



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 1OY5 / pdb_00001oy5
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

<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

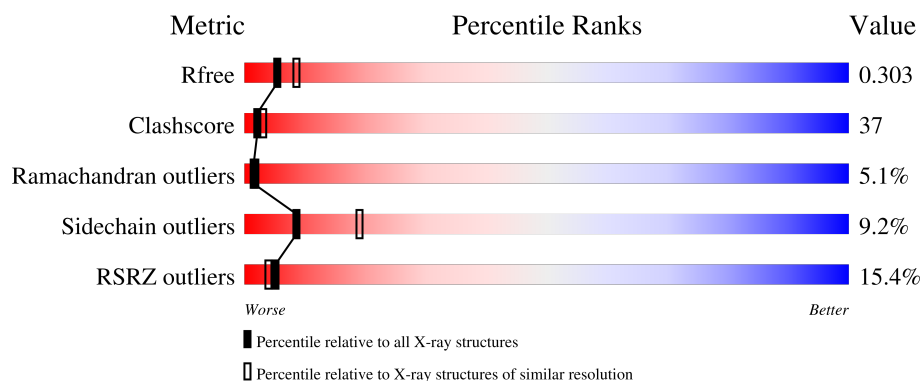
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	257	
1	B	257	
1	C	257	

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			

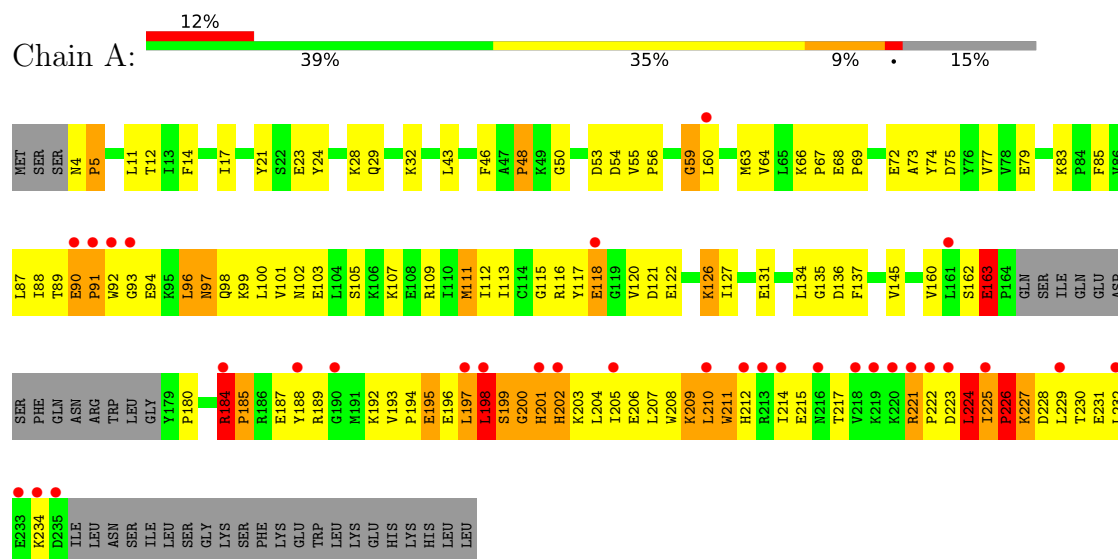
- Molecule 2 is water.

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		

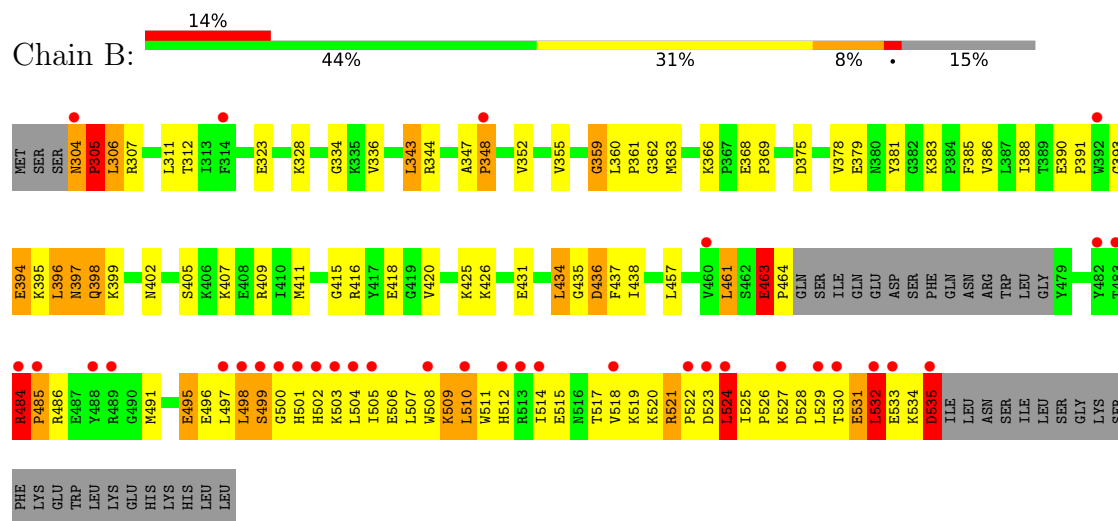
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

