	1:A:160:VAL:O	2.44	0.51
1:A:199:SER:C	1:A:203:LYS:HD2	2.25	0.50
1:B:499:SER:O	1:B:503:LYS:HD2	2.11	0.50
1:A:209:LYS:HA	1:A:209:LYS:HZ2	1.75	0.50
1:C:699:LYS:O	1:C:703:GLU:HG3	2.10	0.50
1:C:604:ASN:N	1:C:605:PRO:HD3	2.26	0.50
1:B:523:ASP:O	1:B:524:LEU:HB2	2.11	0.50
1:A:99:LYS:NZ	1:C:827:LYS:CB	2.74	0.50
1:A:53:ASP:OD2	1:A:63:MET:SD	2.69	0.50
1:B:396:LEU:CD2	1:B:396:LEU:H	2.05	0.50
1:A:231:GLU:HA	1:A:234:LYS:HG2	1.94	0.50
1:C:761:LEU:O	1:C:762:SER:C	2.50	0.50
1:A:87:LEU:O	1:A:112:ILE:HA	2.12	0.50
1:C:806:GLU:O	1:C:809:LYS:N	2.39	0.49
1:C:799:SER:HB2	1:C:802:HIS:CE1	2.43	0.49
1:A:54:ASP:OD2	1:C:784:ARG:HB2	2.12	0.49
1:A:68:GLU:HG3	1:C:788:TYR:CE2	2.47	0.49
1:A:73:ALA:O	1:A:77:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:GLY:C	1:C:660:LEU:HD22	2.33	0.49
1:C:675:ASP:O	1:C:679:GLU:HG3	2.11	0.49
1:C:623:GLU:O	1:C:628:LYS:HD2	2.12	0.49
1:C:810:LEU:HD23	1:C:810:LEU:C	2.33	0.49
1:C:823:ASP:C	1:C:824:LEU:HD23	2.33	0.49
1:A:234:LYS:HE2	1:A:234:LYS:N	2.26	0.49
1:A:93:GLY:C	1:A:94:GLU:OE1	2.51	0.49
1:C:693:GLY:C	1:C:694:GLU:OE1	2.51	0.49
1:A:188:TYR:CE1	1:A:189:ARG:HG2	2.48	0.49
1:A:56:PRO:HA	1:C:782:TYR:O	2.13	0.49
1:C:824:LEU:CB	1:C:826:PRO:HD2	2.43	0.48
1:B:505:ILE:O	1:B:509:LYS:HG2	2.13	0.48
1:C:677:VAL:HG21	1:C:711:MET:CE	2.42	0.48
1:B:336:VAL:CG1	1:B:457:LEU:CD1	2.91	0.48
1:B:461:LEU:HD13	1:B:464:PRO:HB2	1.93	0.48
1:C:604:ASN:N	1:C:605:PRO:HD2	2.27	0.48
1:A:59:GLY:C	1:A:60:LEU:HD22	2.34	0.48
1:A:90:GLU:O	1:A:92:TRP:N	2.47	0.48
1:A:228:ASP:HA	1:A:232:LEU:HG	1.95	0.48
1:C:797:LEU:HA	1:C:807:LEU:HD22	1.95	0.48
1:B:385:PHE:CG	1:B:407:LYS:HE2	2.48	0.48
1:B:520:LYS:C	1:B:522:PRO:HD2	2.34	0.48
1:B:500:GLY:CA	1:B:503:LYS:CB	2.88	0.47
1:B:496:GLU:O	1:B:503:LYS:HD2	2.14	0.47
1:B:508:TRP:HA	1:B:511:TRP:HB2	1.96	0.47
1:A:227:LYS:CG	1:A:231:GLU:HG2	2.40	0.47
1:A:228:ASP:HB3	1:A:232:LEU:CD1	2.42	0.47
1:A:223:ASP:CB	1:A:224:LEU:HD23	2.44	0.47
1:A:21:TYR:CZ	1:C:744:ILE:HD11	2.48	0.47
1:A:201:HIS:C	1:A:203:LYS:H	2.18	0.47
1:C:805:ILE:O	1:C:809:LYS:HG2	2.15	0.47
1:C:606:LEU:C	1:C:606:LEU:HD12	2.34	0.47
1:C:795:GLU:N	1:C:795:GLU:OE1	2.48	0.47
1:B:524:LEU:CD2	1:B:525:ILE:H	2.27	0.46
1:A:99:LYS:HG2	1:A:103:GLU:OE2	2.16	0.46
1:C:823:ASP:OD2	1:C:827:LYS:NZ	2.36	0.46
1:B:336:VAL:HG12	1:B:457:LEU:CD1	2.45	0.46
