



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 PM UTC

PDB ID : 4JSN / pdb_00004jsn
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

<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

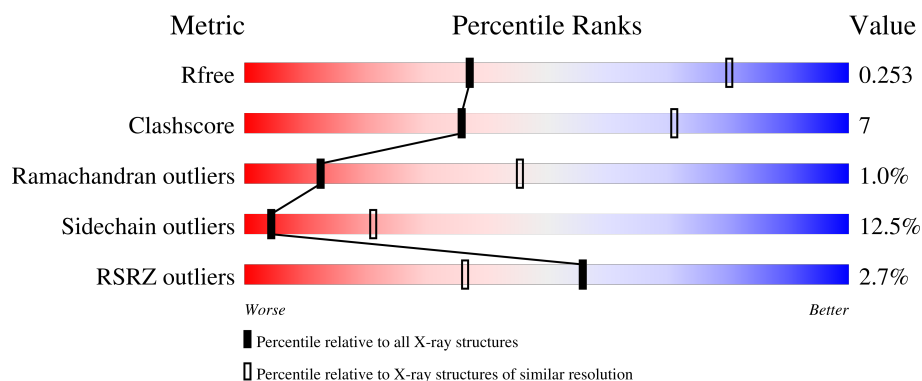
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	1174	4% 67% 20% • 10%
1	B	1174	% 68% 19% • 10%
2	C	326	2% 65% 27% 5% •
2	D	326	2% 66% 27% 5% •

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			

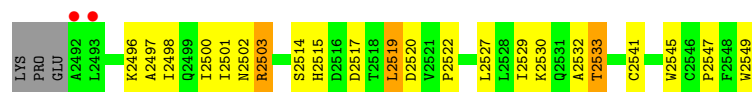
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

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			

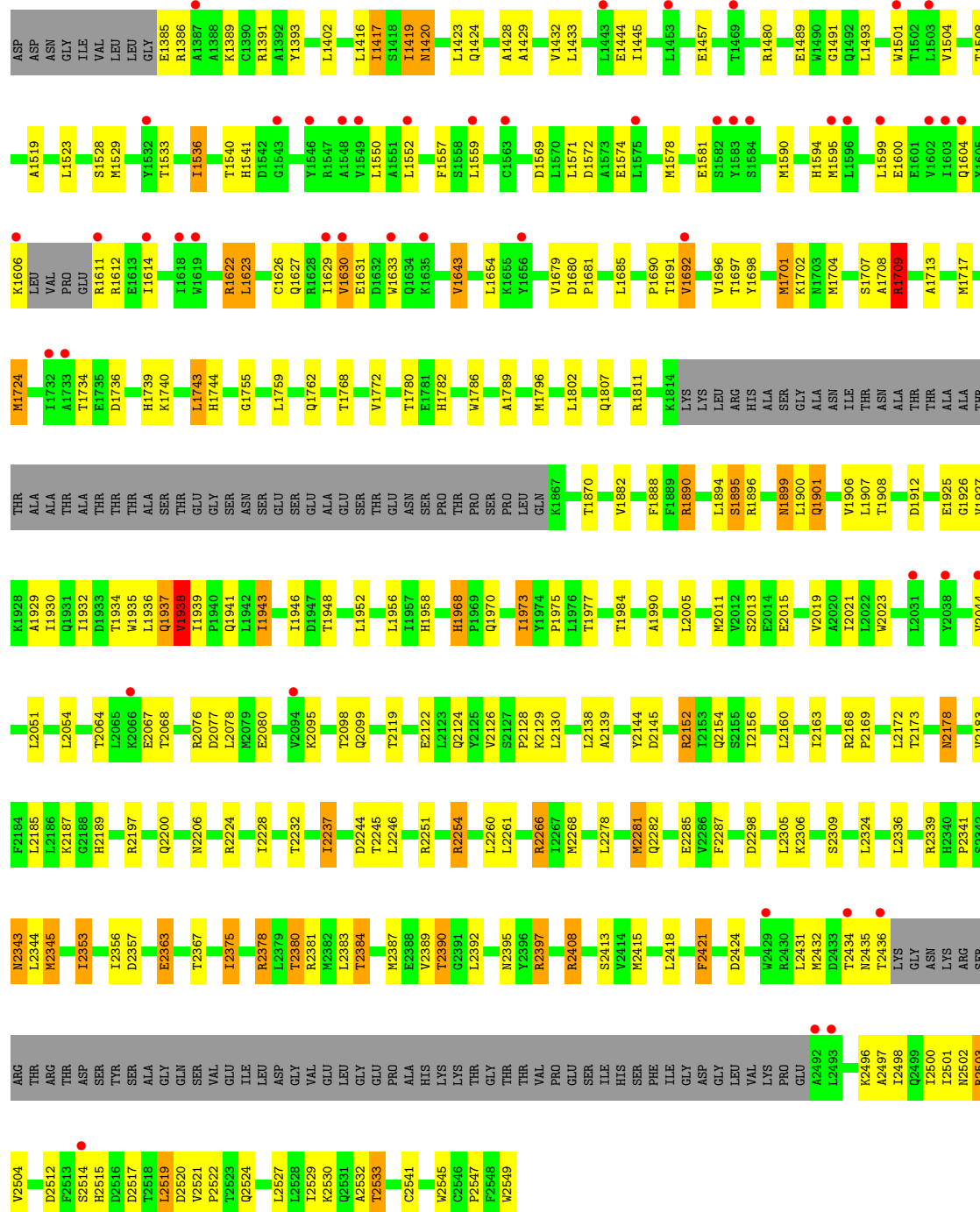
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- Molecule 1: Serine/threonine-protein kinase mTOR