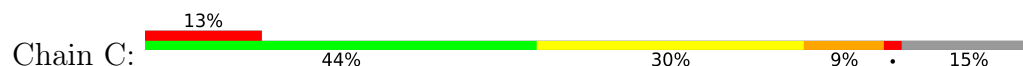
• Molecule 1: tRNA (Guanine-N(1)-)-methyltransferase

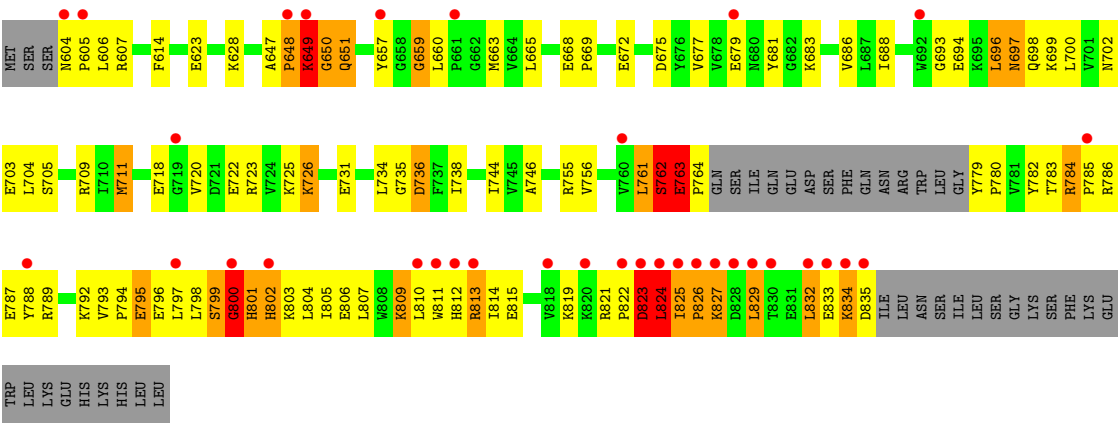


• Molecule 1: tRNA (Guanine-N(1)-)-methyltransferase



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





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 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.60) 99.1 (20.00-2.60)	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	1624 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	1/1811 (0.1%)	1.37	17/2452 (0.7%)
1	B	1.16	4/1810 (0.2%)	1.22	13/2450 (0.5%)
1	C	0.94	2/1811 (0.1%)	1.19	16/2452 (0.7%)
All	All	1.03	7/5432 (0.1%)	1.26	46/7354 (0.6%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	MET	SD-CE	-12.24	1.49	1.79
1	C	711	MET	SD-CE	-10.78	1.52	1.79
1	A	111	MET	SD-CE	-9.02	1.56	1.79
1	B	491	MET	SD-CE	-6.59	1.63	1.79
1	B	344	ARG	C-O	-6.06	1.16	1.24
1	B	461	LEU	CA-C	-5.90	1.45	1.52
1	C	746	ALA	CA-CB	-5.06	1.45	1.53

