



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 PM GMT

PDB ID : 4JSN
Title : structure of mTORdeltaN-mLST8 complex
Authors : Pavletich, N.P.
Deposited on : 2013-03-22
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

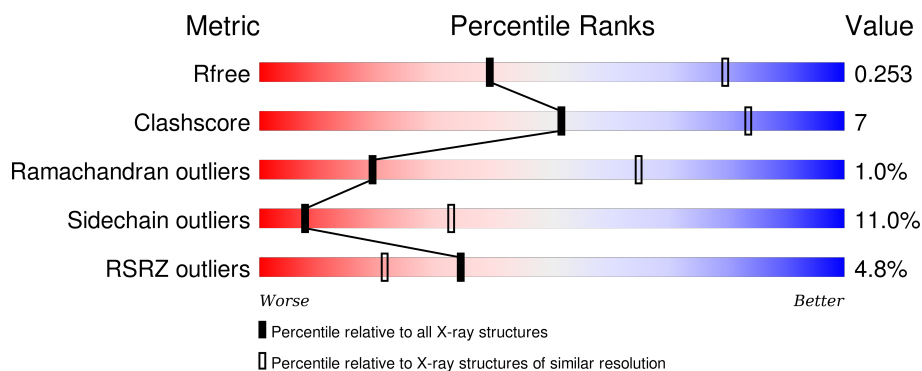
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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>7%</div> <div>68% 19% • 10%</div> </div>
1	B	1174	<div> <div>3%</div> <div>69% 18% • 10%</div> </div>
2	C	326	<div> <div>3%</div> <div>67% 26% • •</div> </div>
2	D	326	<div> <div>2%</div> <div>68% 26% • •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22097 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 Serine/threonine-protein kinase mTOR.

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

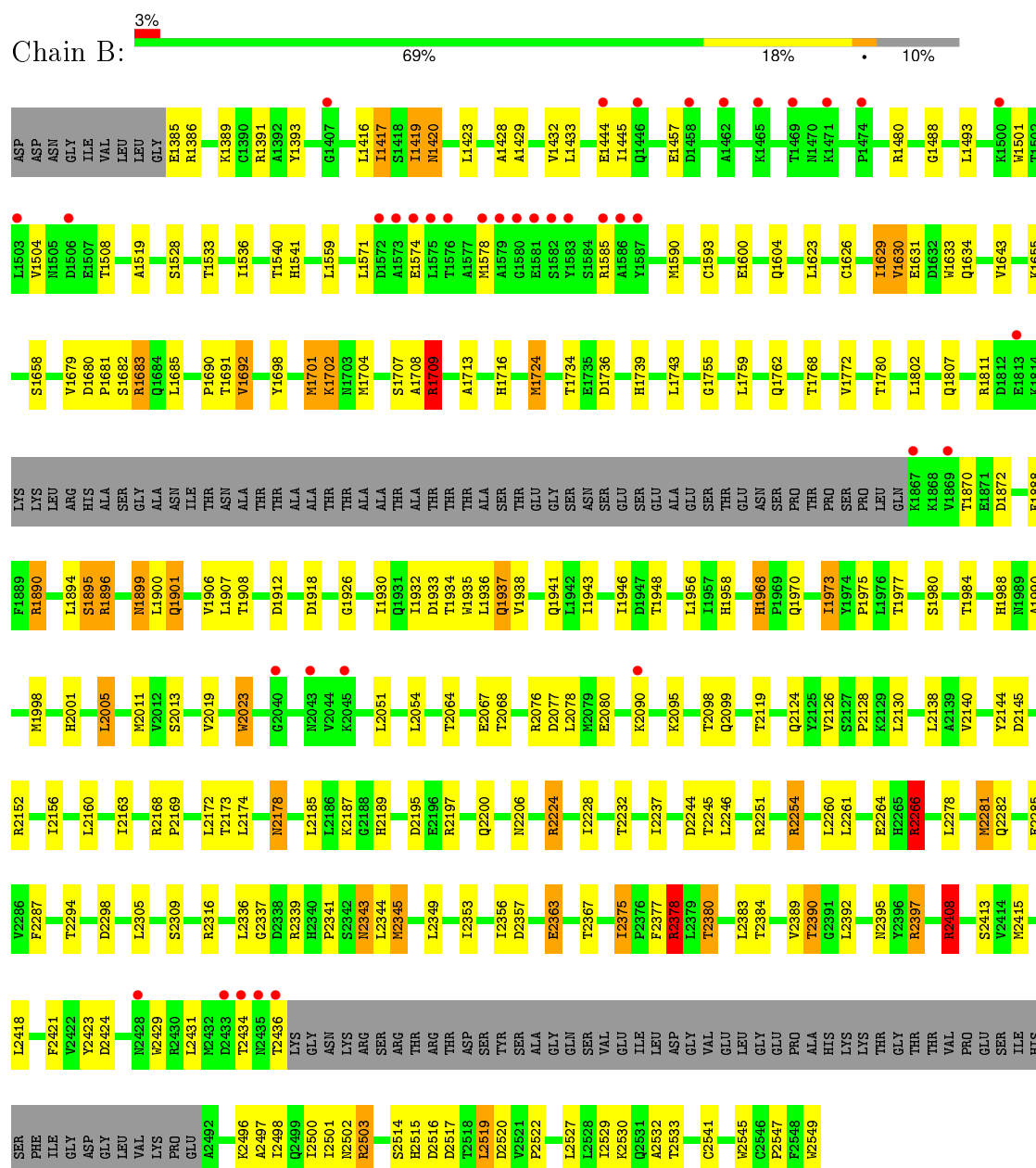
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