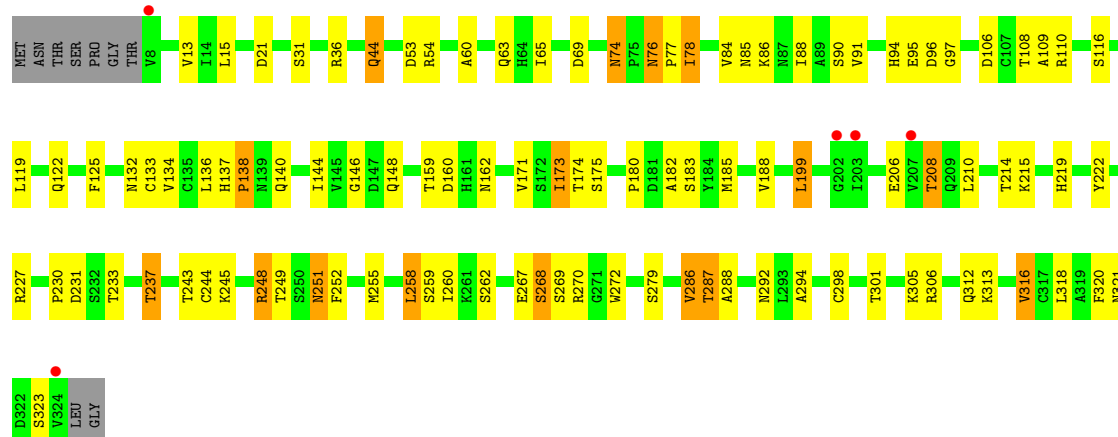




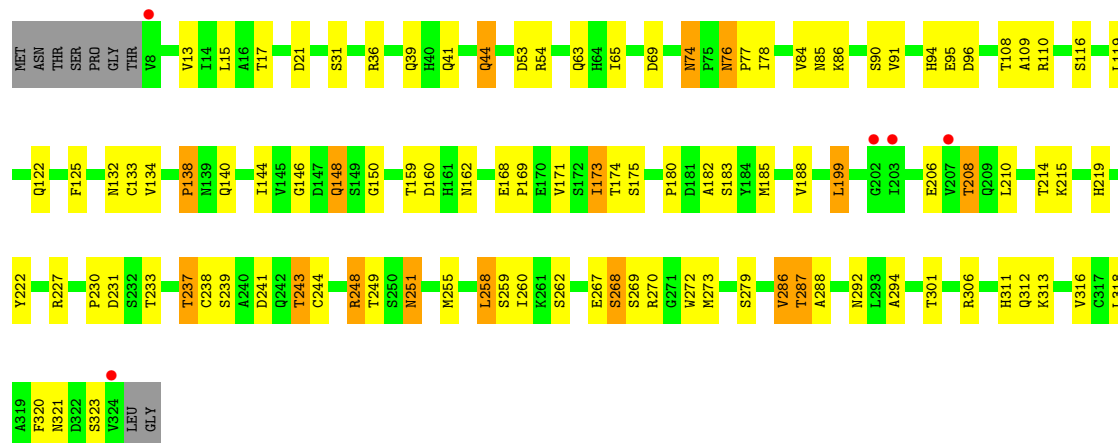
• Molecule 1: Serine/threonine-protein kinase mTOR



• 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	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 3.20 29.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (29.86-3.20) 86.7 (29.86-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.18Å)	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	1857 reflections (2.35%)	wwPDB-VP
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 , 54.5	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	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	2/8772 (0.0%)	1.26	8/11872 (0.1%)
1	B	0.70	1/8805 (0.0%)	1.25	8/11920 (0.1%)
2	C	0.69	0/2514	1.11	6/3426 (0.2%)
2	D	0.72	0/2514	1.13	7/3426 (0.2%)
All	All	0.70	3/22605 (0.0%)	1.22	29/30644 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	ILE	CA-CB	5.58	1.56	1.54
1	B	1939	ILE	CA-CB	5.52	1.56	1.54
1	A	1882	VAL	CA-CB	5.35	1.56	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1938	VAL	CB-CA-C	9.15	119.76	110.70
1	B	1445	ILE	N-CA-C	-8.00	97.05	108.58