1:C:786:ARG:HH11	1:C:786:ARG:HG2	1.80	0.46
1:B:510:LEU:O	1:B:511:TRP:C	2.52	0.46
1:A:77:VAL:HG21	1:A:111:MET:HE3	1.98	0.46
1:B:495:GLU:HA	1:B:498:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:MET:O	1:B:418:GLU:HG2	2.16	0.46
1:A:90:GLU:CD	1:A:92:TRP:NE1	2.68	0.46
1:B:521:ARG:HH11	1:B:521:ARG:HG3	1.81	0.46
1:C:788:TYR:CE1	1:C:789:ARG:CG	2.99	0.46
1:A:228:ASP:O	1:A:232:LEU:HB2	2.15	0.46
1:C:823:ASP:CG	1:C:827:LYS:HZ1	2.16	0.46
1:C:784:ARG:HE	1:C:784:ARG:CA	2.29	0.46
1:B:521:ARG:N	1:B:522:PRO:HD2	2.30	0.46
1:A:24:TYR:HB3	1:C:614:PHE:CE1	2.51	0.46
1:C:825:ILE:HG23	1:C:829:LEU:HD23	1.98	0.45
1:A:88:ILE:HG23	1:A:131:GLU:HG3	1.99	0.45
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.43	0.45
1:A:14:PHE:HB3	1:A:17:ILE:HD12	1.97	0.45
1:A:43:LEU:HD22	1:A:69:PRO:HB2	1.98	0.45
1:B:311:LEU:HG	1:B:343:LEU:HG	1.98	0.45
1:B:304:ASN:CB	1:B:305:PRO:HD3	2.16	0.45
1:C:799:SER:OG	1:C:803:LYS:HE2	2.11	0.45
1:C:803:LYS:HA	1:C:806:GLU:HB3	1.99	0.45
1:A:90:GLU:OE1	1:A:92:TRP:CZ2	2.69	0.45
1:A:115:GLY:O	1:A:116:ARG:HD2	2.16	0.45
1:C:665:LEU:HD12	1:C:720:VAL:HG22	1.99	0.45
1:C:734:LEU:H	1:C:734:LEU:HD12	1.81	0.45
1:B:395:LYS:O	1:B:395:LYS:HG2	2.17	0.45
1:C:702:ASN:O	1:C:705:SER:OG	2.24	0.45
1:A:64:VAL:HG13	1:C:783:THR:CB	2.40	0.45
1:B:497:LEU:HA	1:B:507:LEU:CD2	2.46	0.45
1:B:484:ARG:HB3	1:B:485:PRO:HD3	2.00	0.44
1:B:355:VAL:HG22	1:B:363:MET:HE2	1.99	0.44
1:B:347:ALA:HB2	1:B:352:VAL:HG12	1.98	0.44
1:C:803:LYS:O	1:C:804:LEU:C	2.56	0.44
1:C:806:GLU:HA	1:C:809:LYS:CG	2.47	0.44
1:A:14:PHE:CB	1:A:17:ILE:HD12	2.47	0.44
1:A:83:LYS:O	1:A:109:ARG:NH1	2.49	0.44
1:B:499:SER:O	1:B:503:LYS:CG	2.64	0.44
1:B:394:GLU:HG3	1:B:437:PHE:CZ	2.52	0.44
1:C:763:GLU:O	1:C:764:PRO:C	2.51	0.44
1:B:415:GLY:C	1:B:416:ARG:HG2	2.39	0.44
1:B:366:LYS:NZ	1:B:368:GLU:OE1	2.47	0.44
1:A:89:THR:HG21	1:A:145:VAL:HG12	2.00	0.44
1:C:683:LYS:O	1:C:709:ARG:NH1	2.51	0.44
1:B:506:GLU:HA	1:B:509:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:O	1:B:510:LEU:C	2.56	0.43
1:C:763:GLU:CA	1:C:763:GLU:OE1	2.59	0.43
1:C:700:LEU:O	1:C:704:LEU:HG	2.18	0.43
1:A:118:GLU:N	1:A:118:GLU:OE2	2.51	0.43
1:A:199:SER:OG	1:A:202:HIS:HE1	2.02	0.43
1:A:94:GLU:CD	1:A:94:GLU:N	2.72	0.43
1:C:793:VAL:HG13	1:C:794:PRO:HD2	1.99	0.43
1:A:126:LYS:HA	1:A:126:LYS:HE3	1.99	0.43