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

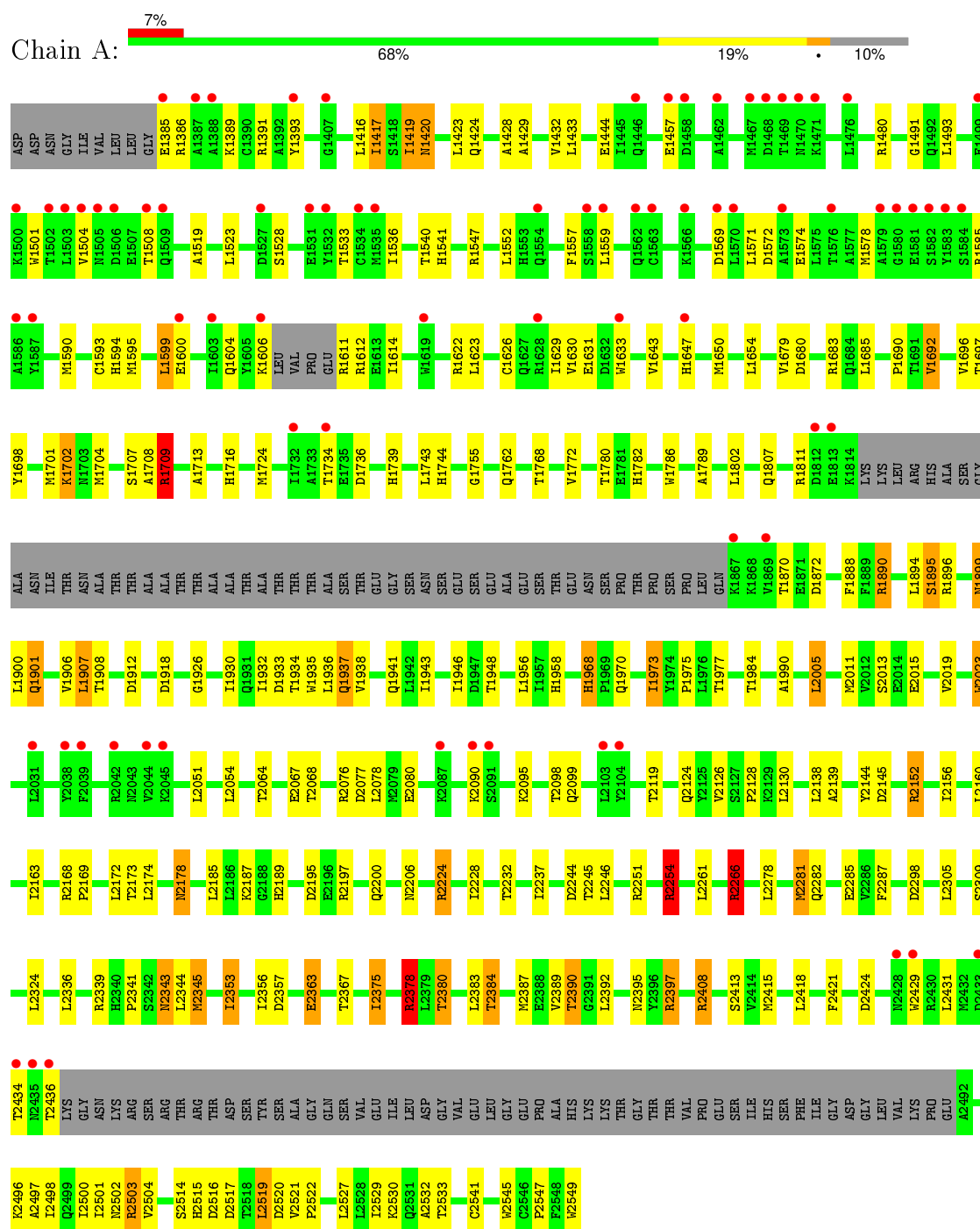
3 Residue-property plots

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

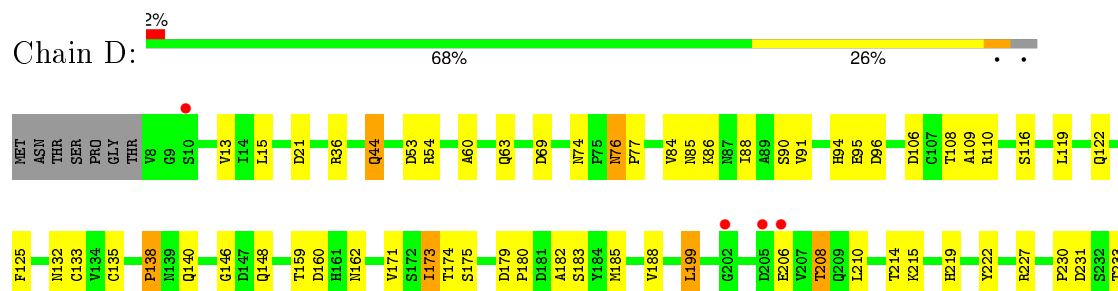
- Molecule 1: Serine/threonine-protein kinase mTOR

