



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:37 am GMT

PDB ID : 4JT6
Title : structure of mTORDeltaN-mLST8-PI-103 complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

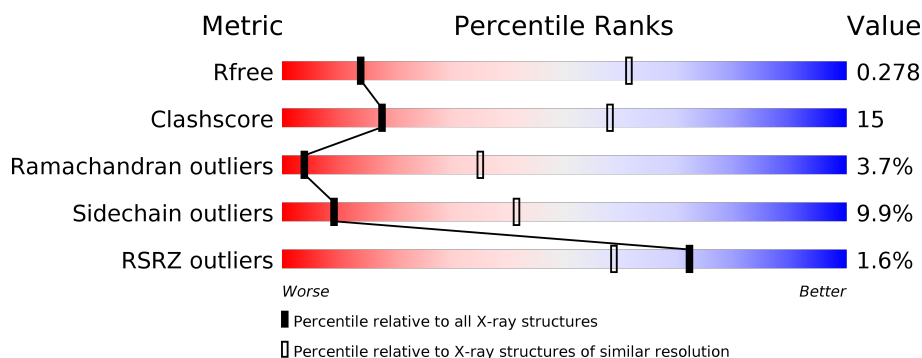
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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	1174	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>25%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	1174	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>5%</div> <div>10%</div> </div> </div>
2	C	326	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>7%</div> <div>.</div> </div> </div>
2	D	326	<div> <div></div> <div> <div></div> <div>55%</div> <div>35%</div> <div>7%</div> <div>..</div> </div> </div>

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.

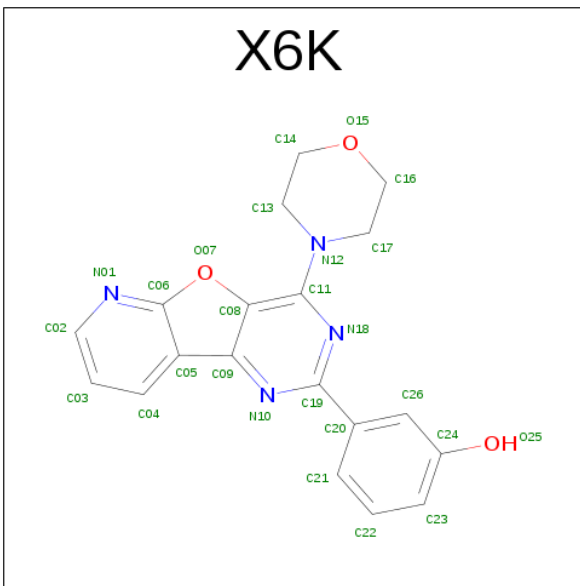
- Molecule 1 is a protein called mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total 8608	C 5472	N 1521	O 1552	S 63	0	0	0
1	A	1054	Total 8577	C 5451	N 1517	O 1546	S 63	0	0	0

- Molecule 2 is a protein called mLST8.

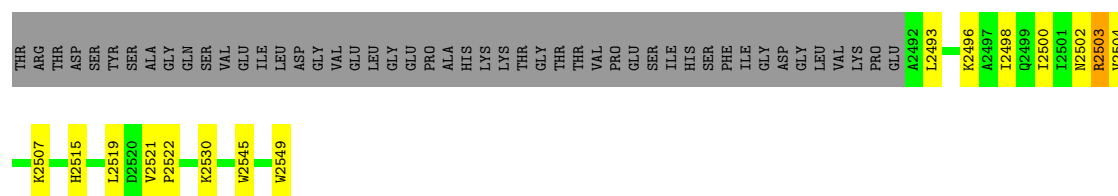
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total 2456	C 1526	N 436	O 476	S 18	0	0	0
2	C	317	Total 2456	C 1526	N 436	O 476	S 18	0	0	0

- Molecule 3 is 3-(4-MORPHOLIN-4-YPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (three-letter code: X6K) (formula: C₁₉H₁₆N₄O₃).



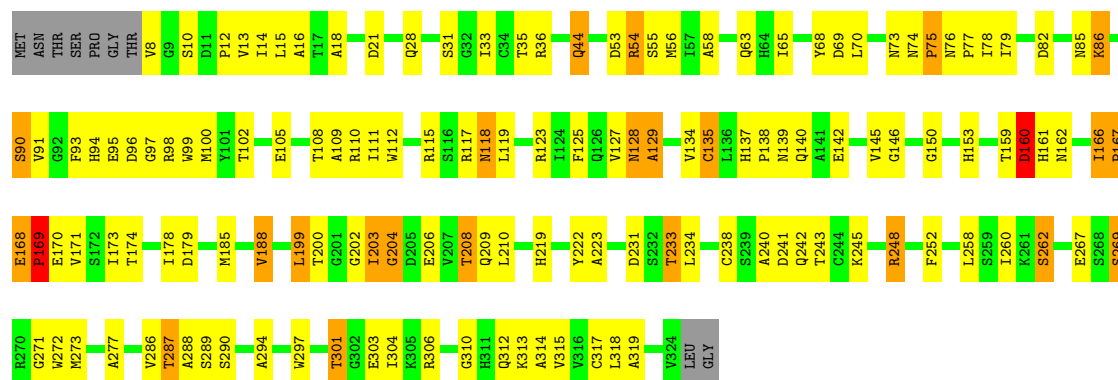
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			26	19	4	3		
3	A	1	Total	C	N	O	0	0
			26	19	4	3		





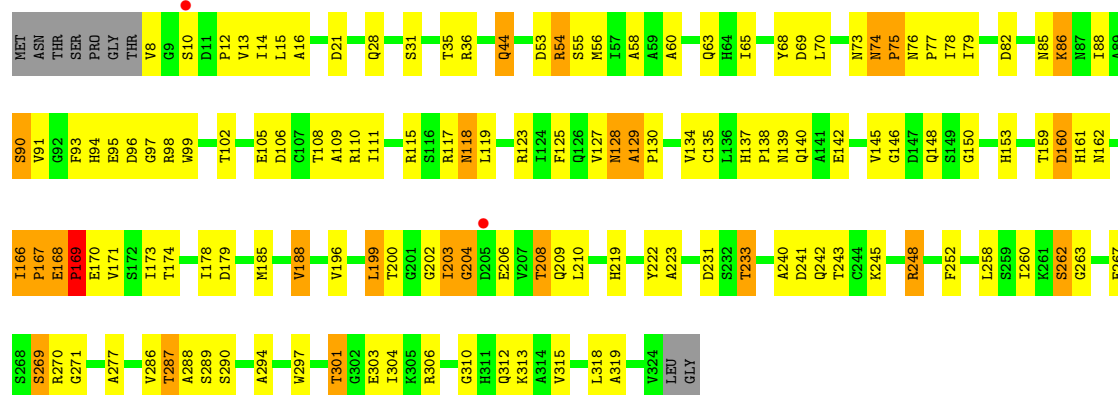
• Molecule 2: mLST8

Chain D: 55% 35% 7% ..



