



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 1U7X / pdb_00001u7x
Title : crystal structure of a mutant M. jannashii tyrosyl-tRNA synthetase specific for O-methyl-tyrosine
Authors : Zhang, Y.; Wang, L.; Schultz, P.G.; Wilson, I.A.
Deposited on : 2004-08-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

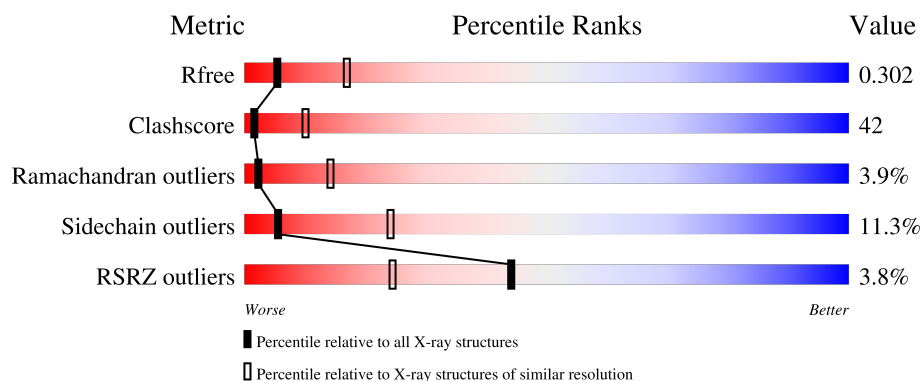
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	312	4% 35% 51% 9% ..
1	B	312	4% 27% 59% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4888 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 Tyrosyl-tRNA synthetase.

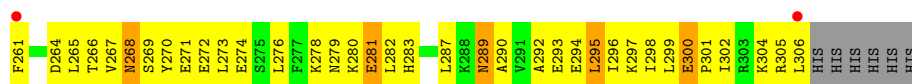
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2446	1566	412	455	13			
1	B	306	Total	C	N	O	S	0	0	0
			2441	1563	411	454	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLN	TYR	engineered mutation	UNP Q57834
A	107	THR	GLU	engineered mutation	UNP Q57834
A	158	ALA	ASP	engineered mutation	UNP Q57834
A	162	PRO	LEU	engineered mutation	UNP Q57834
A	307	HIS	-	expression tag	UNP Q57834
A	308	HIS	-	expression tag	UNP Q57834
A	309	HIS	-	expression tag	UNP Q57834
A	310	HIS	-	expression tag	UNP Q57834
A	311	HIS	-	expression tag	UNP Q57834
A	312	HIS	-	expression tag	UNP Q57834
B	32	GLN	TYR	engineered mutation	UNP Q57834
B	107	THR	GLU	engineered mutation	UNP Q57834
B	158	ALA	ASP	engineered mutation	UNP Q57834
B	162	PRO	LEU	engineered mutation	UNP Q57834
B	307	HIS	-	expression tag	UNP Q57834
B	308	HIS	-	expression tag	UNP Q57834
B	309	HIS	-	expression tag	UNP Q57834
B	310	HIS	-	expression tag	UNP Q57834
B	311	HIS	-	expression tag	UNP Q57834
B	312	HIS	-	expression tag	UNP Q57834

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.37Å 185.00Å 93.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.25 – 3.00 46.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.7 (46.25-3.00) 89.7 (46.25-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.308 0.226 , 0.302	Depositor DCC
R_{free} test set	1471 reflections (9.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4888	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	0.66	3/2487 (0.1%)	1.14	17/3341 (0.5%)
1	B	0.55	3/2482 (0.1%)	1.07	14/3336 (0.4%)
All	All	0.61	6/4969 (0.1%)	1.11	31/6677 (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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLU	C-N	16.13	1.56	1.33
1	A	140	GLU	N-CA	7.00	1.55	1.46
1	B	153	ILE	CA-CB	5.52	1.62	1.54
1	B	177	HIS	ND1-CE1	5.21	1.37	1.32
1	B	289	ASN	CG-OD1	5.20	1.33	1.23
1	A	268	ASN	CG-OD1	5.17	1.33	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	O-C-N	-18.18	98.41	122.59
1	A	143	ASN	CA-C-N	9.09	129.18	119.90
1	A	143	ASN	C-N-CA	9.09	129.18	119.90
1	A	159	ILE	N-CA-C	-7.84	105.07	111.81
1	A	140	GLU	CA-C-N	-7.70	106.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLU	C-N-CA	-7.70	106.83	121.54
1	B	207	SER	N-CA-C	-7.35	103.42	112.38
1	A	36	GLU	N-CA-C	-7.11	101.11	109.93
1	B	176	ILE	N-CA-C	-6.89	104.05	110.53