All (46) 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	A	201	HIS	N-CA-C	-17.60	92.22	114.04
1	A	4	ASN	CA-C-N	11.51	154.63	127.00
1	A	4	ASN	C-N-CA	11.51	154.63	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	824	LEU	N-CA-C	11.49	125.00	108.00
1	C	735	GLY	N-CA-C	-10.16	100.59	112.79
1	C	824	LEU	CB-CA-C	-9.89	102.50	116.34
1	C	799	SER	N-CA-C	-9.42	96.12	109.69
1	B	501	HIS	N-CA-C	-9.38	90.83	110.80
1	B	435	GLY	N-CA-C	-8.84	97.26	112.64
1	A	202	HIS	N-CA-C	-8.82	103.05	112.93
1	C	801	HIS	N-CA-C	-8.61	101.97	111.36
1	A	199	SER	N-CA-C	-8.53	96.48	109.96
1	B	535	ASP	N-CA-CB	7.79	123.74	110.50
1	A	163	GLU	N-CA-C	7.78	127.00	109.81
1	A	226	PRO	N-CA-C	7.38	127.66	112.47
1	A	197	LEU	N-CA-C	-7.05	104.75	113.15
1	C	798	LEU	N-CA-C	7.00	122.07	112.90
1	A	205	ILE	N-CA-C	-6.95	106.01	112.96
1	A	184	ARG	N-CA-C	6.75	124.74	109.81
1	B	502	HIS	N-CA-C	-6.61	104.35	112.88
1	B	386	VAL	N-CA-C	6.49	118.16	108.23
1	B	304	ASN	CA-C-N	6.47	127.93	119.84
1	B	304	ASN	C-N-CA	6.47	127.93	119.84
1	B	510	LEU	N-CA-C	-6.43	103.39	111.11
1	C	802	HIS	N-CA-C	-6.33	106.26	112.97
1	C	681	TYR	N-CA-C	-6.19	100.13	108.86
1	A	198	LEU	N-CA-C	6.05	120.72	112.68
1	C	824	LEU	CA-C-N	5.72	132.72	122.13
1	C	824	LEU	C-N-CA	5.72	132.72	122.13
1	B	420	VAL	N-CA-C	-5.71	100.06	108.85
1	C	800	GLY	N-CA-C	5.64	126.55	113.18
1	B	484	ARG	N-CA-C	5.62	122.22	109.81
1	A	210	LEU	N-CA-C	-5.61	104.54	111.33
1	B	532	LEU	N-CA-C	-5.57	105.59	112.38
1	C	738	ILE	N-CA-C	5.55	115.95	108.17
1	A	5	PRO	CA-N-CD	-5.53	103.76	111.50
1	C	763	GLU	N-CA-C	5.47	121.91	109.81
1	B	438	ILE	N-CA-C	5.33	115.57	108.11
1	C	686	VAL	N-CA-C	5.32	116.38	108.23
1	B	463	GLU	N-CA-C	5.32	121.56	109.81
1	A	225	ILE	CA-C-N	5.28	126.44	119.84
1	A	225	ILE	C-N-CA	5.28	126.44	119.84
1	C	761	LEU	N-CA-C	5.22	121.93	110.80
1	C	823	ASP	CB-CA-C	-5.20	100.07	110.42
1	A	193	VAL	CB-CA-C	-5.14	105.34	110.89

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	153	2
1	B	1767	0	1816	113	0
1	C	1768	0	1818	160	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	402	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 37.