• Molecule 2: mLST8

Chain C: 55% 34% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 3.60 39.64 – 3.58	Depositor EDS
% Data completeness (in resolution range)	75.7 (39.67-3.60) 75.0 (39.64-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.239 , 0.275 0.241 , 0.278	Depositor DCC
R_{free} test set	1294 reflections (3.17%)	DCC
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22149	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0214e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: X6K

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	0.33	0/8772	0.58	1/11872 (0.0%)
1	B	0.33	0/8805	0.58	1/11920 (0.0%)
2	C	0.35	0/2514	0.62	0/3426
2	D	0.38	0/2514	0.63	0/3426
All	All	0.34	0/22605	0.59	2/30644 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	5.36	125.47	111.00
1	B	1915	HIS	N-CA-C	5.30	125.30	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	B	1914	GLY	Peptide
2	C	169	PRO	Peptide
2	D	169	PRO	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	8577	0	8559	229	0
1	B	8608	0	8593	243	0
2	C	2456	0	2341	104	0
2	D	2456	0	2341	109	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
All	All	22149	0	21866	672	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 15.

All (672) 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)
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.47	1.12
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.47	1.12
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.32	1.11
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.33	1.08
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.34	1.06
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.41	1.01
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.42	0.99
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.46	0.95
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.64	0.95
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.47	0.93
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.68	0.91
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.55	0.89
2:C:95:GLU:HB2	2:C:140:GLN:NE2	1.89	0.88
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.54	0.87
2:D:95:GLU:HB2	2:D:140:GLN:NE2	1.89	0.87
1:B:1643:VAL:HG12	1:B:1644:VAL:HG23	1.58	0.85
1:B:2380:THR:HG23	1:B:2549:TRP:O	1.77	0.85
1:A:2503:ARG:HH11	1:A:2507:LYS:HE2	1.43	0.83
1:A:2187:LYS:HZ2	1:A:2187:LYS:HB3	1.42	0.82
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.80	0.81
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.63	0.81
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.64	0.80
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.43	0.80
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.64	0.80
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.63	0.79
1:B:2503:ARG:HH11	1:B:2507:LYS:HE2	1.47	0.79
1:B:1566:LYS:O	1:B:1570:LEU:HG	1.81	0.79
1:A:2503:ARG:NH1	1:A:2507:LYS:HE2	1.98	0.79
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.83	0.79
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.11	0.79
1:A:2380:THR:HG23	1:A:2549:TRP:O	1.84	0.78
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.47	0.78
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.46	0.78
1:A:2146:PRO:O	1:A:2147:ASN:HB2	1.84	0.78
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.66	0.77
2:C:117:ARG:O	2:C:118:ASN:HB2	1.82	0.77
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.13	0.77
2:D:231:ASP:CB	2:D:233:THR:OG1	2.30	0.77
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.20	0.77
1:B:2187:LYS:HB3	1:B:2187:LYS:HZ2	1.49	0.77
2:D:117:ARG:O	2:D:118:ASN:HB2	1.82	0.77
1:B:2146:PRO:O	1:B:2147:ASN:HB2	1.85	0.76
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.66	0.76
2:D:16:ALA:HB3	2:D:319:ALA:HB3	1.68	0.76
1:A:2185:LEU:HD13	1:A:2239:TRP:HZ3	1.49	0.76
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.68	0.76
1:A:1643:VAL:HG12	1:A:1644:VAL:HG23	1.67	0.75
1:B:1926:GLY:O	1:B:1930:ILE:HG22	1.86	0.75
2:C:137:HIS:CD2	2:C:139:ASN:H	2.05	0.74
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.70	0.74
2:D:301:THR:HB	2:D:303:GLU:HG2	1.69	0.74
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.23	0.74
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.70	0.73
2:C:301:THR:HB	2:C:303:GLU:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:ASP:CB	2:C:233:THR:OG1	2.32	0.73
1:A:2095:LYS:O	1:A:2099:GLN:HG2	1.87	0.73
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.71	0.73
2:D:137:HIS:CD2	2:D:139:ASN:H	2.08	0.72
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.72	0.72
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.70	0.72
1:B:2095:LYS:O	1:B:2099:GLN:HG2	1.89	0.72
1:B:2503:ARG:NH1	1:B:2507:LYS:HE2	2.05	0.72
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.72	0.71
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.70	0.71
1:A:1508:THR:O	1:A:1512:MET:HB2	1.90	0.71
1:A:1926:GLY:O	1:A:1930:ILE:HG22	1.90	0.71
1:B:1508:THR:O	1:B:1512:MET:HB2	1.89	0.70
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.20	0.70
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.27	0.70
1:A:2185:LEU:HD13	1:A:2239:TRP:CZ3	2.27	0.69
1:A:2390:THR:O	1:A:2390:THR:HG23	1.91	0.69
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.27	0.69
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.74	0.69
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.74	0.69
1:B:2390:THR:HG23	1:B:2390:THR:O	1.93	0.69
1:B:2187:LYS:HG3	1:B:2237:ILE:HD12	1.75	0.68
1:A:1418:SER:CB	1:A:1581:GLU:HG2	2.19	0.68
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.06	0.68
1:A:1566:LYS:O	1:A:1570:LEU:HG	1.94	0.68
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.28	0.68
1:B:2185:LEU:HD13	1:B:2239:TRP:HZ3	1.57	0.68
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.29	0.68
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.09	0.67
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.76	0.67
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.76	0.67
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.24	0.67
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.26	0.67
1:B:1501:TRP:HH2	1:B:1509:GLN:OE1	1.77	0.67
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.25	0.67
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.95	0.66
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.31	0.66
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.11	0.66
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.31	0.65
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.78	0.65
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.31	0.65
2:C:166:ILE:HG13	2:C:166:ILE:O	1.96	0.65
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.44	0.65
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.96	0.65
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.24	0.65
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.96	0.64
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.29	0.64
2:C:137:HIS:HD2	2:C:139:ASN:H	1.43	0.64
2:D:166:ILE:HG13	2:D:166:ILE:O	1.97	0.64
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.78	0.64
1:A:1913:TYR:O	1:A:1915:HIS:HA	1.97	0.64
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.80	0.64
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	1.98	0.64
1:A:2411:LYS:O	1:A:2415:MET:HG3	1.97	0.64
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.31	0.64
1:A:1734:THR:C	1:A:1736:ASP:H	2.00	0.63
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.28	0.63
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	1.98	0.63
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.98	0.63
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.81	0.63
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.34	0.63
1:B:2169:PRO:HB3	1:B:2187:LYS:HE2	1.80	0.63
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.47	0.63
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.81	0.63
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.98	0.62
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.13	0.62
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.12	0.62
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.29	0.62
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.98	0.62
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.99	0.62
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.81	0.62
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.82	0.62
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.30	0.62
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.99	0.62
1:B:2178:ASN:ND2	1:B:2180:HIS:H	1.97	0.61
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.83	0.61
1:A:2178:ASN:ND2	1:A:2180:HIS:H	1.97	0.61
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.35	0.61
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.30	0.61
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.36	0.61
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:HIS:HD2	2:D:139:ASN:H	1.47	0.61
2:C:168:GLU:N	2:C:169:PRO:HD2	2.16	0.61