1	A	1445	ILE	N-CA-C	-7.60	97.64	108.58
2	D	321	ASN	N-CA-C	7.10	120.05	108.26
2	C	321	ASN	N-CA-C	6.79	119.53	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2381	ARG	N-CA-C	6.78	118.67	111.28
2	C	74	ASN	CA-C-N	-6.45	114.08	120.98
2	C	74	ASN	C-N-CA	-6.45	114.08	120.98
2	D	74	ASN	N-CA-C	6.24	123.61	109.81
1	B	1643	VAL	CB-CA-C	6.16	116.95	110.91
1	A	2381	ARG	N-CA-C	6.13	117.96	111.28
1	A	1643	VAL	CB-CA-C	6.11	116.90	110.91
2	C	74	ASN	N-CA-C	6.01	123.10	109.81
2	C	268	SER	N-CA-C	5.86	123.27	110.80
1	B	2375	ILE	CB-CA-C	5.71	116.47	110.37
2	D	268	SER	N-CA-C	5.67	122.88	110.80
2	D	316	VAL	CB-CA-C	5.49	116.54	110.62
1	B	1973	ILE	N-CA-CB	5.42	117.50	110.57
2	C	239	SER	N-CA-C	5.39	117.38	109.24
1	A	1929	ALA	CA-C-N	5.38	127.91	120.49
1	A	1929	ALA	C-N-CA	5.38	127.91	120.49
1	B	1681	PRO	N-CA-C	-5.34	103.40	111.41
1	B	2421	PHE	N-CA-C	5.30	119.81	113.23
1	A	2421	PHE	N-CA-C	5.28	119.78	113.23
2	D	137	HIS	CA-C-N	5.22	126.37	119.84
2	D	137	HIS	C-N-CA	5.22	126.37	119.84
2	D	78	ILE	CB-CA-C	-5.16	105.26	112.02
1	A	1681	PRO	N-CA-C	-5.12	103.73	111.41
1	B	2375	ILE	N-CA-CB	-5.09	106.16	111.61