All (402) 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:HD23	1:C:696:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:96:LEU:HD23	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:B:396:LEU:H	1:B:396:LEU:HD23	1.24	0.98
1:C:763:GLU:HG3	1:C:763:GLU:O	1.61	0.98
1:C:811:TRP:O	1:C:815:GLU:HB2	1.66	0.95
1:A:223:ASP:C	1:A:224:LEU:HD23	1.92	0.95
1:A:163:GLU:C	1:A:163:GLU:OE1	2.12	0.92
1:C:648:PRO:O	1:C:650:GLY:N	2.02	0.92
1:B:436:ASP:N	1:B:436:ASP:OD1	2.00	0.92
1:A:163:GLU:OE1	1:A:163:GLU:O	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:135:GLY:O	1:A:136:ASP:HB2	1.72	0.89
1:B:355:VAL:HG22	1:B:363:MET:HE1	1.53	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:C:696:LEU:HD23	1:C:696:LEU:N	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:HD12	1:B:434:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:649:LYS:C	1:C:651:GLN:H	1.94	0.75
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:HD23	1:A:96:LEU:N	2.01	0.74
1:A:99:LYS:NZ	1:C:827:LYS:HB3	2.02	0.74
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:O	1:B:532:LEU:HD23	1.88	0.73
1:A:200:GLY:CA	1:A:203:LYS:CB	2.66	0.73
1:A:210:LEU:HG	1:A:214:ILE:HD12	1.71	0.73
1:B:359:GLY:C	1:B:360:LEU:HD22	2.13	0.73
1:C:763:GLU:OE1	1:C:763:GLU:HA	1.87	0.73
1:C:604:ASN:N	1:C:605:PRO:CD	2.52	0.72
1:A:96:LEU:H	1:A:96:LEU:CD2	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:763:GLU:O	1:C:763:GLU:CG	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:B:532:LEU:HD23	1:B:532:LEU:C	2.16	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:C:821:ARG:HB2	1:C:821:ARG:CZ	2.23	0.69
1:A:223:ASP:C	1:A:224:LEU:CD2	2.66	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:784:ARG:O	1:C:785:PRO:C	2.36	0.68
1:A:77:VAL:HG21	1:A:111:MET:CE	2.24	0.68
1:A:90:GLU:OE1	1:A:92:TRP:NE1	2.28	0.67
1:B:499:SER:O	1:B:503:LYS:NZ	2.26	0.67
1:B:305:PRO:HG3	1:B:334:GLY:O	1.95	0.67
1:B:362:GLY:O	1:B:363:MET:HE2	1.94	0.66
1:C:824:LEU:HB2	1:C:826:PRO:HD2	1.78	0.66
1:C:823:ASP:C	1:C:824:LEU:HG	2.20	0.66
1:B:388:ILE:CG2	1:B:431:GLU:HG3	2.26	0.65
1:A:209:LYS:HA	1:A:209:LYS:HZ3	1.60	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:B:402:ASN:O	1:B:405:SER:OG	2.11	0.64
1:C:815:GLU:O	1:C:819:LYS:HG3	1.97	0.64
1:C:647:ALA:C	1:C:648:PRO:O	2.35	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
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:C:832:LEU:C	1:C:832:LEU:CD2	2.72	0.63
1:B:393:GLY:C	1:B:394:GLU:OE1	2.42	0.62
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:823:ASP:C	1:C:824:LEU:CG	2.73	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:A:224:LEU:HG	1:A:226:PRO:HD2	1.82	0.61
1:C:647:ALA:O	1:C:648:PRO:O	2.18	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:832:LEU:HD23	1:C:832:LEU:C	2.26	0.61
1:B:534:LYS:O	1:B:535:ASP:C	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD12	1:A:134:LEU:H	1.66	0.60
1:C:761:LEU:HD22	1:C:764:PRO:CD	2.31	0.60
1:B:383:LYS:O	1:B:409:ARG:NH1	2.35	0.60
1:B:497:LEU:HA	1:B:507:LEU:HD22	1.83	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: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:B:463:GLU:O	1:B:463:GLU:CD	2.46	0.58