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.81	0.60
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.83	0.60
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.83	0.60
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.01	0.60
1:B:1913:TYR:HB3	1:B:1916:TRP:HE1	1.65	0.60
1:A:2187:LYS:NZ	1:A:2187:LYS:HB3	2.16	0.60
1:B:2187:LYS:HB3	1:B:2187:LYS:NZ	2.16	0.60
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.83	0.60
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.82	0.60
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.02	0.60
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.02	0.60
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.85	0.60
1:B:2380:THR:HG23	1:B:2549:TRP:C	2.22	0.59
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.84	0.59
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.37	0.59
2:D:168:GLU:N	2:D:169:PRO:HD2	2.18	0.59
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.30	0.59
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.35	0.59
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.84	0.58
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.03	0.58
2:D:21:ASP:HB3	2:D:313:LYS:H	1.68	0.58
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.68	0.58
2:D:169:PRO:HA	2:D:171:VAL:HG22	1.85	0.58
1:A:2382:MET:SD	1:A:2549:TRP:HA	2.44	0.58
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.85	0.58
1:B:2503:ARG:HH11	1:B:2507:LYS:CE	2.13	0.58
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.69	0.58
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.86	0.58
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.86	0.58
2:C:65:ILE:HD11	2:C:102:THR:HG21	1.85	0.58
2:D:55:SER:O	2:D:56:MET:HG2	2.02	0.58
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.52	0.57
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.38	0.57
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.06	0.57
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.85	0.57
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.86	0.57
1:A:1913:TYR:HB3	1:A:1916:TRP:HE1	1.68	0.57
2:D:65:ILE:HD11	2:D:102:THR:HG21	1.85	0.57
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.52	0.57
1:B:2185:LEU:HD13	1:B:2239:TRP:CZ3	2.39	0.57
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.05	0.57
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.87	0.57
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.05	0.57
2:C:203:ILE:HA	2:C:206:GLU:HG2	1.87	0.57
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.86	0.56
1:A:2336:LEU:HG	1:A:2339:ARG:HD2	1.86	0.56
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.86	0.56
2:C:14:ILE:HD13	2:C:70:LEU:HD13	1.87	0.56
2:C:65:ILE:CD1	2:C:102:THR:HG21	2.35	0.56
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.87	0.56
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.88	0.56
1:B:2015:GLU:OE2	1:B:2127:SER:OG	2.15	0.56
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.87	0.56
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.86	0.56
2:C:21:ASP:HB3	2:C:313:LYS:H	1.70	0.56
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.35	0.56
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.53	0.56
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.71	0.56
2:D:200:THR:O	2:D:208:THR:HA	2.06	0.56
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.06	0.55
2:C:63:GLN:HE21	2:C:86:LYS:H	1.53	0.55
2:D:65:ILE:CD1	2:D:102:THR:HG21	2.36	0.55
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.39	0.55
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.89	0.55
1:B:2382:MET:SD	1:B:2549:TRP:HA	2.46	0.55
1:A:2380:THR:HG23	1:A:2549:TRP:C	2.27	0.55
2:D:231:ASP:HB3	2:D:233:THR:HG1	1.68	0.55
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.55	0.55
1:A:2515:HIS:N	1:A:2515:HIS:ND1	2.54	0.55
1:B:1501:TRP:CH2	1:B:1509:GLN:OE1	2.60	0.55
1:A:1643:VAL:HG12	1:A:1644:VAL:CG2	2.36	0.55
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.10	0.55
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.88	0.55
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.87	0.55
1:B:1417:ILE:HG23	1:B:1432:VAL:HB	1.88	0.55
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.89	0.54
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.07	0.54
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.22	0.54
2:D:63:GLN:HE21	2:D:86:LYS:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.89	0.54
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.72	0.54
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.73	0.54
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.90	0.54
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.38	0.54
1:B:2336:LEU:HG	1:B:2339:ARG:HD2	1.89	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.90	0.54
1:B:1506:ASP:HA	1:B:1509:GLN:HB2	1.90	0.54
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.23	0.54
1:B:1734:THR:C	1:B:1736:ASP:H	2.09	0.53
2:D:82:ASP:H	2:D:119:LEU:HD22	1.73	0.53
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.88	0.53
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.76	0.53
2:C:168:GLU:N	2:C:169:PRO:CD	2.72	0.53
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.90	0.53
1:A:1506:ASP:HA	1:A:1509:GLN:HB2	1.90	0.53
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.55	0.53
2:C:55:SER:O	2:C:56:MET:HG2	2.07	0.53
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.41	0.53
2:D:203:ILE:HA	2:D:206:GLU:HG2	1.91	0.53
2:D:262:SER:OG	2:D:267:GLU:HG2	2.09	0.53
2:C:200:THR:O	2:C:208:THR:HA	2.09	0.53
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.09	0.53
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.90	0.53
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.91	0.53
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.09	0.53
2:D:297:TRP:CZ3	2:D:304:ILE:HG12	2.44	0.53
2:D:56:MET:HB2	2:D:68:TYR:O	2.08	0.53
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.08	0.52
1:A:2078:LEU:HD11	1:A:2107:VAL:HG21	1.90	0.52
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.92	0.52
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.91	0.52
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.43	0.52
1:A:1501:TRP:HH2	1:A:1509:GLN:OE1	1.91	0.52
1:A:1734:THR:O	1:A:1736:ASP:N	2.36	0.52
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.92	0.52
1:B:1654:LEU:HD21	1:B:1696:VAL:HG22	1.91	0.52
1:A:1479:GLY:HA2	1:A:1482:ARG:NH1	2.25	0.52
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.08	0.52
2:C:82:ASP:H	2:C:119:LEU:HD22	1.73	0.52
2:D:14:ILE:HD13	2:D:70:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:ARG:O	2:D:252:PHE:HA	2.10	0.52
1:B:1681:PRO:HG2	1:B:1683:ARG:HG3	1.92	0.52
1:B:2095:LYS:HA	1:B:2098:THR:HG22	1.91	0.52
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.42	0.52
2:D:168:GLU:N	2:D:169:PRO:CD	2.73	0.52
1:A:2401:HIS:HB3	1:A:2521:VAL:HG12	1.91	0.52
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.75	0.52
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.75	0.51
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.93	0.51
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	1.91	0.51
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.40	0.51
1:A:1785:SER:O	1:A:1786:TRP:CB	2.58	0.51
1:B:2319:ASN:HD22	1:B:2352:LYS:HG3	1.75	0.51
1:B:2254:ARG:NH1	1:B:2298:ASP:OD2	2.43	0.51
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.92	0.51
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.45	0.51
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	1.93	0.51
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.09	0.51
2:D:200:THR:HB	2:D:209:GLN:H	1.75	0.51
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	1.93	0.51
1:A:2187:LYS:CG	1:A:2237:ILE:HD12	2.41	0.51
2:C:262:SER:OG	2:C:267:GLU:HG2	2.10	0.51
1:B:1605:TYR:O	1:B:1605:TYR:HD2	1.93	0.51
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.76	0.51
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.75	0.51
1:B:2418:LEU:O	1:B:2422:VAL:HG23	2.11	0.51
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.10	0.51
2:D:203:ILE:HG22	2:D:204:GLY:H	1.76	0.51
1:A:1786:TRP:NE1	1:A:1788:LYS:HB2	2.25	0.51
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.92	0.51
1:B:1783:ASP:O	1:B:1785:SER:N	2.44	0.51
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.92	0.51
1:A:1680:ASP:C	1:A:1682:SER:N	2.65	0.50
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.44	0.50
1:B:1786:TRP:NE1	1:B:1788:LYS:HB2	2.25	0.50
2:C:203:ILE:HG22	2:C:204:GLY:H	1.76	0.50
2:D:287:THR:O	2:D:294:ALA:HA	2.10	0.50
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.10	0.50
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.94	0.50
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.41	0.50
1:B:2401:HIS:HB3	1:B:2521:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1999:CYS:C	1:A:2001:HIS:H	2.15	0.50
1:A:2278:LEU:HB3	1:A:2282:GLN:HB2	1.93	0.50
2:D:203:ILE:HG22	2:D:204:GLY:N	2.26	0.50
1:B:1422:LYS:C	1:B:1424:GLN:H	2.14	0.50
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.94	0.50
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.44	0.50