1	B	177	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	B	270	TYR	N-CA-C	-6.60	104.12	111.71
1	A	142	GLU	N-CA-C	-6.28	103.36	111.02
1	B	99	LYS	N-CA-C	-6.26	100.30	110.20
1	B	210	GLY	N-CA-C	6.15	127.75	113.18
1	B	58	ALA	N-CA-C	-6.05	105.90	113.28
1	B	177	HIS	CB-CG-ND1	5.75	131.33	122.70
1	A	88	TYR	N-CA-C	-5.68	103.86	112.04
1	A	85	ILE	N-CA-C	-5.57	105.30	110.53
1	B	159	ILE	N-CA-C	-5.45	105.06	111.00
1	A	231	CYS	CA-C-N	5.37	126.12	120.11
1	A	231	CYS	C-N-CA	5.37	126.12	120.11
1	B	88	TYR	N-CA-C	-5.29	105.42	111.14
1	A	63	ILE	CB-CA-C	-5.28	104.45	110.73
1	A	247	TYR	N-CA-C	5.24	120.54	113.72
1	A	298	ILE	N-CA-C	5.23	115.44	110.42
1	B	118	VAL	N-CA-C	-5.20	105.42	110.42
1	B	209	LYS	N-CA-C	5.18	121.84	110.80
1	B	247	TYR	N-CA-C	5.17	119.44	113.18
1	A	94	GLU	N-CA-C	-5.16	105.66	111.28
1	B	281	GLU	N-CA-C	-5.13	105.34	111.03
1	A	140	GLU	O-C-N	5.09	129.36	122.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2446	0	2523	196	0
1	B	2441	0	2509	228	0
2	A	1	0	0	0	0
All	All	4888	0	5032	417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (417) 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:176:ILE:HD12	1:A:176:ILE:H	1.12	1.11
1:A:140:GLU:O	1:A:141:ASP:O	1.70	1.07
1:A:139:ARG:O	1:A:140:GLU:HB3	1.57	1.01
1:A:279:ASN:HD21	1:A:281:GLU:HB2	1.24	1.01
1:A:245:ALA:HA	1:A:249:LEU:HD22	1.41	0.98
1:A:131:ARG:HH21	1:A:140:GLU:CD	1.74	0.96
1:B:136:LEU:HD12	1:B:172:GLU:HA	1.50	0.94
1:B:128:LYS:CD	1:B:128:LYS:H	1.81	0.92
1:A:127:LEU:HD11	1:B:127:LEU:HD11	1.50	0.89
1:A:43:LEU:HB2	1:A:205:MET:HE1	1.55	0.87
1:B:128:LYS:H	1:B:128:LYS:HD2	1.37	0.87
1:A:176:ILE:H	1:A:176:ILE:CD1	1.88	0.86
1:B:118:VAL:HG13	1:B:153:ILE:HD11	1.59	0.85
1:B:67:ALA:HB1	1:B:70:HIS:HD2	1.42	0.84
1:B:199:LEU:HD11	1:B:213:ILE:CD1	2.08	0.83
1:B:174:ARG:HA	1:B:192:HIS:CE1	2.13	0.83
1:B:257:ARG:NH1	1:B:265:LEU:HD21	1.94	0.82
1:B:245:ALA:HA	1:B:249:LEU:CD2	2.10	0.82
1:B:232:PRO:HG2	1:B:235:VAL:HB	1.62	0.82
1:B:173:GLN:HA	1:B:173:GLN:HE21	1.44	0.82
1:B:142:GLU:H	1:B:142:GLU:CD	1.84	0.82
1:A:176:ILE:HD12	1:A:176:ILE:N	1.94	0.81
1:B:67:ALA:HB1	1:B:70:HIS:CD2	2.15	0.81
1:B:258:PRO:HB2	1:B:261:PHE:HB2	1.62	0.81
1:A:152:PRO:O	1:A:156:VAL:HG23	1.81	0.81
1:B:53:ILE:O	1:B:56:GLN:HG2	1.81	0.81
1:B:46:TYR:CD1	1:B:96:MET:HE2	2.15	0.79
1:A:300:GLU:HB3	1:A:301:PRO:HD3	1.65	0.78
1:B:19:GLU:O	1:B:23:VAL:HG23	1.83	0.77
1:A:131:ARG:NH2	1:A:140:GLU:OE1	2.17	0.77
1:A:234:GLY:HA2	1:A:277:PHE:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:CD1	1:B:127:LEU:HD11	2.14	0.77
1:A:69:LEU:HD12	1:A:109:GLN:HE21	1.49	0.77
1:B:132:ARG:HH21	1:B:175:LYS:HZ1	1.32	0.77
1:B:197:THR:HB	1:B:243:GLU:OE2	1.86	0.76
1:B:237:GLU:CD	1:B:237:GLU:H	1.94	0.75
1:B:257:ARG:HH22	1:B:281:GLU:HG2	1.51	0.75
1:B:245:ALA:HA	1:B:249:LEU:HD23	1.67	0.75
1:A:132:ARG:HA	1:A:135:GLU:HG3	1.68	0.74
1:A:237:GLU:H	1:A:237:GLU:CD	1.95	0.74
1:B:156:VAL:HG13	1:B:180:ALA:HA	1.69	0.73
1:A:127:LEU:O	1:A:131:ARG:HG3	1.88	0.73
1:A:131:ARG:NH2	1:A:140:GLU:CD	2.45	0.73
1:B:132:ARG:HH21	1:B:175:LYS:NZ	1.86	0.73
1:B:152:PRO:O	1:B:156:VAL:HG23	1.89	0.73
1:B:118:VAL:HA	1:B:153:ILE:HD11	1.71	0.73