1:A:68:GLU:OE2	1:C:785:PRO:HG2	2.19	0.43
1:B:359:GLY:O	1:B:360:LEU:HD22	2.18	0.43
1:A:196:GLU:C	1:A:198:LEU:H	2.22	0.43
1:C:755:ARG:O	1:C:761:LEU:HD12	2.19	0.43
1:A:229:LEU:N	1:A:229:LEU:HD12	2.34	0.43
1:B:390:GLU:HB3	1:B:391:PRO:CD	2.48	0.43
1:C:663:MET:O	1:C:718:GLU:HG2	2.19	0.43
1:C:788:TYR:CD1	1:C:789:ARG:HG2	2.54	0.42
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.84	0.42
1:A:196:GLU:H	1:A:196:GLU:HG3	1.57	0.42
1:C:761:LEU:O	1:C:762:SER:O	2.36	0.42
1:B:525:ILE:N	1:B:526:PRO:CD	2.82	0.42
1:B:398:GLN:O	1:B:402:ASN:ND2	2.52	0.42
1:B:506:GLU:O	1:B:509:LYS:HB2	2.20	0.42
1:B:484:ARG:HE	1:B:484:ARG:CA	2.32	0.42
1:B:378:VAL:O	1:B:381:TYR:O	2.37	0.42
1:C:812:HIS:O	1:C:814:ILE:N	2.53	0.42
1:B:512:HIS:C	1:B:514:ILE:N	2.72	0.42
1:C:803:LYS:HG2	1:C:806:GLU:OE2	2.20	0.42
1:C:783:THR:HG23	1:C:785:PRO:HD2	2.01	0.42
1:A:208:TRP:O	1:A:212:HIS:CD2	2.73	0.42
1:A:225:ILE:H	1:A:226:PRO:CD	2.25	0.42
1:A:221:ARG:N	1:A:222:PRO:HD3	2.35	0.42
1:B:368:GLU:HB2	1:B:369:PRO:HD3	2.01	0.42
1:A:209:LYS:HA	1:A:209:LYS:HZ3	1.79	0.42
1:C:779:TYR:HB3	1:C:815:GLU:HB2	2.02	0.41
1:C:761:LEU:HA	1:C:761:LEU:HD23	1.74	0.41
1:A:96:LEU:N	1:A:96:LEU:CD2	2.71	0.41
1:C:814:ILE:O	1:C:814:ILE:HG22	2.19	0.41
1:C:787:GLU:CG	1:C:792:LYS:HG2	2.49	0.41
1:A:100:LEU:O	1:A:101:VAL:C	2.57	0.41
1:A:200:GLY:HA2	1:A:203:LYS:N	2.36	0.41
1:C:801:HIS:C	1:C:803:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:LEU:HG	1:B:514:ILE:HD12	2.01	0.41
1:B:535:ASP:OD2	1:B:535:ASP:C	2.58	0.41
1:A:203:LYS:HA	1:A:206:GLU:HB3	2.01	0.41
1:A:115:GLY:C	1:A:116:ARG:HG2	2.40	0.41
1:B:343:LEU:HD22	1:B:369:PRO:HB2	2.01	0.41
1:B:512:HIS:C	1:B:514:ILE:H	2.22	0.41
1:A:212:HIS:O	1:A:214:ILE:N	2.54	0.41
1:A:90:GLU:O	1:A:93:GLY:N	2.41	0.41
1:B:385:PHE:CE2	1:B:407:LYS:HE2	2.55	0.41
1:A:187:GLU:CG	1:A:192:LYS:HG2	2.51	0.41
1:A:180:PRO:CB	1:C:722:GLU:HG3	2.24	0.41
1:A:212:HIS:C	1:A:214:ILE:N	2.74	0.41
1:B:306:LEU:HD23	1:B:307:ARG:H	1.86	0.41
1:C:787:GLU:OE2	1:C:792:LYS:HD3	2.20	0.41
1:A:74:TYR:CG	1:A:127:ILE:HD12	2.56	0.41
1:C:797:LEU:HA	1:C:807:LEU:CD2	2.50	0.41
1:B:509:LYS:HA	1:B:509:LYS:HZ2	1.85	0.41
1:A:210:LEU:HG	1:A:214:ILE:CD1	2.45	0.41
1:B:347:ALA:O	1:B:348:PRO:C	2.58	0.41
1:A:66:LYS:HA	1:A:67:PRO:HD3	1.93	0.41
1:B:496:GLU:O	1:B:507:LEU:HD21	2.21	0.40