2:C:31:SER:C	2:C:306:ARG:HD3	2.31	0.50
2:C:200:THR:HB	2:C:209:GLN:H	1.75	0.50
2:C:203:ILE:HG22	2:C:204:GLY:N	2.26	0.50
2:C:297:TRP:CZ3	2:C:304:ILE:HG12	2.46	0.50
1:A:1605:TYR:O	1:A:1605:TYR:HD2	1.94	0.50
1:A:2390:THR:O	1:A:2390:THR:CG2	2.60	0.50
1:B:2168:ARG:O	1:B:2170:ARG:NH1	2.43	0.50
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.77	0.50
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.47	0.50
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.92	0.50
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.93	0.50
1:A:2297:ASP:HB3	1:A:2301:LYS:HD2	1.93	0.50
1:B:2297:ASP:HB3	1:B:2301:LYS:HD2	1.94	0.50
1:A:1422:LYS:C	1:A:1424:GLN:H	2.15	0.50
1:A:1681:PRO:HG2	1:A:1683:ARG:HG3	1.94	0.50
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.42	0.50
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.93	0.50
1:A:1783:ASP:O	1:A:1785:SER:N	2.45	0.49
1:B:1785:SER:O	1:B:1786:TRP:CB	2.60	0.49
1:A:1551:ALA:HB1	1:A:1556:LEU:HB2	1.94	0.49
1:A:1583:TYR:C	1:A:1585:ARG:H	2.16	0.49
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	1.94	0.49
1:A:1514:ARG:HH21	1:A:1540:THR:HG21	1.76	0.49
1:B:2078:LEU:HD11	1:B:2107:VAL:HG21	1.94	0.49
2:D:169:PRO:HA	2:D:171:VAL:H	1.77	0.49
1:A:1443:LEU:HD23	1:A:1452:LYS:HZ3	1.77	0.49
1:B:2170:ARG:HB2	1:B:2186:LEU:HB3	1.94	0.49
2:C:169:PRO:HA	2:C:171:VAL:H	1.77	0.49
2:D:248:ARG:O	2:D:252:PHE:N	2.45	0.49
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.95	0.49
1:A:1796:MET:CE	1:A:1796:MET:HA	2.42	0.49
1:B:1479:GLY:HA2	1:B:1482:ARG:NH1	2.28	0.49
2:C:287:THR:O	2:C:294:ALA:HA	2.11	0.49
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.47	0.49
2:D:53:ASP:C	2:D:55:SER:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1680:ASP:C	1:B:1682:SER:N	2.66	0.49
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.93	0.49
1:B:1583:TYR:C	1:B:1585:ARG:H	2.16	0.49
1:B:1796:MET:HA	1:B:1796:MET:CE	2.43	0.49
2:D:199:LEU:HD22	2:D:210:LEU:CD2	2.43	0.49
1:B:1623:LEU:O	1:B:1633:TRP:HH2	1.96	0.49
2:C:241:ASP:OD2	2:C:243:THR:HB	2.12	0.49
1:A:1443:LEU:CD2	1:A:1452:LYS:HZ3	2.26	0.49
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.77	0.49
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.53	0.49
1:B:1655:LYS:O	1:B:1658:SER:HB3	2.13	0.49
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.93	0.49
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	1.94	0.49
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	1.94	0.48
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.74	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.94	0.48
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.95	0.48
1:A:1514:ARG:NH2	1:A:1540:THR:HG21	2.28	0.48
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.13	0.48
1:B:1796:MET:HE1	1:B:1796:MET:HA	1.96	0.48
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.78	0.48
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.75	0.48
1:B:1443:LEU:CD2	1:B:1452:LYS:HZ3	2.26	0.48
1:B:1443:LEU:HD23	1:B:1452:LYS:HZ3	1.78	0.48
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.34	0.48
2:C:199:LEU:HD22	2:C:210:LEU:CD2	2.44	0.48
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.95	0.48
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.13	0.48
2:C:28:GLN:O	2:C:28:GLN:HG3	2.13	0.48
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.82	0.48
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.44	0.48
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.44	0.48
2:D:231:ASP:CB	2:D:233:THR:HG1	2.26	0.48
2:D:28:GLN:HE21	2:D:33:ILE:HD12	1.78	0.48
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.13	0.48
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.96	0.48
2:C:8:VAL:N	2:C:10:SER:HG	2.12	0.48
1:A:2018:ARG:NH1	1:A:2067:GLU:OE2	2.37	0.47
1:B:1574:GLU:OE2	1:B:1585:ARG:NH1	2.46	0.47
2:C:138:PRO:HD2	2:C:178:ILE:HD13	1.96	0.47
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.35	0.47
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.79	0.47
1:A:2340:HIS:HB2	1:A:2341:PRO:CD	2.45	0.47
1:A:2498:ILE:HG22	1:A:2502:ASN:HD21	1.80	0.47
1:B:1514:ARG:NH2	1:B:1540:THR:HG21	2.30	0.47
2:C:53:ASP:C	2:C:55:SER:H	2.18	0.47
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.23	0.47
1:A:2046:GLY:O	1:A:2050:VAL:HG23	2.14	0.47
1:B:1701:MET:HE1	1:B:1717:MET:N	2.28	0.47
2:D:137:HIS:HD2	2:D:138:PRO:N	2.12	0.47
1:A:1655:LYS:O	1:A:1658:SER:HB3	2.15	0.47
1:B:1920:ASN:O	1:B:1924:VAL:HG23	2.14	0.47
1:B:1999:CYS:C	1:B:2001:HIS:H	2.18	0.47
1:B:2390:THR:O	1:B:2390:THR:CG2	2.62	0.47
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.79	0.47
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.97	0.47
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.97	0.47
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.45	0.47
2:C:248:ARG:O	2:C:252:PHE:N	2.47	0.47
2:C:63:GLN:NE2	2:C:86:LYS:H	2.12	0.47
2:D:56:MET:HA	2:D:70:LEU:HG	1.97	0.47
2:D:8:VAL:N	2:D:10:SER:HG	2.13	0.47
1:B:1904:LEU:O	1:B:1907:LEU:HB2	2.14	0.47
1:A:1481:MET:HA	1:A:1484:LEU:HD12	1.97	0.47
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.97	0.47
1:A:1913:TYR:O	1:A:1914:GLY:C	2.52	0.47
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.49	0.47
2:D:100:MET:HB3	2:D:112:TRP:HB2	1.97	0.47
2:D:233:THR:HB	2:D:234:LEU:HG	1.97	0.47
1:A:2209:LEU:O	1:A:2215:SER:HB2	2.15	0.47
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.97	0.47
1:B:1562:GLN:HB3	1:B:1566:LYS:NZ	2.29	0.47
2:C:137:HIS:HD2	2:C:138:PRO:N	2.13	0.47
1:B:1939:ILE:HA	1:B:1942:LEU:HD12	1.96	0.46
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.98	0.46
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.96	0.46
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.97	0.46
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.14	0.46
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.96	0.46
1:B:1590:MET:HA	1:B:1593:CYS:SG	2.56	0.46
2:C:125:PHE:HE1	2:C:162:ASN:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	2.99	0.46
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.98	0.46
1:B:1913:TYR:O	1:B:1914:GLY:C	2.53	0.46
1:B:2138:LEU:HB3	1:B:2153:ILE:HD12	1.96	0.46
1:B:2340:HIS:HB2	1:B:2341:PRO:CD	2.46	0.46
1:A:1727:GLN:O	1:A:1731:ALA:HB3	2.15	0.46
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.97	0.46
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.15	0.46
3:B:2601:X6K:O07	3:B:2601:X6K:H132	2.16	0.46
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.97	0.46
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.50	0.46
1:B:1717:MET:HG3	1:B:1754:LEU:HG	1.97	0.46
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.36	0.46
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.36	0.46
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.97	0.46
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.56	0.46
1:A:1734:THR:C	1:A:1736:ASP:N	2.68	0.45
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.97	0.45
1:A:2206:ASN:ND2	1:A:2224:ARG:HD2	2.31	0.45
1:B:1427:GLU:OE2	1:B:2322:ARG:NH2	2.49	0.45
2:C:68:TYR:HE2	2:C:77:PRO:HD3	1.82	0.45
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.99	0.45
2:D:28:GLN:O	2:D:28:GLN:HG3	2.15	0.45
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.99	0.45
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	1.98	0.45
2:C:240:ALA:C	2:C:242:GLN:H	2.19	0.45
2:C:102:THR:O	2:C:109:ALA:HA	2.15	0.45
1:A:1705:TRP:HZ2	1:A:1760:ASN:ND2	2.15	0.45
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.98	0.45
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	2.99	0.45
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.75	0.45
1:A:2138:LEU:HB3	1:A:2153:ILE:HD12	1.98	0.45
1:B:1734:THR:O	1:B:1736:ASP:N	2.34	0.45
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.99	0.45
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.52	0.45
1:A:1743:LEU:O	1:A:1747:MET:HG3	2.17	0.45
1:B:2148:GLN:HA	1:B:2149:PRO:HD2	1.85	0.45
2:C:219:HIS:CE1	2:C:245:LYS:HD2	2.51	0.45
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.50	0.45
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.52	0.45
1:B:1578:MET:HB2	1:B:1582:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1602:VAL:HG13	1:B:1643:VAL:HG23	1.99	0.45
1:B:1944:ALA:HA	1:B:2426:LEU:HD11	1.98	0.45
1:A:1957:ILE:HG22	1:A:1961:LEU:HD12	1.99	0.44
1:B:1881:THR:O	1:B:1885:VAL:HG23	2.17	0.44
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.97	0.44
2:C:277:ALA:O	2:C:286:VAL:HG23	2.16	0.44
2:C:58:ALA:HB2	2:C:93:PHE:HZ	1.82	0.44
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.83	0.44
2:D:58:ALA:HB2	2:D:93:PHE:HZ	1.82	0.44
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.51	0.44
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.47	0.44
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	1.99	0.44
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.84	0.44
1:B:1725:GLN:O	1:B:1729:GLN:HG2	2.17	0.44
1:A:1892:ILE:HG21	1:A:1930:ILE:CD1	2.47	0.44
2:C:56:MET:HB2	2:C:68:TYR:O	2.16	0.44
2:D:241:ASP:OD2	2:D:243:THR:HB	2.17	0.44
1:A:1623:LEU:HD13	1:A:1640:ARG:HH12	1.82	0.44