1:B:128:LYS:H	1:B:128:LYS:CE	2.01	0.72
1:A:139:ARG:O	1:A:140:GLU:CB	2.30	0.72
1:A:208:SER:O	1:A:209:LYS:HD2	1.90	0.72
1:A:140:GLU:O	1:A:141:ASP:C	2.32	0.71
1:A:274:GLU:HG2	1:A:278:LYS:HE3	1.73	0.71
1:B:253:LEU:HD23	1:B:253:LEU:H	1.56	0.70
1:A:279:ASN:HD21	1:A:281:GLU:CB	2.04	0.70
1:A:15:ILE:CG2	1:A:15:ILE:O	2.39	0.69
1:A:200:ASP:OD1	1:A:202:GLU:HG2	1.93	0.69
1:B:105:GLY:HA2	1:B:108:PHE:CE1	2.27	0.69
1:B:193:ASN:HD22	1:B:194:PRO:CD	2.06	0.69
1:B:298:ILE:O	1:B:301:PRO:HD2	1.92	0.68
1:A:178:MET:O	1:A:182:GLU:HG2	1.92	0.68
1:A:49:ILE:HD12	1:A:98:LEU:HD22	1.74	0.68
1:A:279:ASN:ND2	1:A:281:GLU:H	1.91	0.68
1:B:142:GLU:CD	1:B:142:GLU:N	2.51	0.68
1:B:55:LEU:HD11	1:B:191:ILE:HD12	1.76	0.68
1:B:1:MET:HE1	1:B:6:MET:HE2	1.76	0.67
1:A:129:ARG:HH21	1:A:132:ARG:HE	1.42	0.67
1:B:128:LYS:HD2	1:B:128:LYS:N	2.08	0.66
1:A:257:ARG:NH1	1:A:261:PHE:HB3	2.11	0.66
1:A:225:LYS:HG2	1:A:228:LYS:HE3	1.78	0.66
1:A:251:TYR:HB3	1:A:252:PRO:HA	1.78	0.66
1:B:134:MET:SD	1:B:151:TYR:HD2	2.17	0.66
1:B:208:SER:O	1:B:209:LYS:CB	2.44	0.66
1:A:96:MET:CE	1:A:215:VAL:HG11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:MET:HE2	1:A:215:VAL:HG11	1.79	0.65
1:A:128:LYS:HD2	1:A:128:LYS:N	2.12	0.65
1:B:118:VAL:CA	1:B:153:ILE:HD11	2.27	0.64
1:B:92:VAL:O	1:B:96:MET:HG3	1.97	0.64
1:B:169:GLY:O	1:B:192:HIS:HA	1.97	0.64
1:B:205:MET:HA	1:B:211:ASN:HD22	1.63	0.64
1:A:8:LYS:O	1:A:11:THR:HG23	1.98	0.64
1:A:260:LYS:HG3	1:A:261:PHE:HD1	1.63	0.64
1:A:171:MET:O	1:A:174:ARG:HG2	1.98	0.63
1:B:53:ILE:HA	1:B:56:GLN:HE21	1.62	0.63
1:B:140:GLU:HG3	1:B:141:ASP:H	1.63	0.63
1:B:193:ASN:HD22	1:B:194:PRO:HD3	1.62	0.63
1:B:276:LEU:HA	1:B:279:ASN:ND2	2.14	0.63
1:B:18:GLU:O	1:B:22:GLU:HG3	1.99	0.63
1:B:172:GLU:HG2	1:B:204:LYS:NZ	2.14	0.63
1:A:228:LYS:HG3	1:A:229:ALA:N	2.12	0.63
1:A:254:THR:HG23	1:A:265:LEU:O	1.99	0.62
1:A:230:TYR:CE1	1:A:232:PRO:HD3	2.34	0.62
1:B:258:PRO:HB2	1:B:261:PHE:CB	2.30	0.62
1:B:229:ALA:CB	1:B:241:ILE:HD11	2.30	0.62
1:B:6:MET:O	1:B:9:ARG:HB3	2.00	0.62
1:A:43:LEU:HB2	1:A:205:MET:CE	2.29	0.62
1:A:131:ARG:NH2	1:A:140:GLU:OE2	2.32	0.62
1:B:118:VAL:CG1	1:B:153:ILE:HD11	2.29	0.61
1:B:132:ARG:NH2	1:B:175:LYS:NZ	2.48	0.61
1:B:256:LYS:HB2	1:B:256:LYS:HZ2	1.66	0.61
1:A:258:PRO:C	1:A:260:LYS:H	2.08	0.60
1:B:109:GLN:NE2	1:B:154:MET:HE1	2.17	0.60
1:A:7:ILE:HD13	1:A:55:LEU:HD23	1.83	0.60
1:A:68:ASP:OD2	1:A:79:LEU:HD22	2.02	0.60
1:A:83:ARG:HB2	1:A:83:ARG:NH1	2.16	0.60
1:A:36:GLU:HA	1:A:67:ALA:HB3	1.83	0.60
1:A:287:LEU:HD22	1:A:291:VAL:HG23	1.84	0.60
1:B:14:ILE:HG12	1:B:191:ILE:HG23	1.83	0.60
1:B:246:LYS:HE3	1:B:247:TYR:CZ	2.37	0.60
1:B:49:ILE:HG23	1:B:98:LEU:HD22	1.84	0.60
1:B:95:ALA:HA	1:B:305:ARG:HD2	1.84	0.59
1:B:118:VAL:HA	1:B:153:ILE:CD1	2.32	0.59
1:B:133:SER:HB3	1:B:176:ILE:HD13	1.84	0.59
1:B:199:LEU:HD11	1:B:213:ILE:HD11	1.84	0.59
1:B:128:LYS:CD	1:B:128:LYS:N	2.58	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PRO:O	1:A:305:ARG:HG2	2.02	0.59
1:A:41:ILE:HD11	1:A:89:ASN:ND2	2.18	0.59
1:A:53:ILE:O	1:A:56:GLN:HB3	2.03	0.59
1:B:67:ALA:CB	1:B:70:HIS:HD2	2.16	0.59