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 [i](#)

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	124	1
1	B	8608	0	8593	120	0
2	C	2456	0	2341	44	0
2	D	2456	0	2341	45	0
All	All	22097	0	21834	321	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 (321) 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:1691:THR:HG23	1:A:1724:MET:HE1	1.58	0.86
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.58	0.84
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.59	0.83
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:2281:MET:HE1	2:D:222:TYR:CD2	2.28	0.68
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:2281:MET:HE1	2:C:222:TYR:CD2	2.33	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:2380:THR:HG23	1:B:2549:TRP:C	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:D:208:THR:HG23	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
1:A:2375:ILE:HD12	1:A:2532:ALA:HA	1.85	0.59
2:C:76:ASN:HB3	2:C:77:PRO:HD3	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:A:2281:MET:HE1	2:C:222:TYR:CG	2.37	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:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.85	0.57
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.51	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:B:2281:MET:HE1	2:D:222:TYR:CG	2.39	0.57
1:A:2345:MET:HE3	1:A:2356:ILE:HG21	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2380:THR:HG23	1:A:2549:TRP:C	2.30	0.56
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.87	0.56
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.20	0.56
2:D:76:ASN:HB3	2:D:77:PRO:HD3	1.88	0.56
2:D:219:HIS:NE2	2:D:237:THR:CG2	2.68	0.56
1:B:1796:MET:HE2	1:B:1796:MET:HA	1.88	0.55
2:D:36:ARG:NH2	2:D:69:ASP:O	2.39	0.55
1:A:2011:MET:HE2	1:A:2129:LYS:HB3	1.88	0.55
1:A:1926:GLY:O	1:A:1930:ILE:HG22	2.06	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
2:D:21:ASP:HB3	2:D:313:LYS:H	1.72	0.55
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.55
1:A:1807:GLN:HE21	1:A:1811:ARG:HH21	1.55	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
1:A:1796:MET:HE2	1:A:1796:MET:HA	1.90	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
1:B:1386:ARG:HA	1:B:1389:LYS:HD2	1.89	0.54
2:D:279:SER:HA	2:D:320:PHE:HE2	1.73	0.54
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.90	0.54
1:B:2251:ARG:HA	1:B:2261:LEU:HD13	1.91	0.53
1:A:1501:TRP:O	1:A:1504:VAL:HG22	2.09	0.53
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.91	0.53
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.91	0.53
1:A:1623:LEU:HG	1:A:1633:TRP:CH2	2.44	0.53
1:B:1501:TRP:O	1:B:1504:VAL:HG22	2.09	0.53
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.42	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:54:ARG:HD2	2:C:323:SER:HB2	1.91	0.52
2:C:63:GLN:HE21	2:C:86:LYS:H	1.57	0.52
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.91	0.52
1:B:2345:MET:HE3	1:B:2356:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1908:THR:O	1:B:1912:ASP:HB2	2.10	0.52
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.43	0.52
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.75	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:2019:VAL:HG22	1:A:2126:VAL:HG12	1.92	0.51
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.10	0.51
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.10	0.51
1:B:1701:MET:HE1	1:B:1717:MET:N	2.26	0.51
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.92	0.51
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.83	0.51
1:A:1701:MET:HE1	1:A:1717:MET:N	2.26	0.51
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.93	0.51
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.11	0.51