1:A:63:MET:O	1:A:117:TYR:HB3	2.04	0.58
1:A:200:GLY:HA2	1:A:203:LYS:HG3	1.84	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:B:306:LEU:HD23	1:B:307:ARG:N	2.19	0.58
1:C:761:LEU:HD13	1:C:764:PRO:HB2	1.85	0.58
1:B:397:ASN:ND2	1:B:399:LYS:HB3	2.19	0.57
1:A:74:TYR:HA	1:A:111:MET:HE1	1.86	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:H	1:B:434:LEU:CD1	2.16	0.57
1:A:11:LEU:HD11	1:A:111:MET:HE2	1.85	0.57
1:C:824:LEU:CG	1:C:826:PRO:HD2	2.35	0.57
1:A:91:PRO:HD3	1:A:115:GLY:HA3	1.86	0.57
1:B:528:ASP:O	1:B:532:LEU:HB3	2.05	0.57
1:B:498:LEU:O	1:B:499:SER:CB	2.47	0.57
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: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:809:LYS:NZ	1:C:809:LYS:HA	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:CD2	1:A:107:LYS:HE2	2.41	0.55
1:B:503:LYS:O	1:B:507:LEU:HG	2.06	0.55
1:A:199:SER:C	1:A:203:LYS:HD2	2.25	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:C:823:ASP:CG	1:C:827:LYS:HZ1	2.12	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:761:LEU:O	1:C:762:SER:C	2.50	0.54
1:C:799:SER:HG	1:C:803:LYS:CE	2.18	0.54
1:A:221:ARG:HB2	1:A:221:ARG:CZ	2.37	0.54
1:B:511:TRP:O	1:B:515:GLU:CB	2.53	0.54
1:C:659:GLY:C	1:C:660:LEU:HD22	2.33	0.54
1:A:77:VAL:HG21	1:A:111:MET:HE3	1.90	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:810:LEU:C	1:C:810:LEU:HD23	2.33	0.54
1:C:832:LEU:O	1:C:832:LEU:CD2	2.53	0.54
1:B:397:ASN:HD21	1:B:399:LYS:HE2	1.71	0.54
1:A:93:GLY:C	1:A:94:GLU:OE1	2.51	0.53
1:C:693:GLY:C	1:C:694:GLU:OE1	2.51	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
1:A:59:GLY:C	1:A:60:LEU:HD22	2.34	0.53
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:B:484:ARG:O	1:B:486:ARG:N	2.42	0.53
1:C:823:ASP:C	1:C:824:LEU:HD23	2.33	0.53
1:C:833:GLU:O	1:C:834:LYS:HB2	2.08	0.53
1:B:520:LYS:C	1:B:522:PRO:HD2	2.34	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:A:201:HIS:C	1:A:203:LYS:H	2.18	0.52
1:B:484:ARG:HE	1:B:484:ARG:HA	1.75	0.52
1:B:434:LEU:HD12	1:B:434:LEU:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:LEU:HD12	1:C:606:LEU:C	2.34	0.51
1:A:46:PHE:O	1:A:48:PRO:HD3	2.10	0.51
1:A:54:ASP:HB3	1:C:783:THR:OG1	2.11	0.51
1:A:97:ASN:HD22	1:A:99:LYS:CB	2.19	0.51
1:C:688:ILE:HG23	1:C:731:GLU:HG3	1.92	0.51
1:C:799:SER:O	1:C:803:LYS:HD2	2.10	0.51
1:C:784:ARG:HB3	1:C:785:PRO:HD3	1.92	0.51
1:C:799:SER:HG	1:C:803:LYS:HE2	1.75	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:B:510:LEU:O	1:B:511:TRP:C	2.52	0.51
1:C:824:LEU:HD23	1:C:824:LEU:N	2.25	0.51
1:A:90:GLU:OE1	1:A:92:TRP:CE2	2.64	0.51
1:A:29:GLN:NE2	1:A:160:VAL:O	2.44	0.51
1:A:90:GLU:CD	1:A:92:TRP:NE1	2.68	0.51
1:B:517:THR:HB	1:B:521:ARG:HH21	1.76	0.51
1:B:499:SER:O	1:B:503:LYS:HD2	2.11	0.50
1:C:604:ASN:N	1:C:605:PRO:HD3	2.26	0.50
1:C:699:LYS:O	1:C:703:GLU:HG3	2.10	0.50
1:B:523:ASP:O	1:B:524:LEU:HB2	2.11	0.50
1:A:53:ASP:OD2	1:A:63:MET:SD	2.69	0.50
1:A:99:LYS:NZ	1:C:827:LYS:CB	2.74	0.50
1:A:231:GLU:HA	1:A:234:LYS:HG2	1.94	0.50
1:B:396:LEU:H	1:B:396:LEU:CD2	2.05	0.50
1:A:87:LEU:O	1:A:112:ILE:HA	2.12	0.50
1:B:509:LYS:HA	1:B:509:LYS:HZ3	1.76	0.49
1:C:806:GLU:O	1:C:809:LYS:N	2.39	0.49