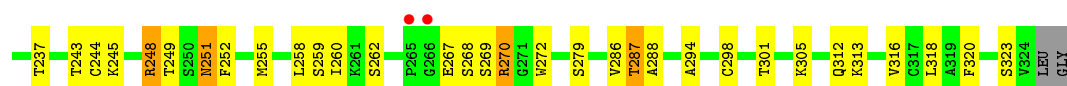


- Molecule 1: Serine/threonine-protein kinase mTOR

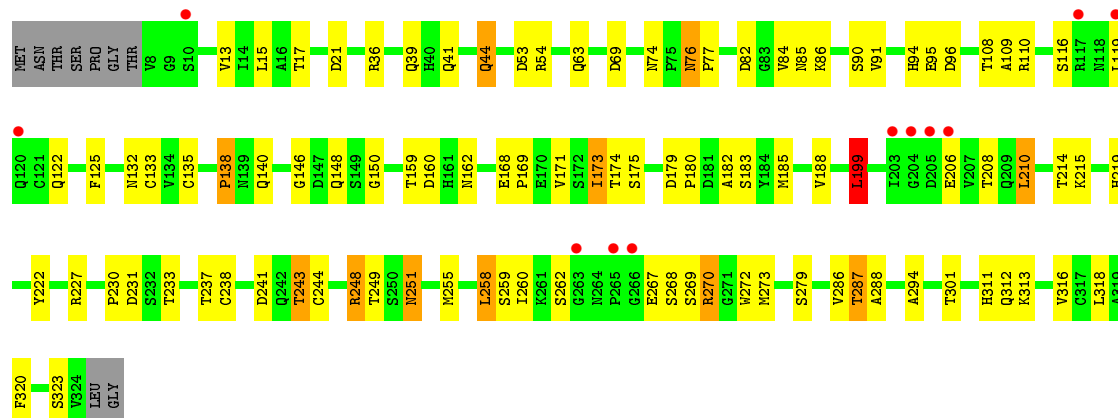


• Molecule 2: Target of rapamycin complex subunit LST8





- Molecule 2: Target of rapamycin complex subunit LST8



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	139.40 Å 163.20 Å 207.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 3.20 29.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (29.86-3.20) 86.5 (29.84-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.18 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.215 , 0.256 0.219 , 0.253	Depositor DCC
R_{free} test set	1855 reflections (2.78%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 75518 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22097	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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 43.98 % 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 1.6294e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/8772	0.85	10/11872 (0.1%)
1	B	0.55	0/8805	0.85	9/11920 (0.1%)
2	C	0.55	0/2514	0.88	2/3426 (0.1%)
2	D	0.58	0/2514	0.90	0/3426
All	All	0.55	0/22605	0.86	21/30644 (0.1%)

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	2
1	B	0	2
2	C	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2378	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	2378	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	2378	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	2378	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	2344	LEU	CA-CB-CG	6.14	129.41	115.30
1	B	2305	LEU	CA-CB-CG	5.86	128.79	115.30
1	B	2344	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	2305	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	2408	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	2005	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2005	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	2254	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	2266	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	2174	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	1445	ILE	N-CA-C	-5.17	97.05	111.00
1	B	1701	MET	CG-SD-CE	-5.10	92.04	100.20
1	B	2266	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	1907	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	1599	LEU	CA-CB-CG	5.02	126.84	115.30
2	C	210	LEU	CA-CB-CG	5.01	126.81	115.30
2	C	199	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	A	1680	ASP	Peptide
1	B	1444	GLU	Peptide
1	B	1680	ASP	Peptide
2	C	267	GLU	Peptide
2	D	267	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	8577	0	8559	114	1
1	B	8608	0	8593	111	0
2	C	2456	0	2341	43	0
2	D	2456	0	2341	43	0
All	All	22097	0	21834	299	1

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 7.