1:A:140:GLU:C	1:A:141:ASP:O	2.45	0.58
1:A:242:MET:HE1	1:A:274:GLU:HA	1.85	0.58
1:A:15:ILE:HG22	1:A:190:CYS:H	1.68	0.58
1:B:199:LEU:HD11	1:B:213:ILE:HD12	1.84	0.58
1:B:172:GLU:HG2	1:B:204:LYS:HZ2	1.68	0.58
1:B:267:VAL:HG12	1:B:272:GLU:HB3	1.83	0.58
1:B:253:LEU:HD23	1:B:267:VAL:HG23	1.85	0.57
1:B:173:GLN:HE21	1:B:173:GLN:CA	2.16	0.57
1:B:257:ARG:HH11	1:B:265:LEU:HD21	1.68	0.57
1:A:208:SER:C	1:A:209:LYS:HD2	2.29	0.57
1:B:140:GLU:HG3	1:B:141:ASP:N	2.20	0.57
1:B:242:MET:HE1	1:B:274:GLU:HA	1.86	0.57
1:A:1:MET:HG2	1:A:2:ASP:N	2.20	0.57
1:A:173:GLN:HA	1:A:176:ILE:HD13	1.86	0.57
1:A:300:GLU:OE2	1:A:304:LYS:HE2	2.05	0.57
1:B:131:ARG:O	1:B:135:GLU:HG3	2.04	0.57
1:B:81:GLU:O	1:B:84:LYS:HG2	2.05	0.57
1:A:109:GLN:O	1:A:110:LEU:HD23	2.05	0.56
1:B:83:ARG:NH1	1:B:83:ARG:HB2	2.20	0.56
1:A:222:ILE:HD13	1:A:295:LEU:CD1	2.35	0.56
1:B:42:HIS:HA	1:B:214:ALA:HA	1.86	0.56
1:B:109:GLN:HA	1:B:114:TYR:CD2	2.41	0.56
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.68	0.56
1:A:15:ILE:O	1:A:15:ILE:HG22	2.04	0.56
1:A:207:SER:C	1:A:209:LYS:H	2.12	0.56
1:A:207:SER:HA	1:A:212:PHE:CD2	2.41	0.55
1:A:279:ASN:O	1:A:280:LYS:HB2	2.05	0.55
1:B:51:LYS:HA	1:B:54:ASP:OD2	2.05	0.55
1:B:211:ASN:O	1:B:212:PHE:HB3	2.05	0.55
1:B:292:ALA:O	1:B:296:ILE:HG13	2.07	0.55
1:A:258:PRO:C	1:A:260:LYS:N	2.64	0.55
1:B:78:GLU:O	1:B:79:LEU:C	2.49	0.55
1:A:19:GLU:O	1:A:23:VAL:HG23	2.06	0.55
1:A:55:LEU:O	1:A:60:PHE:HB2	2.06	0.55
1:A:49:ILE:HD12	1:A:98:LEU:CD2	2.36	0.55
1:A:254:THR:HG23	1:A:266:THR:OG1	2.07	0.55
1:B:29:LYS:O	1:B:60:PHE:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:HB2	1:A:260:LYS:HG2	1.89	0.55
1:B:83:ARG:HD3	1:B:104:TYR:CE2	2.42	0.55
1:B:172:GLU:CD	1:B:172:GLU:H	2.14	0.55
1:B:3:GLU:O	1:B:7:ILE:HG13	2.07	0.55
1:B:132:ARG:NH2	1:B:175:LYS:HZ1	2.02	0.54
1:B:245:ALA:HA	1:B:249:LEU:HD22	1.87	0.54
1:A:170:GLY:HA3	1:A:172:GLU:OE2	2.08	0.54
1:A:214:ALA:HB3	1:A:217:ASP:CG	2.32	0.54
1:A:268:ASN:H	1:A:268:ASN:HD22	1.54	0.54
1:B:228:LYS:HD2	1:B:228:LYS:C	2.33	0.54
1:B:55:LEU:O	1:B:60:PHE:HB2	2.08	0.54
1:B:118:VAL:HG13	1:B:153:ILE:CD1	2.35	0.54
1:B:166:VAL:HG13	1:B:189:VAL:O	2.07	0.53
1:A:73:LEU:HD21	1:B:116:LEU:HD12	1.90	0.53
1:A:12:SER:O	1:A:13:GLU:HB3	2.08	0.53
1:A:132:ARG:HA	1:A:135:GLU:CG	2.36	0.53
1:B:166:VAL:HG22	1:B:189:VAL:HB	1.91	0.53
1:A:92:VAL:O	1:A:95:ALA:HB3	2.09	0.53
1:A:129:ARG:HH21	1:A:132:ARG:NE	2.07	0.53
1:A:269:SER:OG	1:A:272:GLU:HB2	2.09	0.53
1:A:292:ALA:O	1:A:296:ILE:HG13	2.09	0.53
1:B:200:ASP:OD1	1:B:200:ASP:N	2.42	0.53
1:B:253:LEU:CD2	1:B:267:VAL:HG23	2.39	0.53
1:A:88:TYR:O	1:A:92:VAL:HG23	2.09	0.53
1:A:52:MET:HE3	1:A:62:ILE:HD12	1.90	0.52
1:A:222:ILE:HD13	1:A:295:LEU:HD12	1.91	0.52
1:B:153:ILE:HD12	1:B:153:ILE:O	2.09	0.52
1:B:197:THR:HA	1:B:203:GLY:O	2.09	0.52
1:B:68:ASP:OD2	1:B:106:SER:HB3	2.09	0.52
1:B:293:GLU:O	1:B:297:LYS:HG3	2.09	0.52
1:B:301:PRO:O	1:B:305:ARG:HB2	2.09	0.52
1:A:300:GLU:HG2	1:A:303:ARG:NH2	2.24	0.52
1:A:83:ARG:HB2	1:A:83:ARG:CZ	2.39	0.52
1:A:201:GLY:HA3	1:A:230:TYR:CD2	2.44	0.52