1:A:54:ASP:OD2	1:C:784:ARG:HB2	2.12	0.49
1:A:163:GLU:C	1:A:163:GLU:CD	2.77	0.49
1:A:195:GLU:C	1:A:198:LEU:HB2	2.38	0.49
1:C:799:SER:HB2	1:C:802:HIS:CE1	2.43	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
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:803:LYS:O	1:C:804:LEU:C	2.56	0.49
1:A:234:LYS:HE2	1:A:234:LYS:N	2.26	0.49
1:A:56:PRO:HA	1:C:782:TYR:O	2.13	0.49
1:A:188:TYR:CE1	1:A:189:ARG:HG2	2.48	0.49
1:B:505:ILE:O	1:B:509:LYS:HG2	2.13	0.48
1:C:824:LEU:CB	1:C:826:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:CG1	1:B:457:LEU:CD1	2.91	0.48
1:C:677:VAL:HG21	1:C:711:MET:CE	2.42	0.48
1:C:763:GLU:O	1:C:764:PRO:C	2.51	0.48
1:B:461:LEU:HD13	1:B:464:PRO:HB2	1.93	0.48
1:B:509:LYS:O	1:B:510:LEU:C	2.56	0.48
1:C:604:ASN:N	1:C:605:PRO:HD2	2.27	0.48
1:A:94:GLU:N	1:A:94:GLU:CD	2.72	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:B:415:GLY:C	1:B:416:ARG:HG2	2.39	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:500:GLY:CA	1:B:503:LYS:CB	2.88	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: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:21:TYR:CZ	1:C:744:ILE:HD11	2.48	0.47
1:A:196:GLU:C	1:A:198:LEU:H	2.22	0.47
1:A:223:ASP:CB	1:A:224:LEU:HD23	2.44	0.47
1:C:805:ILE:O	1:C:809:LYS:HG2	2.15	0.47
1:C:795:GLU:OE1	1:C:795:GLU:N	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:B:336:VAL:HG12	1:B:457:LEU:CD1	2.45	0.46
1:C:823:ASP:OD2	1:C:827:LYS:NZ	2.36	0.46
1:C:786:ARG:HG2	1:C:786:ARG:HH11	1.80	0.46
1:A:115:GLY:C	1:A:116:ARG:HG2	2.40	0.46
1:B:535:ASP:C	1:B:535:ASP:OD2	2.58	0.46
1:B:363:MET:O	1:B:418:GLU:HG2	2.16	0.46
1:B:495:GLU:HA	1:B:498:LEU:CD1	2.45	0.46
1:A:102:ASN:O	1:A:105:SER:OG	2.30	0.46
1:B:521:ARG:HG3	1:B:521:ARG:HH11	1.81	0.46
1:C:801:HIS:C	1:C:803:LYS:H	2.23	0.46
1:A:228:ASP:O	1:A:232:LEU:HB2	2.15	0.46
1:C:788:TYR:CE1	1:C:789:ARG:CG	2.99	0.46
1:B:512:HIS:C	1:B:514:ILE:H	2.22	0.46
1:A:24:TYR:HB3	1:C:614:PHE:CE1	2.51	0.46
1:B:521:ARG:N	1:B:522:PRO:HD2	2.30	0.46
1:C:784:ARG:HE	1:C:784:ARG:CA	2.29	0.46
1:A:88:ILE:HG23	1:A:131:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:ILE:HG23	1:C:829:LEU:HD23	1.98	0.45
1:A:14:PHE:HB3	1:A:17:ILE:HD12	1.97	0.45
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.43	0.45
1:B:347:ALA:O	1:B:348:PRO:C	2.58	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:512:HIS:C	1:B:514:ILE:N	2.72	0.45
1:B:304:ASN:CB	1:B:305:PRO:HD3	2.16	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:B:395:LYS:O	1:B:395:LYS:HG2	2.17	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: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:100:LEU:O	1:A:101:VAL:C	2.57	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:503:LYS:O	1:B:504:LEU:C	2.59	0.45
1:A:67:PRO:HG3	1:A:121:ASP:CG	2.42	0.45
1:B:497:LEU:HA	1:B:507:LEU:CD2	2.46	0.45
1:B:347:ALA:HB2	1:B:352:VAL:HG12	1.98	0.44
1:B:484:ARG:HB3	1:B:485:PRO:HD3	2.00	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:C:806:GLU:HA	1:C:809:LYS:CG	2.47	0.44
1:C:823:ASP:C	1:C:824:LEU:CD2	2.90	0.44
1:B:394:GLU:HG3	1:B:437:PHE:CZ	2.52	0.44
1:B:499:SER:O	1:B:503:LYS:CG	2.64	0.44