All (299) 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:2380:THR:HG22	1:A:2383:LEU:HG	1.53	0.91
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.52	0.89
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.57	0.87
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.58	0.84
2:C:219:HIS:NE2	2:C:237:THR:HG22	1.97	0.78
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.68	0.76
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.67	0.75
2:D:219:HIS:NE2	2:D:237:THR:HG22	2.02	0.74
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.18	0.73
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.21	0.71
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	0.71
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.25	0.70
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.75	0.69
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.74	0.69
1:B:2380:THR:HG23	1:B:2549:TRP:O	1.94	0.67
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.94	0.67
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.94	0.67
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.42	0.65
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.62	0.65
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.62	0.64
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.79	0.64
1:A:2541:CYS:HB2	1:A:2547:PRO:HG3	1.81	0.63
1:B:2541:CYS:HB2	1:B:2547:PRO:HG3	1.81	0.63
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.34	0.63
2:D:95:GLU:H	2:D:140:GLN:NE2	1.97	0.62
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.34	0.62
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	2.00	0.62
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.15	0.62
2:C:219:HIS:NE2	2:C:237:THR:CG2	2.62	0.62
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	2.01	0.61
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.82	0.61
1:B:2378:ARG:HH11	1:B:2380:THR:HG21	1.65	0.61
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.83	0.61
2:D:208:THR:HG23	2:D:208:THR:O	2.01	0.61
2:D:231:ASP:HB3	2:D:233:THR:OG1	2.01	0.60
2:C:95:GLU:H	2:C:140:GLN:NE2	2.00	0.60
1:B:1900:LEU:HD13	1:B:1937:GLN:HG2	1.82	0.60
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.37	0.60
2:C:231:ASP:HB3	2:C:233:THR:OG1	2.02	0.60
2:C:208:THR:HG23	2:C:208:THR:O	2.02	0.59
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.84	0.59
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:ASN:HB3	2:C:77:PRO:HD3	1.85	0.59
1:A:2375:ILE:HD12	1:A:2532:ALA:HA	1.85	0.59
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.59
1:A:1391:ARG:HH21	1:A:2309:SER:HB3	1.68	0.59
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.68	0.59
1:B:2380:THR:HG23	1:B:2549:TRP:C	2.22	0.58
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.86	0.58
1:A:2251:ARG:HA	1:A:2261:LEU:HD13	1.86	0.58
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.51	0.57
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.85	0.57
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.69	0.57
1:B:1807:GLN:HE21	1:B:1811:ARG:HH21	1.52	0.57
2:D:63:GLN:HE21	2:D:86:LYS:H	1.52	0.57
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.87	0.57
1:A:1571:LEU:HA	1:A:1574:GLU:HB3	1.86	0.57
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.87	0.57
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.85	0.57
1:A:1930:ILE:HD13	1:A:1935:TRP:CZ2	2.40	0.57
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.87	0.56
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.87	0.56
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.87	0.56
2:D:76:ASN:HB3	2:D:77:PRO:HD3	1.88	0.56
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.20	0.56
2:D:219:HIS:NE2	2:D:237:THR:CG2	2.68	0.56
2:D:36:ARG:NH2	2:D:69:ASP:O	2.39	0.55
1:A:1926:GLY:O	1:A:1930:ILE:HG22	2.06	0.55
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.42	0.55
1:B:2375:ILE:HD12	1:B:2532:ALA:HA	1.89	0.55
1:B:1417:ILE:HG23	1:B:1432:VAL:HB	1.89	0.55
1:A:1807:GLN:HE21	1:A:1811:ARG:HH21	1.55	0.55
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.55
2:D:21:ASP:HB3	2:D:313:LYS:H	1.72	0.55
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.07	0.55
1:A:2187:LYS:HD2	1:A:2237:ILE:HD12	1.90	0.54
1:B:1888:PHE:HB3	1:B:1906:VAL:HG23	1.89	0.54
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.89	0.54
2:C:36:ARG:NH2	2:C:69:ASP:O	2.40	0.54
2:C:279:SER:HA	2:C:320:PHE:HE2	1.73	0.54
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.90	0.54
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.90	0.54
1:B:1386:ARG:HA	1:B:1389:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:SER:HA	2:D:320:PHE:HE2	1.73	0.54
1:A:1501:TRP:O	1:A:1504:VAL:HG22	2.09	0.53
1:B:2251:ARG:HA	1:B:2261:LEU:HD13	1.91	0.53
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.91	0.53
1:A:1623:LEU:HG	1:A:1633:TRP:CH2	2.44	0.53
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.91	0.53
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.42	0.53
1:B:1501:TRP:O	1:B:1504:VAL:HG22	2.09	0.53
1:B:1571:LEU:HA	1:B:1574:GLU:HB3	1.91	0.53
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.91	0.53
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.90	0.52
1:B:2520:ASP:OD2	1:B:2522:PRO:HD2	2.10	0.52
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.09	0.52
2:C:63:GLN:HE21	2:C:86:LYS:H	1.57	0.52
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.91	0.52
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.91	0.52
1:A:1654:LEU:HD21	1:A:1696:VAL:HA	1.92	0.52
1:A:2206:ASN:ND2	1:A:2224:ARG:HD2	2.25	0.52
1:B:2095:LYS:HA	1:B:2098:THR:HG22	1.91	0.52
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.43	0.52
1:B:1908:THR:O	1:B:1912:ASP:HB2	2.10	0.52
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.75	0.52
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.44	0.52
1:B:2336:LEU:HG	1:B:2339:ARG:HD2	1.91	0.52
1:A:1386:ARG:HA	1:A:1389:LYS:HD2	1.90	0.51
2:C:21:ASP:HB3	2:C:313:LYS:H	1.75	0.51
1:A:2380:THR:HG23	1:A:2549:TRP:C	2.30	0.51
1:A:2019:VAL:HG22	1:A:2126:VAL:HG12	1.92	0.51
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.10	0.51
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.10	0.51
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.92	0.51
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.11	0.51
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.46	0.50
2:C:248:ARG:HG3	2:C:251:ASN:HD22	1.76	0.50
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.93	0.50
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.92	0.50
1:B:1698:TYR:CE2	1:B:1702:LYS:HD3	2.47	0.50
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.93	0.50
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.93	0.50
1:A:1888:PHE:HB3	1:A:1906:VAL:HG23	1.93	0.50
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1391:ARG:HH21	1:B:2309:SER:HB3	1.76	0.50
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.93	0.50
2:C:287:THR:O	2:C:294:ALA:HA	2.11	0.49
2:D:262:SER:HA	2:D:270:ARG:HH11	1.76	0.49
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.12	0.49
1:A:1416:LEU:O	1:A:1420:ASN:HB2	2.12	0.49
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.92	0.49
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.76	0.49
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.95	0.49
2:D:287:THR:O	2:D:294:ALA:HA	2.13	0.49
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.94	0.49
1:B:1416:LEU:O	1:B:1420:ASN:HB2	2.13	0.49
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.43	0.48
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.94	0.48
1:B:2246:LEU:HD23	1:B:2341:PRO:HB3	1.95	0.48
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.12	0.48
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.13	0.48
1:B:2266:ARG:HH11	1:B:2266:ARG:HB2	1.79	0.48
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.96	0.48