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.93	0.50
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
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:1391:ARG:HH21	1:B:2309:SER:HB3	1.76	0.50
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	1.94	0.50
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.93	0.50
2:D:262:SER:HA	2:D:270:ARG:HH11	1.76	0.49
2:C:287:THR:O	2:C:294:ALA:HA	2.11	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
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.95	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:2246:LEU:HD23	1:B:2341:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1977:THR:HG21	1:A:2013:SER:OG	2.12	0.48
1:B:2266:ARG:HB2	1:B:2266:ARG:HH11	1.79	0.48
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.96	0.48
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.13	0.48
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.46	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:D:94:HIS:CE1	2:D:96:ASP:HB2	2.49	0.47
2:C:248:ARG:HD2	2:C:255:MET:HB2	1.95	0.47
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.97	0.47
1:B:2011:MET:HE2	1:B:2129:LYS:HB3	1.95	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
1:B:2363:GLU:OE1	1:B:2363:GLU:HA	2.14	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: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:2432:MET:HE3	1:B:2435:ASN:HD22	1.80	0.47
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.22	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
1:A:1708:ALA:HB3	1:A:1709:ARG:CZ	2.46	0.47
1:A:1755:GLY:HA2	1:A:1772:VAL:HG12	1.97	0.47
2:C:244:CYS:HB3	2:C:258:LEU:HD12	1.97	0.47
1:B:1708:ALA:HB3	1:B:1709:ARG:CZ	2.46	0.46
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
1:A:2163:ILE:HB	1:A:2169:PRO:HG2	1.97	0.46
2:C:138:PRO:HG2	2:C:182:ALA:HB2	1.96	0.46
2:D:109:ALA:HB3	2:D:125:PHE:HB3	1.96	0.46
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.98	0.46
1:B:2187:LYS:HD2	1:B:2237:ILE:HD12	1.98	0.46
2:D:248:ARG:HG3	2:D:251:ASN:HD22	1.81	0.46
1:A:2197:ARG:NH1	1:A:2424:ASP:OD2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.15	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:B:2514:SER:OG	1:B:2517:ASP:HB2	2.16	0.45
1:A:2497:ALA:O	1:A:2501:ILE:HD12	2.17	0.45
2:C:279:SER:HA	2:C:320:PHE:CE2	2.50	0.45
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.16	0.45
2:C:133:CYS:SG	2:C:175:SER:HA	2.55	0.45
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	1.99	0.45
1:A:2432:MET:HE3	1:A:2435:ASN:HD22	1.82	0.45
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.25	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:B:1716:HIS:CE1	1:A:2266:ARG:HE	2.35	0.44
1:A:1970:GLN:HA	1:A:1973:ILE:HD11	1.98	0.44
1:A:2285:GLU:HG3	2:C:272:TRP:CE2	2.52	0.44
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.37	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
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.90	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
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:1755:GLY:HA2	1:B:1772:VAL:HG12	1.99	0.44
1:B:1393:TYR:O	1:B:1419:ILE:HD11	2.18	0.44
1:B:1926:GLY:O	1:B:1930:ILE:HG22	2.17	0.44
1:B:1998:MET:HA	1:B:2001:HIS:CE1	2.53	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:2512:ASP:CG	1:A:2524:GLN:HE21	2.26	0.44
1:B:1970:GLN:HA	1:B:1973:ILE:HD11	1.98	0.43
2:D:95:GLU:C	2:D:97:GLY:H	2.25	0.43
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.44	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.18	0.43
2:D:95:GLU:H	2:D:140:GLN:HE22	1.66	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:31:SER:C	2:D:306:ARG:HD3	2.44	0.43