1:C:823:ASP:CG	1:C:827:LYS:NZ	2.75	0.44
1:A:212:HIS:C	1:A:214:ILE:N	2.74	0.44
1:A:89:THR:HG21	1:A:145:VAL:HG12	2.00	0.44
1:B:366:LYS:NZ	1:B:368:GLU:OE1	2.47	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
1:C:700:LEU:O	1:C:704:LEU:HG	2.18	0.43
1:C:763:GLU:OE1	1:C:763:GLU:CA	2.59	0.43
1:A:118:GLU:OE2	1:A:118:GLU:N	2.51	0.43
1:A:126:LYS:HE3	1:A:126:LYS:HA	1.99	0.43
1:A:199:SER:OG	1:A:202:HIS:HE1	2.02	0.43
1:C:793:VAL:HG13	1:C:794:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:531:GLU:C	1:B:533:GLU:N	2.76	0.43
1:A:120:VAL:O	1:A:121:ASP:C	2.59	0.43
1:B:394:GLU:CD	1:B:394:GLU:N	2.76	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:755:ARG:O	1:C:761:LEU:HD12	2.19	0.43
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.84	0.42
1:C:788:TYR:CD1	1:C:789:ARG:HG2	2.54	0.42
1:A:196:GLU:H	1:A:196:GLU:HG3	1.57	0.42
1:B:525:ILE:N	1:B:526:PRO:CD	2.82	0.42
1:C:761:LEU:O	1:C:762:SER:O	2.36	0.42
1:B:398:GLN:O	1:B:402:ASN:ND2	2.52	0.42
1:B:378:VAL:O	1:B:381:TYR:O	2.37	0.42
1:B:484:ARG:HE	1:B:484:ARG:CA	2.32	0.42
1:B:506:GLU:O	1:B:509:LYS:HB2	2.20	0.42
1:C:812:HIS:O	1:C:814:ILE:N	2.53	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:B:484:ARG:O	1:B:485:PRO:C	2.60	0.42
1:C:783:THR:HG23	1:C:785:PRO:HD2	2.01	0.42
1:C:803:LYS:HG2	1:C:806:GLU:OE2	2.20	0.42
1:C:825:ILE:O	1:C:826:PRO:C	2.63	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:B:425:LYS:HE3	1:B:431:GLU:CD	2.45	0.42
1:C:779:TYR:HB3	1:C:815:GLU:HB2	2.02	0.41
1:C:809:LYS:O	1:C:810:LEU:C	2.63	0.41
1:A:96:LEU:N	1:A:96:LEU:CD2	2.71	0.41
1:C:761:LEU:HA	1:C:761:LEU:HD23	1.74	0.41
1:C:787:GLU:CG	1:C:792:LYS:HG2	2.49	0.41
1:C:814:ILE:O	1:C:814:ILE:HG22	2.19	0.41
1:A:200:GLY:HA2	1:A:203:LYS:N	2.36	0.41
1:B:510:LEU:HG	1:B:514:ILE:HD12	2.01	0.41
1:A:203:LYS:HA	1:A:206:GLU:HB3	2.01	0.41
1:B:343:LEU:HD22	1:B:369:PRO:HB2	2.01	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:A:187:GLU:CG	1:A:192:LYS:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PHE:CE2	1:B:407:LYS:HE2	2.55	0.41
1:A:74:TYR:CG	1:A:127:ILE:HD12	2.56	0.41
1:A:180:PRO:CB	1:C:722:GLU:HG3	2.24	0.41
1:A:209:LYS:O	1:A:210:LEU:C	2.63	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:66:LYS:HA	1:A:67:PRO:HD3	1.93	0.41
1:A:210:LEU:HG	1:A:214:ILE:CD1	2.45	0.41
1:C:797:LEU:HA	1:C:807:LEU:CD2	2.50	0.41
1:B:496:GLU:O	1:B:507:LEU:HD21	2.21	0.40
1:C:833:GLU:OE1	1:C:833:GLU:N	2.54	0.40
1:C:834:LYS:O	1:C:835:ASP:C	2.65	0.40
1:A:54:ASP:OD1	1:A:55:VAL:N	2.49	0.40
1:A:196:GLU:C	1:A:198:LEU:N	2.78	0.40
1:A:199:SER:CB	1:A:202:HIS:HE1	2.35	0.40
1:C:784:ARG:HA	1:C:784:ARG:NE	2.33	0.40
1:C:812:HIS:C	1:C:814:ILE:N	2.79	0.40
1:A:187:GLU:HG3	1:A:192:LYS:HG2	2.04	0.40
1:A:197:LEU:HG	1:A:210:LEU:HD13	2.03	0.40
1:A:217:THR:HA	1:A:221:ARG:NH2	2.37	0.40
1:B:396:LEU:N	1:B:396:LEU:CD2	2.76	0.40
1:C:787:GLU:HG3	1:C:792: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 [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	214/257 (83%)	179 (84%)	23 (11%)	12 (6%)	1	1
1	B	214/257 (83%)	183 (86%)	23 (11%)	8 (4%)	2	3
1	C	214/257 (83%)	178 (83%)	23 (11%)	13 (6%)	1	1
All	All	642/771 (83%)	540 (84%)	69 (11%)	33 (5%)	1	2