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.46	0.48
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.48	0.48
1:A:1908:THR:O	1:A:1912:ASP:HB2	2.14	0.48
1:B:2498:ILE:HG22	1:B:2502:ASN:HD21	1.78	0.47
2:C:248:ARG:HD2	2:C:255:MET:HB2	1.95	0.47
1:B:1701:MET:HE1	1:B:1716:HIS:CB	2.44	0.47
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.49	0.47
2:C:262:SER:HA	2:C:270:ARG:HH11	1.78	0.47
1:A:2266:ARG:HH11	1:A:2266:ARG:HB2	1.78	0.47
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.50	0.47
2:D:279:SER:HA	2:D:320:PHE:CE2	2.50	0.47
1:B:2363:GLU:OE1	1:B:2363:GLU:HA	2.14	0.47
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.15	0.47
2:D:138:PRO:HG2	2:D:182:ALA:HB2	1.95	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.97	0.47
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.96	0.47
1:A:2246:LEU:HD23	1:A:2341:PRO:HB3	1.97	0.47
1:B:2285:GLU:HG3	2:D:272:TRP:CE2	2.49	0.47
2:C:244:CYS:HB3	2:C:258:LEU:HD12	1.97	0.47
1:A:1755:GLY:HA2	1:A:1772:VAL:HG12	1.97	0.47
1:A:1708:ALA:HB3	1:A:1709:ARG:CZ	2.46	0.47
1:B:1708:ALA:HB3	1:B:1709:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.50	0.46
1:B:2339:ARG:NH2	1:B:2343:ASN:HB3	2.30	0.46
2:C:138:PRO:HG2	2:C:182:ALA:HB2	1.96	0.46
1:A:2163:ILE:HB	1:A:2169:PRO:HG2	1.97	0.46
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.98	0.46
2:D:109:ALA:HB3	2:D:125:PHE:HB3	1.96	0.46
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.83	0.46
1:B:2187:LYS:HD2	1:B:2237:ILE:HD12	1.98	0.46
1:A:2197:ARG:NH1	1:A:2424:ASP:OD2	2.48	0.46
2:D:248:ARG:HG3	2:D:251:ASN:HD22	1.81	0.46
1:B:2408:ARG:NH2	1:B:2519:LEU:O	2.48	0.46
1:B:2130:LEU:HD22	1:B:2156:ILE:HD13	1.98	0.46
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.15	0.46
1:A:1701:MET:HE1	1:A:1716:HIS:CB	2.46	0.46
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.81	0.46
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.31	0.45
1:B:2163:ILE:HB	1:B:2169:PRO:HG2	1.98	0.45
1:A:2497:ALA:O	1:A:2501:ILE:HD12	2.17	0.45
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.16	0.45
2:C:279:SER:HA	2:C:320:PHE:CE2	2.50	0.45
2:C:133:CYS:SG	2:C:175:SER:HA	2.55	0.45
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.16	0.45
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	1.99	0.45
1:B:2529:ILE:O	1:B:2533:THR:HB	2.16	0.45
1:B:1930:ILE:HD13	1:B:1935:TRP:CZ2	2.52	0.45
1:B:2023:TRP:CD2	1:B:2067:GLU:HG2	2.52	0.45
1:A:2051:LEU:HA	1:A:2054:LEU:HD12	1.99	0.45
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.52	0.44
1:A:2498:ILE:HG22	1:A:2502:ASN:HD21	1.81	0.44
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.37	0.44
1:B:1716:HIS:CE1	1:A:2266:ARG:HE	2.35	0.44
1:A:2285:GLU:HG3	2:C:272:TRP:CE2	2.52	0.44
1:A:1970:GLN:HA	1:A:1973:ILE:HD11	1.98	0.44
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.99	0.44
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.17	0.44
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.53	0.44
2:C:132:ASN:HD21	2:C:148:GLN:HG2	1.82	0.44
1:B:1488:GLY:HA3	1:B:1634:GLN:HE22	1.83	0.44
1:A:1393:TYR:O	1:A:1419:ILE:HD11	2.17	0.44
1:B:1755:GLY:HA2	1:B:1772:VAL:HG12	1.99	0.44
1:B:1926:GLY:O	1:B:1930:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1998:MET:HA	1:B:2001:HIS:CE1	2.53	0.44
1:B:1393:TYR:O	1:B:1419:ILE:HD11	2.18	0.44
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	1.99	0.44
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	1.99	0.44
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.48	0.43
2:C:241:ASP:OD2	2:C:243:THR:HB	2.17	0.43
1:B:1970:GLN:HA	1:B:1973:ILE:HD11	1.98	0.43
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	2.01	0.43
1:B:2390:THR:HG23	1:B:2390:THR:O	2.17	0.43
1:A:2408:ARG:NH2	1:A:2519:LEU:O	2.51	0.43
1:A:1698:TYR:CE2	1:A:1702:LYS:HD3	2.53	0.43
2:D:95:GLU:H	2:D:140:GLN:HE22	1.66	0.43
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.18	0.43
1:A:1600:GLU:O	1:A:1604:GLN:HG2	2.19	0.43
1:B:1980:SER:O	1:B:1988:HIS:HB2	2.18	0.43
2:D:44:GLN:HG3	2:D:44:GLN:H	1.41	0.43
2:C:17:THR:HG22	2:C:311:HIS:CE1	2.54	0.43
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.43
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.22	0.43
1:A:1936:LEU:HD21	1:A:1968:HIS:CD2	2.54	0.42
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.33	0.42
1:A:2520:ASP:OD2	1:A:2522:PRO:HD2	2.20	0.42
1:B:2281:MET:HA	1:B:2281:MET:CE	2.49	0.42
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.99	0.42
1:A:1697:THR:O	1:A:1701:MET:HG3	2.19	0.42
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.54	0.42
1:A:1533:THR:HA	1:A:1536:ILE:HD12	2.01	0.42
1:A:1744:HIS:O	1:A:1782:HIS:HB3	2.19	0.42
1:B:1691:THR:HG23	1:B:1724:MET:HE3	2.02	0.42
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.52	0.42
1:A:2178:ASN:HD22	1:A:2178:ASN:H	1.67	0.42
2:D:248:ARG:O	2:D:252:PHE:HA	2.20	0.42
1:A:2375:ILE:HD13	1:A:2375:ILE:HA	1.82	0.42
1:A:2529:ILE:O	1:A:2533:THR:HB	2.19	0.42
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.20	0.42
1:A:2287:PHE:HE1	1:A:2547:PRO:HB2	1.85	0.42
2:C:168:GLU:HA	2:C:169:PRO:HD3	1.92	0.42
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.20	0.42
2:D:133:CYS:SG	2:D:175:SER:HA	2.60	0.42
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
1:A:1786:TRP:CE3	1:A:1789:ALA:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2324:LEU:HD13	1:A:2353:ILE:HD13	2.02	0.41
1:B:2375:ILE:HG23	1:B:2377:PHE:O	2.20	0.41
1:A:2336:LEU:HG	1:A:2339:ARG:HD2	2.02	0.41
1:B:2178:ASN:H	1:B:2178:ASN:HD22	1.67	0.41
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.41
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	2.01	0.41
1:A:2139:ALA:HA	1:A:2152:ARG:HA	2.03	0.41
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.20	0.41
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	2.01	0.41
1:A:1698:TYR:O	1:A:1702:LYS:HG2	2.21	0.41
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.84	0.41
1:B:2375:ILE:HA	1:B:2375:ILE:HD13	1.81	0.41
2:D:244:CYS:HB3	2:D:258:LEU:HD12	2.02	0.41
2:C:109:ALA:HB3	2:C:125:PHE:HB3	2.01	0.41
1:B:1681:PRO:O	1:B:1683:ARG:HB2	2.20	0.41
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.85	0.41
1:A:1552:LEU:HD22	1:A:1606:LYS:HD3	2.03	0.41
2:C:94:HIS:CD2	2:C:140:GLN:HE21	2.39	0.41
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
1:A:2015:GLU:O	1:A:2019:VAL:HG23	2.21	0.41
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	2.02	0.41
1:A:1768:THR:O	1:A:1772:VAL:HG22	2.20	0.41
1:A:2384:THR:O	1:A:2387:MET:HB2	2.21	0.41
1:B:2497:ALA:O	1:B:2501:ILE:HD12	2.21	0.41
2:C:39:GLN:HB3	2:C:41:GLN:HE21	1.86	0.41
1:B:2140:VAL:HG13	1:B:2174:LEU:HD12	2.03	0.41
1:B:2051:LEU:HA	1:B:2054:LEU:HD12	2.03	0.41
1:B:2287:PHE:HE1	1:B:2547:PRO:HB2	1.85	0.41
1:A:1900:LEU:HD13	1:A:1937:GLN:HG2	2.01	0.41
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	2.03	0.41
2:C:238:CYS:HB3	2:C:273:MET:O	2.21	0.40
1:B:1533:THR:HA	1:B:1536:ILE:HD12	2.02	0.40
1:B:1936:LEU:HD21	1:B:1968:HIS:CD2	2.56	0.40
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	2.02	0.40
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.25	0.40
2:C:150:GLY:HA2	2:C:173:ILE:HG23	2.03	0.40
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	2.04	0.40
1:A:2390:THR:O	1:A:2390:THR:HG23	2.21	0.40
1:A:1557:PHE:HE2	1:A:1606:LYS:HG3	1.86	0.40
1:B:1600:GLU:O	1:B:1604:GLN:HG2	2.21	0.40
1:B:2316:ARG:HH21	1:B:2349:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:ASN:HB3	2:C:77:PRO:HD2	2.02	0.40
1:B:1941:GLN:NE2	1:B:2200:GLN:HE22	2.15	0.40
1:A:2278:LEU:HD22	1:A:2282:GLN:HB3	2.03	0.40
1:B:2423:TYR:CE1	1:B:2501:ILE:HD13	2.56	0.40
1:A:1569:ASP:HA	1:A:1572:ASP:HB2	2.03	0.40
1:A:1491:GLY:HA2	1:A:1523:LEU:HD11	2.03	0.40
1:B:1895:SER:HB2	1:B:1896:ARG:H	1.79	0.40
2:D:298:CYS:HB2	2:D:305:LYS:HE3	2.04	0.40
1:A:1647:HIS:HA	1:A:1650:MET:HE2	2.02	0.40
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.04	0.40
2:D:60:ALA:HB1	2:D:88:ILE:HG22	2.03	0.40