2:D:44:GLN:H	2:D:44:GLN:HG3	1.41	0.43
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.43
2:C:17:THR:HG22	2:C:311:HIS:CE1	2.54	0.43
1:B:1701:MET:HB3	1:B:1701:MET:HE2	1.41	0.43
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.33	0.42
1:A:1936:LEU:HD21	1:A:1968:HIS:CD2	2.54	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: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:2339:ARG:NH2	1:B:2356:ILE:O	2.52	0.42
1:A:2178:ASN:H	1:A:2178:ASN:HD22	1.67	0.42
2:D:248:ARG:O	2:D:252:PHE:HA	2.20	0.42
1:B:2281:MET:HA	1:B:2281:MET:HE3	2.02	0.42
1:A:2375:ILE:HD13	1:A:2375:ILE:HA	1.82	0.42
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.20	0.42
1:A:2529:ILE:O	1:A:2533:THR:HB	2.19	0.42
1:A:2287:PHE:HE1	1:A:2547:PRO:HB2	1.85	0.42
2:D:133:CYS:SG	2:D:175:SER:HA	2.60	0.42
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.20	0.42
2:C:168:GLU:HA	2:C:169:PRO:HD3	1.92	0.42
1:A:1786:TRP:CE3	1:A:1789:ALA:HB2	2.54	0.41
1:A:2324:LEU:HD13	1:A:2353:ILE:HD13	2.02	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
1:B:2178:ASN:HD22	1:B:2178:ASN:H	1.67	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:1762:GLN:HB2	1:B:1768:THR:HG21	2.01	0.41
1:A:2268:MET:HE3	1:A:2287:PHE:HA	2.02	0.41
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2139:ALA:HA	1:A:2152:ARG:HA	2.03	0.41
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	2.01	0.41
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.84	0.41
1:A:1698:TYR:O	1:A:1702:LYS:HG2	2.21	0.41
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.20	0.41
1:B:1681:PRO:O	1:B:1683:ARG:HB2	2.20	0.41
1:B:2375:ILE:HD13	1:B:2375:ILE:HA	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:A:1552:LEU:HD22	1:A:1606:LYS:HD3	2.03	0.41
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.85	0.41
1:B:2051:LEU:HA	1:B:2054:LEU:HD12	2.03	0.41
1:B:2140:VAL:HG13	1:B:2174:LEU:HD12	2.03	0.41
1:B:2245:THR:HG22	1:B:2345:MET:HE2	2.02	0.41
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	2.02	0.41
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
1:B:2497:ALA:O	1:B:2501:ILE:HD12	2.21	0.41
1:A:1768:THR:O	1:A:1772:VAL:HG22	2.20	0.41
1:A:2015:GLU:O	1:A:2019:VAL:HG23	2.21	0.41
1:A:2384:THR:O	1:A:2387:MET:HB2	2.21	0.41
2:C:31:SER:C	2:C:306:ARG:HD3	2.46	0.41
2:C:39:GLN:HB3	2:C:41:GLN:HE21	1.86	0.41
2:C:94:HIS:CD2	2:C:140:GLN:HE21	2.39	0.41
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	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:1529:MET:HE3	1:B:1550:LEU:HG	2.03	0.40
1:B:1533:THR:HA	1:B:1536:ILE:HD12	2.02	0.40
2:C:238:CYS:HB3	2:C:273:MET:O	2.21	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: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
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	2.04	0.40
1:A:1557:PHE:HE2	1:A:1606:LYS:HG3	1.86	0.40
2:C:150:GLY:HA2	2:C:173:ILE:HG23	2.03	0.40
1:B:1941:GLN:NE2	1:B:2200:GLN:HE22	2.15	0.40
1:B:2423:TYR:CE1	1:B:2501:ILE:HD13	2.56	0.40
1:A:1491:GLY:HA2	1:A:1523:LEU:HD11	2.03	0.40
1:A:1569:ASP:HA	1:A:1572:ASP:HB2	2.03	0.40
1:A:2278:LEU:HD22	1:A:2282:GLN:HB3	2.03	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:1895:SER:HB2	1:B:1896:ARG:H	1.79	0.40
2:D:60:ALA:HB1	2:D:88:ILE:HG22	2.03	0.40
2:D:298:CYS:HB2	2:D:305:LYS:HE3	2.04	0.40
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.04	0.40
1:A:2390:THR:O	1:A:2390:THR:HG23	2.21	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 [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%)	967 (92%)	72 (7%)	7 (1%)	18	52
1	B	1052/1174 (90%)	967 (92%)	77 (7%)	8 (1%)	16	50
2	C	315/326 (97%)	285 (90%)	24 (8%)	6 (2%)	6	33
2	D	315/326 (97%)	284 (90%)	24 (8%)	7 (2%)	5	29
All	All	2728/3000 (91%)	2503 (92%)	197 (7%)	28 (1%)	12	45