1:B:212:PHE:CD1	1:B:212:PHE:C	2.87	0.52
1:A:238:GLY:O	1:A:240:PRO:HD3	2.10	0.52
1:A:73:LEU:C	1:A:75:GLN:H	2.18	0.52
1:B:65:LEU:HD13	1:B:103:VAL:HG23	1.92	0.52
1:B:279:ASN:OD1	1:B:281:GLU:HB2	2.09	0.52
1:A:258:PRO:CB	1:A:260:LYS:HG2	2.40	0.51
1:B:249:LEU:HD11	1:B:294:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD13	1:A:149:VAL:HG11	1.91	0.51
1:B:295:LEU:HD22	1:B:299:LEU:HD11	1.92	0.51
1:B:72:TYR:CD1	1:B:72:TYR:C	2.87	0.51
1:B:239:ASN:O	1:B:243:GLU:HG3	2.10	0.51
1:B:11:THR:HG22	1:B:13:GLU:H	1.74	0.51
1:B:4:PHE:O	1:B:8:LYS:HB2	2.09	0.51
1:A:80:ASP:OD1	1:A:81:GLU:N	2.44	0.51
1:B:205:MET:HA	1:B:211:ASN:ND2	2.25	0.51
1:A:252:PRO:HB3	1:A:268:ASN:HA	1.93	0.51
1:B:83:ARG:HB2	1:B:83:ARG:HH11	1.75	0.51
1:B:126:THR:HB	1:B:128:LYS:CD	2.41	0.51
1:A:257:ARG:HH12	1:A:261:PHE:HD2	1.59	0.50
1:B:128:LYS:H	1:B:128:LYS:HE3	1.76	0.50
1:B:33:ILE:HG22	1:B:52:MET:HE2	1.93	0.50
1:B:36:GLU:O	1:B:37:PRO:C	2.51	0.50
1:A:298:ILE:O	1:A:301:PRO:HD2	2.12	0.50
1:B:4:PHE:CD1	1:B:4:PHE:C	2.89	0.50
1:A:65:LEU:HD12	1:A:66:LEU:N	2.27	0.50
1:A:239:ASN:HB3	1:A:242:MET:HB2	1.92	0.50
1:A:271:GLU:CD	1:A:271:GLU:H	2.19	0.50
1:A:137:ILE:HD11	1:A:173:GLN:OE1	2.11	0.50
1:A:222:ILE:HG21	1:A:295:LEU:HD12	1.93	0.50
1:B:257:ARG:CZ	1:B:265:LEU:HD11	2.42	0.50
1:A:10:ASN:ND2	1:A:247:TYR:CD1	2.80	0.50
1:A:258:PRO:O	1:A:260:LYS:N	2.45	0.50
1:B:229:ALA:HB3	1:B:241:ILE:HD11	1.94	0.50
1:A:71:ALA:O	1:A:76:LYS:HB2	2.11	0.49
1:A:129:ARG:NH2	1:A:132:ARG:HE	2.08	0.49
1:B:96:MET:HE3	1:B:215:VAL:HG11	1.93	0.49
1:B:155:GLN:O	1:B:158:ALA:HB3	2.12	0.49
1:A:43:LEU:CB	1:A:205:MET:HE1	2.35	0.49
1:A:71:ALA:HB3	1:A:82:ILE:HD13	1.94	0.49
1:B:129:ARG:HG3	1:B:179:LEU:HD21	1.94	0.49
1:B:295:LEU:HD22	1:B:299:LEU:CD1	2.42	0.49
1:B:290:ALA:O	1:B:294:GLU:HB2	2.11	0.49
1:B:77:GLY:HA3	1:B:82:ILE:HG13	1.94	0.49
1:B:268:ASN:N	1:B:268:ASN:HD22	2.11	0.49
1:A:33:ILE:HB	1:A:168:VAL:HB	1.93	0.49
1:A:237:GLU:CD	1:A:237:GLU:N	2.68	0.49
1:B:96:MET:HG2	1:B:302:ILE:HD13	1.94	0.49
1:A:260:LYS:HG3	1:A:261:PHE:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HA	1:A:228:LYS:HE3	1.94	0.49
1:A:201:GLY:HA3	1:A:230:TYR:HD2	1.77	0.48
1:B:126:THR:HB	1:B:128:LYS:HD3	1.95	0.48
1:B:177:HIS:O	1:B:178:MET:C	2.55	0.48
1:B:225:LYS:O	1:B:228:LYS:HG3	2.13	0.48
1:B:236:VAL:CG2	1:B:278:LYS:HG3	2.44	0.48
1:B:246:LYS:HE3	1:B:247:TYR:OH	2.13	0.48
1:A:266:THR:HG22	1:A:266:THR:O	2.14	0.48
1:B:159:ILE:CG2	1:B:188:VAL:HG11	2.43	0.48
1:B:105:GLY:HA3	1:B:109:GLN:OE1	2.14	0.48
1:B:46:TYR:O	1:B:50:LYS:HG3	2.14	0.47
1:B:128:LYS:N	1:B:128:LYS:HE3	2.29	0.47
1:A:123:LEU:HD13	1:B:147:ALA:CB	2.44	0.47
1:B:48:GLN:C	1:B:50:LYS:N	2.69	0.47
1:A:78:GLU:O	1:A:82:ILE:HG13	2.14	0.47
1:A:117:ASN:O	1:A:120:ARG:HB2	2.14	0.47
1:B:219:PRO:O	1:B:223:ARG:HG3	2.15	0.47
1:A:81:GLU:HA	1:A:84:LYS:HE2	1.97	0.47
1:B:229:ALA:HB1	1:B:241:ILE:HD11	1.97	0.47
1:A:7:ILE:HD13	1:A:55:LEU:CD2	2.44	0.47
1:A:7:ILE:CD1	1:A:55:LEU:HD23	2.43	0.47
1:B:52:MET:HE3	1:B:62:ILE:HG23	1.95	0.47
1:B:206:SER:C	1:B:208:SER:N	2.72	0.47
1:A:15:ILE:HG21	1:A:181:ARG:HD2	1.96	0.47