All (1) 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:1612:ARG:NH2	1:A:1612:ARG:NH2[2_554]	1.96	0.24

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	1046/1174 (89%)	967 (92%)	72 (7%)	7 (1%)	26	72
1	B	1052/1174 (90%)	967 (92%)	77 (7%)	8 (1%)	24	69
2	C	315/326 (97%)	285 (90%)	24 (8%)	6 (2%)	10	50
2	D	315/326 (97%)	284 (90%)	24 (8%)	7 (2%)	8	45
All	All	2728/3000 (91%)	2503 (92%)	197 (7%)	28 (1%)	19	65

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1630	VAL
1	B	1692	VAL
1	B	1937	GLN
2	D	74	ASN
1	A	1692	VAL
1	A	1937	GLN
2	C	74	ASN
2	D	268	SER
1	A	1630	VAL
1	A	1709	ARG
2	C	268	SER
1	B	1578	MET
1	B	1709	ARG
1	A	1578	MET
1	B	1707	SER
2	D	269	SER
1	A	1707	SER
2	C	206	GLU
2	C	269	SER
1	B	2357	ASP
2	D	76	ASN
2	D	106	ASP
2	D	138	PRO
2	D	206	GLU
1	A	2357	ASP
2	C	76	ASN
2	C	138	PRO
1	B	1682	SER

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%)	831 (90%)	96 (10%)	9	35
1	B	931/1024 (91%)	834 (90%)	97 (10%)	9	35
2	C	269/276 (98%)	233 (87%)	36 (13%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	269/276 (98%)	234 (87%)	35 (13%)	5	24
All	All	2396/2600 (92%)	2132 (89%)	264 (11%)	8	33

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1385	GLU
1	B	1417	ILE
1	B	1419	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1433	LEU
1	B	1457	GLU
1	B	1480	ARG
1	B	1508	THR
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU
1	B	1585	ARG
1	B	1590	MET
1	B	1593	CYS
1	B	1626	CYS
1	B	1629	ILE
1	B	1643	VAL
1	B	1655	LYS
1	B	1658	SER
1	B	1679	VAL
1	B	1683	ARG
1	B	1685	LEU
1	B	1702	LYS
1	B	1709	ARG
1	B	1724	MET
1	B	1734	THR
1	B	1736	ASP
1	B	1780	THR
1	B	1802	LEU
1	B	1870	THR
1	B	1872	ASP
1	B	1890	ARG
1	B	1895	SER
1	B	1896	ARG