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

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Mol	Chain	Res	Type
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%)	819 (88%)	108 (12%)	5	23
1	B	931/1024 (91%)	821 (88%)	110 (12%)	5	23
2	C	269/276 (98%)	228 (85%)	41 (15%)	3	14
2	D	269/276 (98%)	228 (85%)	41 (15%)	3	14
All	All	2396/2600 (92%)	2096 (88%)	300 (12%)	4	21

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1385	GLU
1	B	1402	LEU
1	B	1417	ILE
1	B	1419	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1424	GLN
1	B	1433	LEU
1	B	1457	GLU
1	B	1480	ARG
1	B	1489	GLU
1	B	1508	THR
1	B	1528	SER
1	B	1536	ILE
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU
1	B	1581	GLU
1	B	1590	MET
1	B	1622	ARG
1	B	1623	LEU
1	B	1626	CYS
1	B	1627	GLN
1	B	1629	ILE
1	B	1630	VAL
1	B	1636	ILE
1	B	1643	VAL
1	B	1679	VAL
1	B	1685	LEU
1	B	1701	MET
1	B	1709	ARG
1	B	1724	MET
1	B	1734	THR
1	B	1736	ASP
1	B	1740	LYS
1	B	1743	LEU
1	B	1780	THR
1	B	1802	LEU
1	B	1870	THR
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	1925	GLU
1	B	1927	VAL
1	B	1932	ILE
1	B	1938	VAL
1	B	1943	ILE
1	B	1948	THR
1	B	1952	LEU
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	2005	LEU
1	B	2021	ILE
1	B	2044	VAL
1	B	2068	THR
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2080	GLU
1	B	2119	THR
1	B	2124	GLN
1	B	2138	LEU
1	B	2145	ASP
1	B	2152	ARG
1	B	2154	GLN
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2183	VAL
1	B	2185	LEU
1	B	2189	HIS
1	B	2228	ILE
1	B	2232	THR
1	B	2237	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET

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Mol	Chain	Res	Type
1	B	2305	LEU
1	B	2306	LYS
1	B	2343	ASN
1	B	2344	LEU
1	B	2345	MET
1	B	2353	ILE
1	B	2363	GLU
1	B	2364	VAL
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	2431	LEU
1	B	2434	THR
1	B	2436	THR
1	B	2503	ARG
1	B	2515	HIS
1	B	2519	LEU
1	B	2527	LEU
1	B	2530	LYS
1	B	2533	THR
2	D	13	VAL
2	D	44	GLN
2	D	53	ASP
2	D	65	ILE
2	D	78	ILE
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	134	VAL
2	D	136	LEU
2	D	144	ILE
2	D	159	THR

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Mol	Chain	Res	Type
2	D	160	ASP
2	D	162	ASN
2	D	171	VAL
2	D	173	ILE
2	D	174	THR
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	208	THR
2	D	214	THR
2	D	215	LYS
2	D	227	ARG
2	D	237	THR
2	D	243	THR
2	D	248	ARG
2	D	249	THR
2	D	251	ASN
2	D	258	LEU
2	D	259	SER
2	D	260	ILE
2	D	286	VAL
2	D	287	THR
2	D	292	ASN
2	D	301	THR
2	D	312	GLN
1	A	1385	GLU
1	A	1402	LEU
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	1489	GLU
1	A	1508	THR
1	A	1528	SER
1	A	1536	ILE
1	A	1540	THR
1	A	1541	HIS
1	A	1559	LEU