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
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

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Mol	Chain	Res	Type
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%)	178 (91%)	18 (9%)	8	19
1	B	196/233 (84%)	175 (89%)	21 (11%)	6	14
1	C	196/233 (84%)	181 (92%)	15 (8%)	12	27
All	All	588/699 (84%)	534 (91%)	54 (9%)	8	19

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	32	LYS
1	A	72	GLU
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	198	LEU
1	A	209	LYS
1	A	211	TRP
1	A	221	ARG
1	A	224	LEU
1	A	226	PRO
1	A	227	LYS
1	B	305	PRO
1	B	306	LEU
1	B	312	THR

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Mol	Chain	Res	Type
1	B	343	LEU
1	B	394	GLU
1	B	396	LEU
1	B	397	ASN
1	B	398	GLN
1	B	426	LYS
1	B	434	LEU
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	518	VAL
1	B	521	ARG
1	B	524	LEU
1	B	532	LEU
1	B	535	ASP
1	C	649	LYS
1	C	696	LEU
1	C	697	ASN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	202	HIS
1	B	397	ASN
1	B	502	HIS
1	C	604	ASN

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Mol	Chain	Res	Type
1	C	629	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/257 (84%)	0.78	32 (14%) 6 4	19, 29, 40, 53	0
1	B	218/257 (84%)	0.60	35 (16%) 4 3	16, 27, 41, 47	0
1	C	218/257 (84%)	0.75	34 (15%) 5 4	20, 30, 39, 41	0
All	All	654/771 (84%)	0.71	101 (15%) 5 4	16, 28, 40, 53	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	7.7
1	A	223	ASP	6.0
1	A	233	GLU	5.7
1	A	232	LEU	5.5
1	B	522	PRO	5.4
1	C	823	ASP	5.3
1	B	532	LEU	4.9
1	B	535	ASP	4.8
1	B	529	LEU	4.6
1	A	91	PRO	4.6
1	A	213	ARG	4.5
1	A	220	LYS	4.5
1	C	834	LYS	4.4
1	C	826	PRO	4.4
1	A	161	LEU	4.3
1	A	225	ILE	4.2
1	B	510	LEU	4.2
1	B	304	ASN	4.1
1	C	800	GLY	4.0
1	B	530	THR	3.9
1	C	832	LEU	3.9
1	A	235	ASP	3.9
1	A	210	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	219	LYS	3.9
1	C	785	PRO	3.8
1	B	523	ASP	3.7
1	A	92	TRP	3.7
1	A	197	LEU	3.7
1	B	513	ARG	3.7
1	C	827	LYS	3.6
1	C	829	LEU	3.6
1	C	661	PRO	3.6
1	C	835	ASP	3.5
1	C	822	PRO	3.5
1	B	460	VAL	3.5
1	B	484	ARG	3.4
1	A	93	GLY	3.4
1	B	533	GLU	3.3
1	A	216	ASN	3.3
1	C	810	LEU	3.2
1	B	512	HIS	3.2
1	C	833	GLU	3.2
1	C	649	LYS	3.1
1	A	229	LEU	3.1
1	C	812	HIS	3.1
1	B	488	TYR	3.0
1	B	485	PRO	2.9
1	C	820	LYS	2.9
1	A	205	ILE	2.9
1	C	648	PRO	2.9
1	B	500	GLY	2.9
1	C	830	THR	2.9
1	A	184	ARG	2.8
1	A	234	LYS	2.8
1	B	483	THR	2.8
1	C	825	ILE	2.8
1	B	524	LEU	2.7
1	A	190	GLY	2.7
1	A	202	HIS	2.7
1	C	818	VAL	2.7
1	B	482	TYR	2.7
1	B	505	ILE	2.7
1	C	824	LEU	2.7
1	A	90	GLU	2.7
1	C	811	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	760	VAL	2.7
1	B	508	TRP	2.6
1	C	802	HIS	2.6
1	C	813	ARG	2.6
1	C	828	ASP	2.6
1	B	489	ARG	2.5
1	B	501	HIS	2.5
1	B	499	SER	2.5
1	B	518	VAL	2.5
1	B	527	LYS	2.5
1	B	348	PRO	2.4
1	A	214	ILE	2.4
1	C	604	ASN	2.4
1	B	392	TRP	2.4
1	C	692	TRP	2.4
1	B	314	PHE	2.4
1	B	497	LEU	2.4
1	B	498	LEU	2.4
1	A	212	HIS	2.4
1	C	788	TYR	2.3
1	A	60	LEU	2.3
1	C	719	GLY	2.3
1	B	502	HIS	2.3
1	C	679	GLU	2.3
1	C	797	LEU	2.2
1	A	118	GLU	2.2
1	A	218	VAL	2.2
1	A	201	HIS	2.2
1	B	503	LYS	2.2
1	B	514	ILE	2.2
1	C	605	PRO	2.1
1	A	188	TYR	2.1
1	A	221	ARG	2.1
1	A	198	LEU	2.1
1	B	504	LEU	2.0
1	C	657	TYR	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 [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.