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.99	0.44
2:C:248:ARG:O	2:C:252:PHE:HA	2.17	0.44
2:D:238:CYS:HB3	2:D:273:MET:O	2.17	0.44
1:A:1590:MET:HA	1:A:1593:CYS:SG	2.57	0.44
1:A:1623:LEU:HD22	1:A:1652:THR:HG23	1.99	0.44
1:A:2157:ALA:HB3	1:A:2173:THR:HG23	1.99	0.44
1:B:1882:VAL:HG12	1:B:1886:GLN:NE2	2.33	0.44
1:B:2297:ASP:O	1:B:2298:ASP:C	2.55	0.44
1:B:2362:PHE:O	1:B:2364:VAL:N	2.50	0.44
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.44
1:A:1778:ALA:O	1:A:1782:HIS:HD2	2.01	0.44
1:A:1701:MET:HE1	1:A:1717:MET:N	2.33	0.44
1:A:1725:GLN:O	1:A:1729:GLN:HG2	2.17	0.44
1:A:1705:TRP:CZ2	1:A:1760:ASN:ND2	2.85	0.44
1:B:1974:TYR:O	1:B:1978:VAL:HG23	2.18	0.44
2:D:63:GLN:NE2	2:D:86:LYS:H	2.15	0.44
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.00	0.44
1:A:2401:HIS:HB3	1:A:2521:VAL:CG1	2.47	0.44
2:D:31:SER:C	2:D:306:ARG:HD3	2.38	0.44
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.99	0.43
1:B:1571:LEU:HA	1:B:1574:GLU:HB3	2.00	0.43
1:A:1796:MET:HE2	1:A:1796:MET:HA	2.00	0.43
1:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	2.15	0.43
1:B:2418:LEU:HD13	1:B:2504:VAL:HG11	1.99	0.43
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.19	0.43
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	1.99	0.43
1:B:1915:HIS:CE1	1:B:1919:VAL:HG11	2.53	0.43
1:B:2187:LYS:O	1:B:2234:SER:HA	2.18	0.43
2:D:102:THR:O	2:D:109:ALA:HA	2.17	0.43
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.54	0.43
2:C:15:LEU:HD11	2:C:286:VAL:HG11	2.00	0.43
2:D:117:ARG:O	2:D:118:ASN:CB	2.60	0.43
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.19	0.43
1:A:2187:LYS:NZ	1:A:2187:LYS:CB	2.81	0.43
1:A:2297:ASP:O	1:A:2298:ASP:C	2.56	0.43
2:D:12:PRO:O	2:D:54:ARG:NH2	2.51	0.43
1:A:1490:TRP:CE3	1:A:1519:ALA:HA	2.53	0.43
1:A:2115:LEU:HA	1:A:2115:LEU:HD23	1.94	0.43
1:A:1687:HIS:HA	1:A:1688:PRO:HD2	1.80	0.43
1:B:1605:TYR:O	1:B:1605:TYR:CD2	2.70	0.43
1:B:2324:LEU:HA	1:B:2353:ILE:HG21	2.00	0.43
1:B:2430:ARG:HG3	1:B:2430:ARG:H	1.65	0.43
2:C:202:GLY:O	2:C:203:ILE:O	2.37	0.43
2:C:28:GLN:HG3	2:C:31:SER:HG	1.84	0.43
2:C:86:LYS:HB3	2:C:105:GLU:HB2	2.01	0.43
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	2.01	0.43
1:B:1621:GLU:C	1:B:1623:LEU:H	2.21	0.43
1:B:1691:THR:HG22	1:B:1691:THR:O	2.19	0.43
1:B:1727:GLN:O	1:B:1731:ALA:HB3	2.18	0.43
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.83	0.43
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.83	0.43
2:C:117:ARG:O	2:C:118:ASN:CB	2.61	0.43
1:A:1621:GLU:C	1:A:1623:LEU:H	2.22	0.43
1:A:2162:VAL:CG1	1:A:2168:ARG:HG2	2.49	0.43
1:B:1973:ILE:HG13	1:B:1973:ILE:H	1.52	0.43
1:B:2187:LYS:CB	1:B:2187:LYS:NZ	2.82	0.43
1:B:2387:MET:HE1	1:B:2396:TYR:HB2	2.00	0.43
2:D:127:VAL:HG11	2:D:153:HIS:HE1	1.81	0.43
2:C:36:ARG:NH2	2:C:69:ASP:O	2.52	0.43
2:C:74:ASN:H	2:C:75:PRO:CD	2.32	0.43
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	2.00	0.42
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.77	0.42
1:B:2162:VAL:CG1	1:B:2168:ARG:HG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2260:LEU:HB3	1:B:2263:ILE:HD12	2.01	0.42
2:C:12:PRO:O	2:C:54:ARG:NH2	2.52	0.42
1:A:2187:LYS:HG3	1:A:2237:ILE:CD1	2.49	0.42
1:B:2209:LEU:O	1:B:2215:SER:HB2	2.19	0.42
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	2.01	0.42
2:D:128:ASN:O	2:D:129:ALA:HB3	2.18	0.42
2:D:202:GLY:HA3	2:D:208:THR:H	1.84	0.42
2:D:277:ALA:O	2:D:286:VAL:HG23	2.19	0.42
1:A:1726:GLN:HG2	1:A:1729:GLN:HE21	1.84	0.42
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.83	0.42
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.19	0.42
1:B:1425:GLN:HG2	1:B:2314:PHE:HZ	1.84	0.42
1:B:1629:ILE:O	1:B:1630:VAL:C	2.57	0.42
1:B:1970:GLN:HA	1:B:1973:ILE:HD11	2.01	0.42
1:B:1977:THR:HG22	1:B:1981:LYS:HE2	2.00	0.42
1:B:2165:SER:OG	1:B:2166:LYS:N	2.52	0.42
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.55	0.42
2:C:137:HIS:CD2	2:C:138:PRO:N	2.88	0.42
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.33	0.42
1:B:1418:SER:O	1:B:1421:ASN:HB2	2.19	0.42
1:B:1784:ARG:HA	1:B:1784:ARG:HD3	1.85	0.42
1:B:2387:MET:CE	1:B:2396:TYR:HB2	2.50	0.42
2:D:188:VAL:HG13	2:D:223:ALA:HB3	2.00	0.42
1:A:1605:TYR:O	1:A:1605:TYR:CD2	2.71	0.42
2:D:28:GLN:HG3	2:D:31:SER:HG	1.85	0.42
1:A:2287:PHE:O	1:A:2291:VAL:HG23	2.19	0.42
1:B:1562:GLN:HB3	1:B:1566:LYS:HZ1	1.84	0.42
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.29	0.42
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.20	0.42
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.34	0.42
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.29	0.42
2:D:137:HIS:CD2	2:D:138:PRO:N	2.88	0.42
1:A:1920:ASN:O	1:A:1924:VAL:HG23	2.19	0.42
1:A:2084:TRP:HB3	1:A:2096:ASP:O	2.20	0.42
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.19	0.42
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.54	0.42
1:B:2299:LEU:O	1:B:2303:LEU:HG	2.19	0.42
2:C:202:GLY:HA3	2:C:208:THR:H	1.84	0.42
1:A:1418:SER:O	1:A:1421:ASN:HB2	2.19	0.42
1:A:2165:SER:OG	1:A:2166:LYS:N	2.53	0.42
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.85	0.42
1:B:2401:HIS:HB3	1:B:2521:VAL:CG1	2.49	0.42
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	2.17	0.42
1:B:1400:LYS:HD2	1:B:1412:ILE:HG23	2.01	0.42
2:C:90:SER:O	2:C:102:THR:HA	2.20	0.42
2:D:138:PRO:HD2	2:D:178:ILE:HD13	2.02	0.42
1:B:1892:ILE:HG21	1:B:1930:ILE:CD1	2.50	0.41
2:C:289:SER:O	2:C:315:VAL:HB	2.20	0.41
1:B:2064:THR:HG21	1:B:2126:VAL:O	2.20	0.41
1:B:2152:ARG:HG2	1:B:2177:SER:OG	2.20	0.41
2:D:240:ALA:C	2:D:242:GLN:H	2.23	0.41
2:D:15:LEU:HD11	2:D:286:VAL:HG11	2.02	0.41
1:A:2152:ARG:HG2	1:A:2177:SER:OG	2.20	0.41
1:B:1474:PRO:HB3	1:B:1505:ASN:HD22	1.85	0.41
1:B:2293:ASN:O	1:B:2294:THR:HG23	2.20	0.41
2:C:56:MET:HA	2:C:70:LEU:HG	2.02	0.41
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.35	0.41
1:B:1716:HIS:CE1	1:A:2266:ARG:HE	2.38	0.41
2:C:128:ASN:O	2:C:129:ALA:HB3	2.19	0.41
2:D:90:SER:O	2:D:102:THR:HA	2.20	0.41
2:D:142:GLU:OE2	2:D:208:THR:HB	2.20	0.41
2:D:262:SER:CB	2:D:267:GLU:HG2	2.51	0.41
1:B:1732:ILE:CD1	1:B:1740:LYS:HB2	2.50	0.41
1:B:2498:ILE:HG22	1:B:2502:ASN:HD21	1.86	0.41
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.55	0.41
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.20	0.41
2:C:60:ALA:HB1	2:C:88:ILE:HG22	2.02	0.41
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.55	0.41
2:D:290:SER:HA	2:D:314:ALA:HB1	2.03	0.41
2:D:289:SER:O	2:D:315:VAL:HB	2.20	0.41
2:D:86:LYS:HB3	2:D:105:GLU:HB2	2.03	0.41
2:C:127:VAL:HG11	2:C:153:HIS:HE1	1.82	0.41
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.03	0.41
1:A:2080:GLU:O	1:A:2083:GLU:HB3	2.21	0.41
1:B:1901:GLN:HG3	1:B:2413:SER:CA	2.39	0.41
1:B:2016:LEU:O	1:B:2186:LEU:HD21	2.20	0.41
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.56	0.41
1:A:1772:VAL:HA	1:A:1775:TYR:HD1	1.86	0.41
1:A:1904:LEU:O	1:A:1907:LEU:HB2	2.21	0.41
3:A:2601:X6K:O07	3:A:2601:X6K:H132	2.20	0.41
1:B:2082:GLN:HB3	1:B:2082:GLN:HE21	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:VAL:HB	2:C:318:LEU:HD13	2.03	0.41
2:D:82:ASP:HB2	2:D:119:LEU:HD13	2.01	0.41
2:D:125:PHE:HE1	2:D:162:ASN:HB2	1.86	0.41
1:A:1973:ILE:HG13	1:A:1973:ILE:H	1.56	0.41
1:A:2401:HIS:O	1:A:2405:GLU:HB2	2.21	0.41
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.85	0.41
1:B:1681:PRO:O	1:B:1682:SER:C	2.59	0.41
2:D:75:PRO:HB2	2:D:76:ASN:H	1.63	0.41
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.86	0.41
1:A:1552:LEU:HD11	1:A:1603:ILE:HG13	2.02	0.41
1:B:1715:GLN:HG3	1:A:2260:LEU:HD23	2.02	0.41
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.01	0.41
1:B:2167:GLN:O	1:B:2168:ARG:C	2.60	0.40
2:C:262:SER:HB2	2:C:263:GLY:H	1.58	0.40
2:D:248:ARG:O	2:D:252:PHE:CA	2.69	0.40
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.22	0.40
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.40
1:A:1545:PHE:CE1	1:A:1599:LEU:HD22	2.57	0.40
1:A:1623:LEU:CD2	1:A:1652:THR:HG23	2.51	0.40
1:A:2121:LEU:HA	1:A:2121:LEU:HD23	1.94	0.40
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.83	0.40
1:B:1772:VAL:HA	1:B:1775:TYR:HD1	1.86	0.40
1:B:2401:HIS:O	1:B:2405:GLU:HB2	2.21	0.40
2:C:95:GLU:CB	2:C:140:GLN:HE22	2.24	0.40
1:A:1588:GLY:O	1:A:1591:VAL:HB	2.22	0.40
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.86	0.40
1:A:1728:ALA:HB2	1:A:1743:LEU:HD23	2.03	0.40
1:B:1501:TRP:O	1:B:1501:TRP:HE3	2.05	0.40
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.21	0.40
1:B:1687:HIS:HA	1:B:1688:PRO:HD2	1.81	0.40
1:B:1734:THR:C	1:B:1736:ASP:N	2.74	0.40
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.21	0.40
2:C:142:GLU:OE2	2:C:208:THR:HB	2.21	0.40
2:C:68:TYR:CE2	2:C:77:PRO:HD3	2.57	0.40
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.22	0.40
1:A:1721:VAL:HG11	1:A:1751:PHE:CE2	2.57	0.40
1:A:1999:CYS:C	1:A:2001:HIS:N	2.75	0.40
1:A:2082:GLN:HE21	1:A:2082:GLN:HB3	1.63	0.40
1:B:1688:PRO:HG3	1:A:2270:ARG:HA	2.03	0.40
1:A:2299:LEU:O	1:A:2303:LEU:HG	2.21	0.40
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2311:GLU:HG2	1:B:2312:VAL:N	2.37	0.40
2:D:18:ALA:HB3	2:D:317:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