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Mol	Chain	Res	Type
1	B	1899	ASN
1	B	1901	GLN
1	B	1918	ASP
1	B	1932	ILE
1	B	1933	ASP
1	B	1948	THR
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2023	TRP
1	B	2068	THR
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2080	GLU
1	B	2090	LYS
1	B	2119	THR
1	B	2124	GLN
1	B	2138	LEU
1	B	2145	ASP
1	B	2152	ARG
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2185	LEU
1	B	2189	HIS
1	B	2195	ASP
1	B	2224	ARG
1	B	2228	ILE
1	B	2232	THR
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2343	ASN
1	B	2345	MET
1	B	2353	ILE
1	B	2363	GLU

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Mol	Chain	Res	Type
1	B	2367	THR
1	B	2375	ILE
1	B	2378	ARG
1	B	2380	THR
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2415	MET
1	B	2429	TRP
1	B	2431	LEU
1	B	2434	THR
1	B	2436	THR
1	B	2503	ARG
1	B	2515	HIS
1	B	2516	ASP
1	B	2519	LEU
1	B	2527	LEU
1	B	2530	LYS
2	D	13	VAL
2	D	44	GLN
2	D	53	ASP
2	D	84	VAL
2	D	85	ASN
2	D	90	SER
2	D	91	VAL
2	D	116	SER
2	D	119	LEU
2	D	122	GLN
2	D	135	CYS
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	171	VAL
2	D	173	ILE
2	D	174	THR
2	D	179	ASP
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	208	THR
2	D	214	THR

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Mol	Chain	Res	Type
2	D	215	LYS
2	D	227	ARG
2	D	243	THR
2	D	248	ARG
2	D	249	THR
2	D	251	ASN
2	D	259	SER
2	D	260	ILE
2	D	270	ARG
2	D	287	THR
2	D	301	THR
2	D	312	GLN
1	A	1385	GLU
1	A	1417	ILE
1	A	1419	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1424	GLN
1	A	1433	LEU
1	A	1457	GLU
1	A	1480	ARG
1	A	1508	THR
1	A	1528	SER
1	A	1540	THR
1	A	1541	HIS
1	A	1547	ARG
1	A	1559	LEU
1	A	1585	ARG
1	A	1590	MET
1	A	1593	CYS
1	A	1626	CYS
1	A	1629	ILE
1	A	1643	VAL
1	A	1679	VAL
1	A	1683	ARG
1	A	1685	LEU
1	A	1702	LYS
1	A	1709	ARG
1	A	1724	MET
1	A	1734	THR
1	A	1736	ASP
1	A	1780	THR

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Mol	Chain	Res	Type
1	A	1802	LEU
1	A	1870	THR
1	A	1872	ASP
1	A	1890	ARG
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1901	GLN
1	A	1918	ASP
1	A	1932	ILE
1	A	1933	ASP
1	A	1948	THR
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2023	TRP
1	A	2068	THR
1	A	2076	ARG
1	A	2077	ASP
1	A	2078	LEU
1	A	2080	GLU
1	A	2090	LYS
1	A	2119	THR
1	A	2124	GLN
1	A	2138	LEU
1	A	2145	ASP
1	A	2152	ARG
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2224	ARG
1	A	2228	ILE
1	A	2232	THR
1	A	2244	ASP
1	A	2254	ARG
1	A	2266	ARG

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Mol	Chain	Res	Type
1	A	2281	MET
1	A	2343	ASN
1	A	2345	MET
1	A	2353	ILE
1	A	2363	GLU
1	A	2367	THR
1	A	2375	ILE
1	A	2378	ARG
1	A	2380	THR
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2415	MET
1	A	2429	TRP
1	A	2431	LEU
1	A	2434	THR
1	A	2436	THR
1	A	2503	ARG
1	A	2515	HIS
1	A	2516	ASP
1	A	2519	LEU
1	A	2527	LEU
1	A	2530	LYS
2	C	13	VAL
2	C	44	GLN
2	C	53	ASP
2	C	82	ASP
2	C	84	VAL
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
2	C	116	SER
2	C	119	LEU
2	C	122	GLN
2	C	135	CYS
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	171	VAL
2	C	173	ILE
2	C	174	THR

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Mol	Chain	Res	Type
2	C	179	ASP
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	214	THR
2	C	215	LYS
2	C	227	ARG
2	C	243	THR
2	C	248	ARG
2	C	249	THR
2	C	251	ASN
2	C	258	LEU
2	C	259	SER
2	C	260	ILE
2	C	270	ARG
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 (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1492	GLN
1	B	1496	GLN
1	B	1541	HIS
1	B	1594	HIS
1	B	1693	HIS
1	B	1760	ASN
1	B	1782	HIS
1	B	1807	GLN
1	B	1941	GLN
1	B	1968	HIS
1	B	2001	HIS
1	B	2082	GLN
1	B	2167	GLN
1	B	2178	ASN
1	B	2319	ASN
1	B	2343	ASN
1	B	2395	ASN
1	B	2502	ASN
2	D	22	HIS
2	D	30	HIS