1:C:833:GLU:N	1:C:833:GLU:OE1	2.54	0.40
1:A:199:SER:CB	1:A:202:HIS:HE1	2.35	0.40
1:A:54:ASP:OD1	1:A:55:VAL:N	2.49	0.40
1:C:784:ARG:NE	1:C:784:ARG:HA	2.33	0.40
1:A:197:LEU:HG	1:A:210:LEU:HD13	2.03	0.40
1:B:396:LEU:CD2	1:B:396:LEU:N	2.76	0.40
1:A:217:THR:HA	1:A:221:ARG:NH2	2.37	0.40
1:C:787:GLU:HG3	1:C:792:LYS:HG2	2.04	0.40
1:A:187:GLU:HG3	1:A:192:LYS:HG2	2.04	0.40
1:C:800:GLY:O	1:C:804:LEU:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:NE2	1:C:756:VAL:O[1_554]	1.96	0.24
1:A:79:GLU:O	1:C:672:GLU:OE2[4_445]	2.09	0.11

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	214/257 (83%)	179 (84%)	23 (11%)	12 (6%)	2	2
1	B	214/257 (83%)	183 (86%)	23 (11%)	8 (4%)	4	5
1	C	214/257 (83%)	178 (83%)	23 (11%)	13 (6%)	2	2
All	All	642/771 (83%)	540 (84%)	69 (11%)	33 (5%)	2	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	162	SER
1	A	163	GLU
1	B	305	PRO
1	B	463	GLU
1	C	648	PRO
1	C	649	LYS
1	C	762	SER
1	C	834	LYS
1	A	48	PRO
1	A	50	GLY
1	A	59	GLY
1	A	224	LEU
1	B	524	LEU
1	B	531	GLU
1	C	650	GLY
1	C	659	GLY
1	A	185	PRO
1	B	359	GLY
1	B	361	PRO
1	C	651	GLN
1	C	800	GLY
1	C	813	ARG
1	C	823	ASP

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Mol	Chain	Res	Type
1	A	91	PRO
1	A	200	GLY
1	B	485	PRO
1	A	194	PRO
1	C	826	PRO
1	C	825	ILE
1	B	348	PRO
1	C	763	GLU
1	A	226	PRO

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	196/233 (84%)	179 (91%)	17 (9%)	13	24
1	B	196/233 (84%)	179 (91%)	17 (9%)	13	24
1	C	196/233 (84%)	180 (92%)	16 (8%)	14	27
All	All	588/699 (84%)	538 (92%)	50 (8%)	13	25

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	32	LYS
1	A	90	GLU
1	A	96	LEU
1	A	97	ASN
1	A	118	GLU
1	A	126	LYS
1	A	163	GLU
1	A	184	ARG
1	A	195	GLU
1	A	209	LYS
1	A	211	TRP
1	A	221	ARG

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	226	PRO
1	A	227	LYS
1	A	235	ASP
1	B	305	PRO
1	B	306	LEU
1	B	312	THR
1	B	343	LEU
1	B	396	LEU
1	B	397	ASN
1	B	398	GLN
1	B	426	LYS
1	B	436	ASP
1	B	484	ARG
1	B	495	GLU
1	B	498	LEU
1	B	499	SER
1	B	509	LYS
1	B	521	ARG
1	B	524	LEU
1	B	535	ASP
1	C	649	LYS
1	C	696	LEU
1	C	697	ASN
1	C	716	ARG
1	C	726	LYS
1	C	736	ASP
1	C	762	SER
1	C	784	ARG
1	C	795	GLU
1	C	809	LYS
1	C	813	ARG
1	C	823	ASP
1	C	824	LEU
1	C	827	LYS
1	C	829	LEU
1	C	832	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS

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Mol	Chain	Res	Type
1	A	202	HIS
1	B	397	ASN
1	C	697	ASN
1	C	702	ASN
1	C	802	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 carbohydrates 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	218/257 (84%)	0.64	37 (16%) 2 1	19, 29, 40, 53	0
1	B	218/257 (84%)	0.34	26 (11%) 6 4	16, 27, 41, 47	0
1	C	218/257 (84%)	0.63	33 (15%) 3 1	20, 30, 39, 41	0
All	All	654/771 (84%)	0.54	96 (14%) 3 2	16, 28, 40, 53	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	14.3
1	C	823	ASP	12.2
1	A	223	ASP	11.1
1	B	501	HIS	8.3
1	A	232	LEU	8.1
1	C	661	PRO	7.4
1	B	502	HIS	7.2
1	C	826	PRO	7.2
1	A	202	HIS	7.1
1	B	535	ASP	6.9
1	B	523	ASP	6.8
1	C	812	HIS	6.5
1	B	532	LEU	6.3
1	C	822	PRO	5.9
1	A	161	LEU	5.8
1	A	233	GLU	5.7
1	B	522	PRO	5.7
1	A	91	PRO	5.7
1	C	827	LYS	5.6
1	B	529	LEU	4.9
1	A	219	LYS	4.9
1	A	225	ILE	4.7
1	C	833	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	208	TRP	4.5
1	A	213	ARG	4.4
1	A	210	LEU	4.4
1	C	811	TRP	4.3
1	A	220	LYS	4.3
1	C	802	HIS	4.2
1	C	829	LEU	4.1
1	C	649	LYS	4.1
1	A	184	ARG	4.0
1	C	760	VAL	3.9
1	B	533	GLU	3.9
1	A	201	HIS	3.9
1	A	205	ILE	3.8
1	C	604	ASN	3.7
1	B	510	LEU	3.7
1	B	503	LYS	3.7
1	C	805	ILE	3.6
1	B	534	LYS	3.6
1	A	164	PRO	3.5
1	A	186	ARG	3.4
1	A	218	VAL	3.4
1	A	92	TRP	3.4
1	A	197	LEU	3.3
1	A	212	HIS	3.3
1	B	512	HIS	3.3
1	B	524	LEU	3.1
1	B	511	TRP	3.1
1	B	513	ARG	3.1
1	A	204	LEU	3.1
1	A	207	LEU	3.1
1	A	215	GLU	3.1
1	C	804	LEU	3.0
1	B	526	PRO	3.0
1	A	199	SER	3.0
1	B	304	ASN	3.0
1	A	216	ASN	2.9
1	A	211	TRP	2.9
1	B	527	LYS	2.9
1	C	818	VAL	2.9
1	C	801	HIS	2.8
1	A	163	GLU	2.8
1	C	605	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	832	LEU	2.7
1	C	797	LEU	2.7
1	A	61	PRO	2.7
1	C	657	TYR	2.7
1	B	508	TRP	2.6
1	A	226	PRO	2.6
1	A	206	GLU	2.6
1	A	60	LEU	2.5
1	B	392	TRP	2.5
1	C	785	PRO	2.5
1	A	224	LEU	2.3
1	B	460	VAL	2.3
1	C	803	LYS	2.3
1	B	504	LEU	2.3
1	B	348	PRO	2.3
1	C	692	TRP	2.3
1	A	195	GLU	2.2
1	C	658	GLY	2.2
1	A	62	GLY	2.2
1	B	500	GLY	2.2
1	B	530	THR	2.2
1	C	813	ARG	2.2
1	C	810	LEU	2.2
1	C	820	LYS	2.1
1	C	784	ARG	2.1
1	C	651	GLN	2.1
1	C	762	SER	2.1
1	C	764	PRO	2.0
1	B	531	GLU	2.0
1	A	90	GLU	2.0
1	C	783	THR	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 carbohydrates 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.