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	1046/1174 (89%)	936 (90%)	74 (7%)	36 (3%)	4	38
1	B	1052/1174 (90%)	941 (89%)	77 (7%)	34 (3%)	5	38
2	C	315/326 (97%)	271 (86%)	28 (9%)	16 (5%)	2	26
2	D	315/326 (97%)	272 (86%)	27 (9%)	16 (5%)	2	26
All	All	2728/3000 (91%)	2420 (89%)	206 (8%)	102 (4%)	4	35

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1709	ARG
1	B	1896	ARG
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
2	D	75	PRO
2	D	97	GLY
2	D	203	ILE
1	A	1525	GLN
1	A	1630	VAL

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Mol	Chain	Res	Type
1	A	1650	MET
1	A	1709	ARG
1	A	1896	ARG
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
2	C	97	GLY
2	C	203	ILE
1	B	1444	GLU
1	B	1445	ILE
1	B	1682	SER
1	B	1735	GLU
1	B	1784	ARG
1	B	1914	GLY
1	B	2357	ASP
2	D	35	THR
2	D	74	ASN
2	D	118	ASN
2	D	167	PRO
2	D	204	GLY
1	A	1444	GLU
1	A	1445	ILE
1	A	1682	SER
1	A	1735	GLU
1	A	1784	ARG
1	A	1914	GLY
1	A	2357	ASP
1	A	2364	VAL
2	C	35	THR
2	C	74	ASN
2	C	75	PRO
2	C	118	ASN
2	C	167	PRO
2	C	204	GLY
1	B	1707	SER
1	B	1734	THR
1	B	2000	GLU
1	B	2001	HIS
1	B	2093	ASN
1	B	2364	VAL
2	D	54	ARG
2	D	208	THR