1:B:300:GLU:OE2	1:B:304:LYS:HD2	2.14	0.47
1:B:127:LEU:HB2	1:B:128:LYS:HZ1	1.80	0.47
1:A:128:LYS:O	1:A:132:ARG:HG3	2.15	0.47
1:A:169:GLY:O	1:A:192:HIS:HA	2.15	0.46
1:A:304:LYS:C	1:A:306:LEU:H	2.23	0.46
1:B:82:ILE:O	1:B:83:ARG:C	2.58	0.46
1:B:178:MET:HE2	1:B:182:GLU:OE2	2.15	0.46
1:A:70:HIS:O	1:A:74:ASN:HB2	2.15	0.46
1:B:53:ILE:HG12	1:B:56:GLN:NE2	2.30	0.46
1:B:73:LEU:C	1:B:75:GLN:H	2.23	0.46
1:B:134:MET:SD	1:B:137:ILE:HD12	2.54	0.46
1:B:168:VAL:HG12	1:B:169:GLY:N	2.30	0.46
1:B:118:VAL:CB	1:B:153:ILE:HD11	2.46	0.46
1:A:90:LYS:HG2	1:A:94:GLU:OE1	2.15	0.46
1:B:161:TYR:HB3	1:B:162:PRO:HD3	1.97	0.46
1:B:176:ILE:O	1:B:179:LEU:HB2	2.15	0.46
1:A:46:TYR:O	1:A:50:LYS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLN:HG2	1:B:114:TYR:CZ	2.51	0.46
1:B:230:TYR:CE1	1:B:232:PRO:HD3	2.51	0.46
1:A:267:VAL:HG23	1:A:267:VAL:O	2.16	0.46
1:B:20:LEU:O	1:B:23:VAL:HB	2.16	0.46
1:B:148:GLU:O	1:B:152:PRO:HD2	2.16	0.46
1:B:267:VAL:HG12	1:B:272:GLU:CB	2.45	0.46
1:A:146:VAL:O	1:A:149:VAL:HG22	2.16	0.45
1:B:127:LEU:H	1:B:128:LYS:HZ2	1.64	0.45
1:B:242:MET:O	1:B:245:ALA:HB3	2.17	0.45
1:A:151:TYR:N	1:A:152:PRO:HD2	2.31	0.45
1:A:217:ASP:HB3	1:A:221:GLU:HB2	1.97	0.45
1:B:300:GLU:HB3	1:B:301:PRO:HD3	1.97	0.45
1:B:128:LYS:CE	1:B:128:LYS:N	2.77	0.45
1:B:218:SER:O	1:B:221:GLU:N	2.50	0.45
1:A:143:ASN:HA	1:A:144:PRO:HD2	1.70	0.45
1:B:48:GLN:O	1:B:52:MET:HG2	2.16	0.45
1:A:207:SER:C	1:A:209:LYS:N	2.75	0.45
1:A:287:LEU:HD22	1:A:291:VAL:CG2	2.46	0.45
1:B:82:ILE:O	1:B:85:ILE:N	2.49	0.45
1:B:178:MET:O	1:B:181:ARG:HB3	2.17	0.45
1:B:260:LYS:H	1:B:260:LYS:HG2	1.61	0.45
1:B:304:LYS:C	1:B:306:LEU:H	2.24	0.45
1:A:105:GLY:HA2	1:A:108:PHE:CE2	2.52	0.45
1:B:78:GLU:O	1:B:80:ASP:N	2.50	0.45
1:B:126:THR:OG1	1:B:129:ARG:HB2	2.16	0.45
1:B:134:MET:SD	1:B:151:TYR:CD2	3.06	0.45
1:B:273:LEU:HD12	1:B:282:LEU:CD2	2.46	0.45
1:B:49:ILE:O	1:B:49:ILE:HG22	2.16	0.44
1:B:136:LEU:HD13	1:B:136:LEU:O	2.17	0.44
1:A:65:LEU:HD13	1:A:103:VAL:HG23	1.99	0.44
1:B:151:TYR:N	1:B:152:PRO:HD2	2.32	0.44
1:A:15:ILE:O	1:A:16:SER:HB3	2.18	0.44
1:A:8:LYS:HG2	1:A:14:ILE:HD12	1.99	0.44
1:A:126:THR:OG1	1:A:129:ARG:HB2	2.17	0.44
1:A:212:PHE:CD1	1:A:212:PHE:C	2.95	0.44
1:A:259:GLU:CD	1:A:259:GLU:H	2.25	0.44
1:A:260:LYS:HB2	1:A:260:LYS:HE3	1.77	0.44
1:B:178:MET:O	1:B:182:GLU:HG3	2.17	0.44
1:A:246:LYS:HB2	1:A:270:TYR:CZ	2.52	0.44
1:A:73:LEU:HD21	1:B:116:LEU:CD1	2.47	0.44
1:A:174:ARG:HB3	1:A:192:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:NH1	1:A:9:ARG:HG2	2.33	0.44
1:A:198:GLY:HA2	1:A:205:MET:HG2	1.99	0.44
1:A:303:ARG:O	1:A:306:LEU:HB2	2.18	0.44
1:B:18:GLU:HG3	1:B:19:GLU:H	1.82	0.43
1:B:89:ASN:N	1:B:89:ASN:HD22	2.16	0.43
1:A:1:MET:HG2	1:A:2:ASP:H	1.80	0.43
1:A:160:HIS:HB2	1:A:184:LEU:HD13	1.99	0.43
1:A:176:ILE:CD1	1:A:176:ILE:N	2.65	0.43
1:B:1:MET:CE	1:B:6:MET:HG3	2.48	0.43
1:A:219:PRO:HB3	1:A:296:ILE:HD13	2.00	0.43
1:B:35:PHE:CE2	1:B:49:ILE:HD11	2.53	0.43
1:B:252:PRO:HA	1:B:267:VAL:O	2.19	0.43
1:A:15:ILE:O	1:A:15:ILE:HG23	2.16	0.43
1:A:53:ILE:HG12	1:A:56:GLN:NE2	2.33	0.43
1:A:257:ARG:NH1	1:A:261:PHE:HD2	2.16	0.43