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Mol	Chain	Res	Type
2	D	41	GLN
2	D	63	GLN
2	D	94	HIS
2	D	137	HIS
2	D	140	GLN
2	D	251	ASN
2	D	311	HIS
2	D	312	GLN
1	A	1492	GLN
1	A	1496	GLN
1	A	1541	HIS
1	A	1594	HIS
1	A	1693	HIS
1	A	1760	ASN
1	A	1782	HIS
1	A	1807	GLN
1	A	1941	GLN
1	A	1968	HIS
1	A	2001	HIS
1	A	2082	GLN
1	A	2178	ASN
1	A	2319	ASN
1	A	2343	ASN
1	A	2395	ASN
1	A	2502	ASN
2	C	22	HIS
2	C	41	GLN
2	C	63	GLN
2	C	94	HIS
2	C	137	HIS
2	C	140	GLN
2	C	251	ASN
2	C	311	HIS
2	C	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1054/1174 (89%)	0.15	77 (7%) 18 10	38, 86, 178, 243	0
1	B	1058/1174 (90%)	-0.12	38 (3%) 46 31	28, 72, 150, 238	0
2	C	317/326 (97%)	-0.06	11 (3%) 48 32	40, 77, 147, 222	0
2	D	317/326 (97%)	-0.35	6 (1%) 70 55	27, 52, 116, 192	0
All	All	2746/3000 (91%)	-0.04	132 (4%) 34 21	27, 74, 170, 243	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1579	ALA	8.7
1	A	1580	GLY	7.4
1	B	1580	GLY	6.8
1	A	1559	LEU	6.5
1	B	2436	THR	6.1
1	A	1503	LEU	5.8
1	A	1558	SER	5.7
1	A	2434	THR	5.5
2	C	119	LEU	5.4
1	A	1579	ALA	5.2
1	A	2038	TYR	5.1
1	A	1469	THR	5.1
1	B	2434	THR	5.1
2	C	206	GLU	5.0
1	A	1582	SER	5.0
1	A	1619	TRP	4.7
1	A	2436	THR	4.7
1	B	1469	THR	4.6
2	C	204	GLY	4.5
1	B	2435	ASN	4.5
1	B	1503	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	1506	ASP	4.4
2	D	206	GLU	4.4
2	C	205	ASP	4.3
1	A	1586	ALA	4.2
2	D	265	PRO	4.1
1	A	1576	THR	4.1
1	B	2433	ASP	4.1
1	A	1573	ALA	4.1
1	A	1581	GLU	3.9
1	B	1869	VAL	3.8
1	A	1600	GLU	3.8
1	B	1581	GLU	3.7
1	A	1583	TYR	3.7
1	A	1584	SER	3.7
1	A	1468	ASP	3.6
1	A	2435	ASN	3.5
1	B	1582	SER	3.5
1	A	1499	GLU	3.4
1	A	2044	VAL	3.4
2	C	10	SER	3.3
1	A	1531	GLU	3.3
1	B	1586	ALA	3.2
1	A	2428	ASN	3.2
1	B	1578	MET	3.2
2	C	117	ARG	3.1
2	D	205	ASP	3.1
1	A	2091	SER	3.1
1	A	2090	LYS	3.1
1	B	1587	TYR	3.1
1	A	1606	LYS	3.1
1	A	1569	ASP	3.1
1	A	1812	ASP	3.1
1	A	1502	THR	3.0
1	B	1446	GLN	3.0
1	A	1385	GLU	3.0
2	C	265	PRO	3.0
1	A	1554	GLN	3.0
1	A	1633	TRP	3.0
1	B	2090	LYS	2.9
1	B	2045	LYS	2.9
2	C	203	ILE	2.9
1	A	1393	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1505	ASN	2.8
1	B	1465	LYS	2.8
1	A	1647	HIS	2.8
1	B	1471	LYS	2.8
1	A	1563	CYS	2.8
1	A	1867	LYS	2.7
1	B	1583	TYR	2.7
1	A	1387	ALA	2.7
1	A	2042	ARG	2.7
1	A	1587	TYR	2.6
1	B	1458	ASP	2.6
1	B	1575	LEU	2.6
2	C	266	GLY	2.6
1	A	2433	ASP	2.6
1	A	1628	ARG	2.5
1	A	1506	ASP	2.5
2	D	266	GLY	2.5
1	A	1562	GLN	2.5
2	C	120	GLN	2.5
2	D	202	GLY	2.5
1	A	1566	LYS	2.5
1	A	1471	LYS	2.5
1	A	1467	MET	2.5
1	A	1869	VAL	2.5
1	A	1734	THR	2.5
1	B	1573	ALA	2.4
1	A	1532	TYR	2.4
1	A	2039	PHE	2.4
1	A	1500	LYS	2.4
1	A	1570	LEU	2.4
1	A	1509	GLN	2.4
1	A	2031	LEU	2.4
1	B	1867	LYS	2.4
1	B	1585	ARG	2.4
1	A	1527	ASP	2.4
1	B	1813	GLU	2.3
1	A	1476	LEU	2.3
2	C	263	GLY	2.3
1	A	1470	ASN	2.3
1	A	2087	LYS	2.3
1	B	2428	ASN	2.3
1	A	1508	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	10	SER	2.3
1	A	2103	LEU	2.3
1	A	2429	TRP	2.3
1	A	1457	GLU	2.2
1	B	1407	GLY	2.2
1	B	1500	LYS	2.2
1	B	2043	ASN	2.2
1	B	2040	GLY	2.2
1	B	1444	GLU	2.2
1	B	1462	ALA	2.1
1	B	1576	THR	2.1
1	A	1732	ILE	2.1
1	A	1535	MET	2.1
1	A	1407	GLY	2.1
1	A	1446	GLN	2.1
1	A	2045	LYS	2.1
1	A	1458	ASP	2.1
1	A	1388	ALA	2.1
1	A	1603	ILE	2.1
1	A	2104	TYR	2.0
1	A	1534	CYS	2.0
1	B	1574	GLU	2.0
1	A	1813	GLU	2.0
1	B	1572	ASP	2.0
1	B	1474	PRO	2.0
1	A	1504	VAL	2.0
1	A	1462	ALA	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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.