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Mol	Chain	Res	Type
1	A	1707	SER
1	A	1734	THR
1	A	1786	TRP
1	A	2000	GLU
1	A	2001	HIS
1	A	2093	ASN
2	C	208	THR
1	B	1423	LEU
1	B	1786	TRP
1	B	1934	THR
1	B	2362	PHE
2	D	169	PRO
2	D	269	SER
1	A	1423	LEU
1	A	1934	THR
1	A	1937	GLN
2	C	54	ARG
2	C	73	ASN
2	C	169	PRO
2	C	269	SER
1	B	1454	HIS
1	B	1470	ASN
1	B	1512	MET
1	B	2363	GLU
2	D	73	ASN
2	D	160	ASP
1	A	1470	ASN
1	A	1512	MET
1	A	1933	ASP
1	A	1987	ARG
1	A	2362	PHE
2	C	270	ARG
1	B	1680	ASP
1	B	1933	ASP
1	A	1454	HIS
1	A	1503	LEU
1	A	1680	ASP
2	D	129	ALA
2	D	310	GLY
1	A	1688	PRO
2	C	129	ALA
1	A	2141	PRO

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Mol	Chain	Res	Type
2	C	310	GLY
1	B	1426	PRO
1	B	2141	PRO
1	B	2163	ILE
1	A	1426	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	927/1024 (90%)	837 (90%)	90 (10%)	9	42
1	B	931/1024 (91%)	840 (90%)	91 (10%)	9	42
2	C	269/276 (98%)	241 (90%)	28 (10%)	8	39
2	D	269/276 (98%)	241 (90%)	28 (10%)	8	39
All	All	2396/2600 (92%)	2159 (90%)	237 (10%)	9	41

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1445	ILE
1	B	1457	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1558	SER
1	B	1559	LEU
1	B	1590	MET
1	B	1630	VAL
1	B	1650	MET

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Mol	Chain	Res	Type
1	B	1675	LEU
1	B	1679	VAL
1	B	1680	ASP
1	B	1685	LEU
1	B	1724	MET
1	B	1736	ASP
1	B	1740	LYS
1	B	1749	ARG
1	B	1780	THR
1	B	1796	MET
1	B	1878	LEU
1	B	1879	MET
1	B	1895	SER
1	B	1896	ARG
1	B	1898	ASN
1	B	1899	ASN
1	B	1912	ASP
1	B	1916	TRP
1	B	1932	ILE
1	B	1956	LEU
1	B	1968	HIS
1	B	1970	GLN
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2001	HIS
1	B	2005	LEU
1	B	2011	MET
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2080	GLU
1	B	2082	GLN
1	B	2090	LYS
1	B	2093	ASN
1	B	2102	ASP
1	B	2124	GLN
1	B	2136	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2165	SER

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Mol	Chain	Res	Type
1	B	2166	LYS
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2187	LYS
1	B	2189	HIS
1	B	2195	ASP
1	B	2214	THR
1	B	2223	GLN
1	B	2224	ARG
1	B	2228	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2301	LYS
1	B	2311	GLU
1	B	2318	THR
1	B	2363	GLU
1	B	2378	ARG
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2401	HIS
1	B	2408	ARG
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2503	ARG
1	B	2519	LEU
1	B	2530	LYS
2	D	13	VAL
2	D	44	GLN
2	D	79	ILE
2	D	85	ASN
2	D	86	LYS
2	D	90	SER
2	D	91	VAL
2	D	128	ASN
2	D	135	CYS