1:B:111:ASP:O	1:B:112:LYS:C	2.60	0.43
1:A:30:SER:OG	1:A:164:VAL:HA	2.17	0.43
1:B:222:ILE:O	1:B:226:ILE:HG12	2.19	0.43
1:B:1:MET:O	1:B:2:ASP:C	2.62	0.43
1:A:46:TYR:HD1	1:A:96:MET:SD	2.42	0.43
1:A:69:LEU:HD12	1:A:109:GLN:HB2	2.01	0.43
1:A:140:GLU:O	1:A:140:GLU:HG3	2.18	0.43
1:A:294:GLU:O	1:A:298:ILE:HG13	2.18	0.43
1:B:141:ASP:O	1:B:142:GLU:C	2.61	0.43
1:B:153:ILE:HD12	1:B:153:ILE:C	2.44	0.43
1:A:9:ARG:HG2	1:A:9:ARG:HH11	1.84	0.42
1:A:245:ALA:CA	1:A:249:LEU:HD22	2.30	0.42
1:A:246:LYS:HB2	1:A:270:TYR:CE2	2.54	0.42
1:B:261:PHE:HE1	1:B:283:HIS:CG	2.37	0.42
1:A:300:GLU:HB3	1:A:301:PRO:CD	2.43	0.42
1:B:15:ILE:HD13	1:B:15:ILE:HA	1.78	0.42
1:B:33:ILE:HD11	1:B:48:GLN:OE1	2.19	0.42
1:B:35:PHE:O	1:B:66:LEU:HA	2.19	0.42
1:B:89:ASN:O	1:B:90:LYS:C	2.61	0.42
1:B:193:ASN:HD22	1:B:194:PRO:HD2	1.81	0.42
1:A:263:GLY:O	1:A:265:LEU:HG	2.19	0.42
1:B:56:GLN:HA	1:B:60:PHE:O	2.20	0.42
1:B:70:HIS:NE2	1:B:155:GLN:NE2	2.66	0.42
1:B:121:LEU:HB2	1:B:153:ILE:HD13	2.01	0.42
1:A:132:ARG:O	1:A:135:GLU:HB2	2.20	0.42
1:A:216:ASP:HA	1:A:303:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:TYR:CD1	1:B:157:ASN:ND2	2.88	0.42
1:B:242:MET:CE	1:B:274:GLU:HA	2.49	0.42
1:A:13:GLU:OE2	1:A:174:ARG:NH1	2.45	0.42
1:B:240:PRO:HA	1:B:243:GLU:OE2	2.19	0.42
1:A:1:MET:CG	1:A:2:ASP:N	2.81	0.42
1:B:253:LEU:HD23	1:B:253:LEU:N	2.29	0.42
1:A:133:SER:HA	1:A:175:LYS:HB3	2.00	0.42
1:A:162:PRO:HB2	1:A:164:VAL:HG13	2.02	0.42
1:A:270:TYR:O	1:A:271:GLU:C	2.62	0.42
1:B:31:ALA:HB2	1:B:166:VAL:HB	2.02	0.42
1:B:218:SER:O	1:B:219:PRO:C	2.61	0.42
1:B:233:ALA:C	1:B:235:VAL:H	2.28	0.42
1:B:56:GLN:CA	1:B:62:ILE:HD11	2.50	0.42
1:A:62:ILE:HG21	1:A:98:LEU:HD11	2.03	0.41
1:A:140:GLU:O	1:A:140:GLU:CG	2.68	0.41
1:A:147:ALA:HB3	1:B:123:LEU:HD13	2.02	0.41
1:B:170:GLY:HA3	1:B:172:GLU:OE2	2.19	0.41
1:A:130:ALA:O	1:A:133:SER:HB2	2.20	0.41
1:B:90:LYS:O	1:B:94:GLU:HG3	2.21	0.41
1:B:212:PHE:CD1	1:B:212:PHE:O	2.73	0.41
1:A:166:VAL:HG22	1:A:189:VAL:HB	2.02	0.41
1:A:256:LYS:O	1:A:257:ARG:HB2	2.19	0.41
1:B:138:ALA:O	1:B:139:ARG:C	2.63	0.41
1:B:256:LYS:H	1:B:256:LYS:NZ	2.17	0.41
1:B:1:MET:HE1	1:B:6:MET:HG3	2.02	0.41
1:B:127:LEU:HA	1:B:127:LEU:HD22	1.82	0.41
1:A:199:LEU:HD22	1:A:229:ALA:HB2	2.03	0.41
1:A:294:GLU:O	1:A:295:LEU:C	2.63	0.41
1:B:17:GLU:O	1:B:20:LEU:N	2.53	0.41
1:B:29:LYS:HD2	1:B:60:PHE:CE1	2.56	0.41
1:A:32:GLN:HB2	1:A:164:VAL:HG11	2.02	0.41
1:A:104:TYR:C	1:A:106:SER:N	2.79	0.41
1:B:8:LYS:HA	1:B:14:ILE:HD11	2.03	0.41
1:B:16:SER:OG	1:B:19:GLU:CD	2.64	0.41
1:B:85:ILE:HA	1:B:85:ILE:HD13	1.84	0.41
1:A:1:MET:CG	1:A:2:ASP:H	2.34	0.41
1:A:85:ILE:O	1:A:88:TYR:HB3	2.21	0.41
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.94	0.41
1:B:162:PRO:HG2	1:B:164:VAL:HG13	2.03	0.41
1:B:255:ILE:HD13	1:B:282:LEU:HD21	2.02	0.41
1:A:151:TYR:CD1	1:A:151:TYR:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:O	1:A:240:PRO:HD2	2.22	0.40
1:B:276:LEU:HA	1:B:279:ASN:HD21	1.84	0.40
1:A:249:LEU:HD12	1:A:298:ILE:CD1	2.51	0.40
1:B:254:THR:CG2	1:B:266:THR:HG23	2.51	0.40
1:B:279:ASN:O	1:B:280:LYS:HB2	2.21	0.40