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Mol	Chain	Res	Type
2	D	159	THR
2	D	160	ASP
2	D	161	HIS
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	174	THR
2	D	179	ASP
2	D	188	VAL
2	D	199	LEU
2	D	233	THR
2	D	248	ARG
2	D	260	ILE
2	D	262	SER
2	D	269	SER
2	D	287	THR
2	D	301	THR
2	D	312	GLN
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1427	GLU
1	A	1443	LEU
1	A	1445	ILE
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1528	SER
1	A	1541	HIS
1	A	1590	MET
1	A	1630	VAL
1	A	1650	MET
1	A	1675	LEU
1	A	1679	VAL
1	A	1680	ASP
1	A	1685	LEU
1	A	1736	ASP
1	A	1740	LYS
1	A	1749	ARG
1	A	1780	THR
1	A	1796	MET

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Mol	Chain	Res	Type
1	A	1878	LEU
1	A	1879	MET
1	A	1895	SER
1	A	1896	ARG
1	A	1898	ASN
1	A	1899	ASN
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1956	LEU
1	A	1968	HIS
1	A	1970	GLN
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2001	HIS
1	A	2005	LEU
1	A	2011	MET
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2080	GLU
1	A	2082	GLN
1	A	2090	LYS
1	A	2093	ASN
1	A	2102	ASP
1	A	2124	GLN
1	A	2136	LEU
1	A	2138	LEU
1	A	2152	ARG
1	A	2165	SER
1	A	2166	LYS
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2183	VAL
1	A	2187	LYS
1	A	2189	HIS
1	A	2195	ASP
1	A	2214	THR

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Mol	Chain	Res	Type
1	A	2223	GLN
1	A	2224	ARG
1	A	2228	ILE
1	A	2232	THR
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2301	LYS
1	A	2311	GLU
1	A	2318	THR
1	A	2363	GLU
1	A	2378	ARG
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2401	HIS
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2503	ARG
1	A	2519	LEU
1	A	2530	LYS
2	C	13	VAL
2	C	44	GLN
2	C	79	ILE
2	C	85	ASN
2	C	86	LYS
2	C	90	SER
2	C	91	VAL
2	C	128	ASN
2	C	135	CYS
2	C	159	THR
2	C	160	ASP
2	C	161	HIS
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	174	THR

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Mol	Chain	Res	Type
2	C	179	ASP
2	C	188	VAL
2	C	199	LEU
2	C	233	THR
2	C	248	ARG
2	C	260	ILE
2	C	262	SER
2	C	269	SER
2	C	287	THR
2	C	301	THR
2	C	312	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	B	1496	GLN
1	B	1505	ASN
1	B	1594	HIS
1	B	1695	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1886	GLN
1	B	1898	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1968	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2178	ASN
1	B	2189	HIS
1	B	2223	GLN
1	B	2319	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
1	B	2502	ASN
2	D	30	HIS
2	D	63	GLN
2	D	64	HIS

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Mol	Chain	Res	Type
2	D	71	ASN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN
2	D	122	GLN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	311	HIS
2	D	312	GLN
1	A	1496	GLN
1	A	1594	HIS
1	A	1687	HIS
1	A	1729	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1898	ASN
1	A	1899	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1968	HIS
1	A	1970	GLN
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2178	ASN
1	A	2189	HIS
1	A	2319	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2428	ASN
1	A	2502	ASN
2	C	30	HIS
2	C	63	GLN
2	C	64	HIS
2	C	71	ASN
2	C	85	ASN
2	C	94	HIS
2	C	118	ASN
2	C	122	GLN
2	C	137	HIS
2	C	140	GLN

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Mol	Chain	Res	Type
2	C	153	HIS
2	C	311	HIS
2	C	312	GLN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	X6K	A	2601	-	26,30,30	1.07	1 (3%)	30,43,43	1.83	9 (30%)
3	X6K	B	2601	-	26,30,30	1.01	1 (3%)	30,43,43	1.92	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X6K	A	2601	-	-	0/8/16/16	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X6K	B	2601	-	-	0/8/16/16	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	X6K	C11-N18	2.63	1.36	1.32
3	A	2601	X6K	C11-N18	2.72	1.36	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	X6K	N10-C19-N18	-5.91	121.49	126.08
3	A	2601	X6K	N10-C19-N18	-5.00	122.20	126.08
3	A	2601	X6K	C03-C04-C05	-3.94	114.15	120.81
3	B	2601	X6K	C03-C04-C05	-3.34	115.17	120.81
3	B	2601	X6K	C14-C13-N12	-3.25	104.14	109.98
3	A	2601	X6K	C14-C13-N12	-2.70	105.12	109.98
3	B	2601	X6K	C05-C06-N01	-2.53	120.73	124.94
3	A	2601	X6K	C17-N12-C11	-2.19	112.36	118.81
3	B	2601	X6K	C16-C17-N12	-2.19	106.04	109.98
3	A	2601	X6K	C05-C06-N01	-2.13	121.40	124.94
3	A	2601	X6K	C17-N12-C13	-2.09	107.14	111.57
3	A	2601	X6K	C20-C19-N18	2.14	120.80	117.29
3	B	2601	X6K	C04-C05-C06	2.43	123.11	118.36
3	A	2601	X6K	C11-N18-C19	2.63	121.65	116.24
3	A	2601	X6K	C04-C05-C06	2.71	123.65	118.36
3	B	2601	X6K	C11-N18-C19	3.31	123.05	116.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	X6K	1	0
3	B	2601	X6K	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1054/1174 (89%)	-0.17	26 (2%) 58 43	26, 57, 146, 187	0
1	B	1058/1174 (90%)	-0.29	17 (1%) 72 59	21, 48, 126, 166	0
2	C	317/326 (97%)	-0.25	2 (0%) 89 81	30, 58, 103, 126	0
2	D	317/326 (97%)	-0.39	0 100 100	23, 40, 83, 138	0
All	All	2746/3000 (91%)	-0.25	45 (1%) 72 59	21, 51, 137, 187	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1580	GLY	7.2
1	A	1580	GLY	6.5
1	B	1581	GLU	5.5
1	A	1581	GLU	4.9
1	A	1584	SER	4.9
1	B	1582	SER	4.0
1	B	2433	ASP	3.9
1	A	2435	ASN	3.6
1	B	2436	THR	3.5
1	B	2434	THR	3.4
1	B	1469	THR	3.4
1	B	1446	GLN	3.3
1	A	2433	ASP	3.2
1	A	1583	TYR	3.1
1	A	1730	HIS	3.1
1	A	1867	LYS	3.0
1	A	1585	ARG	2.9
1	A	1619	TRP	2.8
1	A	1582	SER	2.8
1	B	2435	ASN	2.8
1	A	1868	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1558	SER	2.7
1	A	2038	TYR	2.6
1	A	1469	THR	2.6
1	B	1573	ALA	2.6
1	A	2436	THR	2.5
1	B	1867	LYS	2.5
1	A	1554	GLN	2.5
1	B	1577	ALA	2.5
1	A	2092	GLY	2.4
1	B	1607	LEU	2.4
1	A	2044	VAL	2.4
1	B	1584	SER	2.3
1	A	2043	ASN	2.3
2	C	10	SER	2.2
1	B	1579	ALA	2.2
1	A	1385	GLU	2.1
1	B	1470	ASN	2.1
1	A	2049	GLU	2.1
1	A	1386	ARG	2.0
1	A	1587	TYR	2.0
1	B	1504	VAL	2.0
2	C	205	ASP	2.0
1	A	1603	ILE	2.0
1	A	2434	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	X6K	A	2601	26/26	0.95	0.20	-0.16	32,35,35,36	0
3	X6K	B	2601	26/26	0.96	0.20	-0.22	24,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.