1:A:144:PRO:O	1:B:128:LYS:NZ	2.53	0.40
1:B:24:LEU:HD23	1:B:60:PHE:HE1	1.86	0.40
1:B:102:TYR:CD1	1:B:102:TYR:N	2.90	0.40
1:A:4:PHE:CG	1:A:21:ARG:NH1	2.90	0.40
1:A:27:ASP:N	1:A:27:ASP:OD1	2.49	0.40
1:A:93:PHE:HB3	1:A:98:LEU:HD23	2.03	0.40
1:A:117:ASN:O	1:A:118:VAL:C	2.64	0.40
1:A:133:SER:HA	1:A:175:LYS:CB	2.51	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.40
1:B:127:LEU:CB	1:B:128:LYS:HZ1	2.35	0.40
1:A:49:ILE:HG23	1:A:98:LEU:HD22	2.04	0.40
1:B:237:GLU:CD	1:B:237:GLU:N	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/312 (97%)	255 (84%)	35 (12%)	14 (5%)	2	11
1	B	304/312 (97%)	263 (86%)	31 (10%)	10 (3%)	3	17
All	All	608/624 (97%)	518 (85%)	66 (11%)	24 (4%)	2	14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	140	GLU
1	A	141	ASP
1	B	79	LEU
1	B	209	LYS
1	A	77	GLY
1	A	229	ALA
1	B	16	SER
1	A	74	ASN
1	A	75	GLN
1	A	266	THR
1	A	305	ARG
1	B	109	GLN
1	B	199	LEU
1	B	264	ASP
1	A	112	LYS
1	A	259	GLU
1	B	76	LYS
1	B	139	ARG
1	B	212	PHE
1	A	257	ARG
1	B	137	ILE
1	A	15	ILE
1	A	262	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/273 (97%)	237 (89%)	29 (11%)	6	26
1	B	264/273 (97%)	233 (88%)	31 (12%)	5	23
All	All	530/546 (97%)	470 (89%)	60 (11%)	5	24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	8	LYS
1	A	15	ILE
1	A	20	LEU
1	A	50	LYS
1	A	69	LEU
1	A	83	ARG
1	A	123	LEU
1	A	125	THR
1	A	127	LEU
1	A	129	ARG
1	A	140	GLU
1	A	141	ASP
1	A	143	ASN
1	A	148	GLU
1	A	154	MET
1	A	155	GLN
1	A	166	VAL
1	A	172	GLU
1	A	174	ARG
1	A	176	ILE
1	A	237	GLU
1	A	249	LEU
1	A	257	ARG
1	A	268	ASN
1	A	272	GLU
1	A	279	ASN
1	A	287	LEU
1	A	289	ASN
1	B	8	LYS
1	B	18	GLU
1	B	20	LEU
1	B	69	LEU
1	B	83	ARG
1	B	123	LEU
1	B	127	LEU
1	B	128	LYS
1	B	133	SER
1	B	136	LEU
1	B	140	GLU
1	B	142	GLU
1	B	148	GLU
1	B	153	ILE

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Mol	Chain	Res	Type
1	B	172	GLU
1	B	173	GLN
1	B	186	LYS
1	B	193	ASN
1	B	196	LEU
1	B	202	GLU
1	B	228	LYS
1	B	237	GLU
1	B	249	LEU
1	B	256	LYS
1	B	268	ASN
1	B	269	SER
1	B	271	GLU
1	B	287	LEU
1	B	289	ASN
1	B	295	LEU
1	B	300	GLU

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	70	HIS
1	A	75	GLN
1	A	109	GLN
1	A	177	HIS
1	A	268	ASN
1	A	279	ASN
1	B	32	GLN
1	B	56	GLN
1	B	57	ASN
1	B	74	ASN
1	B	155	GLN
1	B	173	GLN
1	B	193	ASN
1	B	211	ASN
1	B	268	ASN

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	306/312 (98%)	0.04	11 (3%) 46 26	2, 29, 80, 132	0
1	B	306/312 (98%)	0.24	12 (3%) 43 24	10, 38, 74, 98	0
All	All	612/624 (98%)	0.14	23 (3%) 44 24	2, 34, 76, 132	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	4.3
1	A	140	GLU	3.5
1	A	257	ARG	3.2
1	A	206	SER	3.1
1	B	140	GLU	2.9
1	A	208	SER	2.9
1	B	306	LEU	2.9
1	B	261	PHE	2.5
1	A	265	LEU	2.5
1	A	267	VAL	2.4
1	B	77	GLY	2.3
1	B	141	ASP	2.3
1	A	266	THR	2.3
1	A	138	ALA	2.2
1	B	1	MET	2.2
1	B	57	ASN	2.2
1	B	210	GLY	2.2
1	A	75	GLN	2.2
1	B	135	GLU	2.2
1	B	129	ARG	2.2
1	A	285	MET	2.1
1	A	261	PHE	2.1
1	B	208	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	A	500	1/1	0.97	0.04	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.