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Mol	Chain	Res	Type
1	A	1581	GLU
1	A	1590	MET
1	A	1622	ARG
1	A	1623	LEU
1	A	1626	CYS
1	A	1627	GLN
1	A	1629	ILE
1	A	1630	VAL
1	A	1643	VAL
1	A	1679	VAL
1	A	1685	LEU
1	A	1701	MET
1	A	1709	ARG
1	A	1724	MET
1	A	1734	THR
1	A	1736	ASP
1	A	1740	LYS
1	A	1743	LEU
1	A	1780	THR
1	A	1802	LEU
1	A	1870	THR
1	A	1890	ARG
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1901	GLN
1	A	1925	GLU
1	A	1927	VAL
1	A	1932	ILE
1	A	1938	VAL
1	A	1943	ILE
1	A	1948	THR
1	A	1952	LEU
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	2005	LEU
1	A	2021	ILE
1	A	2044	VAL
1	A	2068	THR
1	A	2076	ARG

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Mol	Chain	Res	Type
1	A	2077	ASP
1	A	2078	LEU
1	A	2080	GLU
1	A	2119	THR
1	A	2122	GLU
1	A	2124	GLN
1	A	2138	LEU
1	A	2145	ASP
1	A	2152	ARG
1	A	2154	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2183	VAL
1	A	2185	LEU
1	A	2189	HIS
1	A	2228	ILE
1	A	2232	THR
1	A	2237	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2305	LEU
1	A	2306	LYS
1	A	2343	ASN
1	A	2344	LEU
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	2431	LEU
1	A	2434	THR

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Mol	Chain	Res	Type
1	A	2436	THR
1	A	2503	ARG
1	A	2515	HIS
1	A	2519	LEU
1	A	2527	LEU
1	A	2530	LYS
1	A	2533	THR
2	C	13	VAL
2	C	44	GLN
2	C	53	ASP
2	C	65	ILE
2	C	78	ILE
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	134	VAL
2	C	144	ILE
2	C	148	GLN
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	171	VAL
2	C	173	ILE
2	C	174	THR
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	208	THR
2	C	214	THR
2	C	215	LYS
2	C	227	ARG
2	C	237	THR
2	C	243	THR
2	C	248	ARG
2	C	249	THR
2	C	251	ASN
2	C	258	LEU
2	C	259	SER

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Mol	Chain	Res	Type
2	C	260	ILE
2	C	286	VAL
2	C	287	THR
2	C	292	ASN
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1496	GLN
1	B	1525	GLN
1	B	1541	HIS
1	B	1562	GLN
1	B	1594	HIS
1	B	1727	GLN
1	B	1729	GLN
1	B	1739	HIS
1	B	1758	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1807	GLN
1	B	1920	ASN
1	B	1941	GLN
1	B	1968	HIS
1	B	2001	HIS
1	B	2028	HIS
1	B	2082	GLN
1	B	2114	GLN
1	B	2124	GLN
1	B	2161	GLN
1	B	2167	GLN
1	B	2178	ASN
1	B	2265	HIS
1	B	2319	ASN
1	B	2343	ASN
1	B	2395	ASN
1	B	2428	ASN
1	B	2435	ASN
1	B	2494	ASN
1	B	2502	ASN
2	D	22	HIS

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Mol	Chain	Res	Type
2	D	30	HIS
2	D	41	GLN
2	D	63	GLN
2	D	73	ASN
2	D	94	HIS
2	D	128	ASN
2	D	132	ASN
2	D	140	GLN
2	D	251	ASN
2	D	264	ASN
2	D	311	HIS
2	D	312	GLN
1	A	1541	HIS
1	A	1594	HIS
1	A	1670	HIS
1	A	1693	HIS
1	A	1727	GLN
1	A	1739	HIS
1	A	1758	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1803	HIS
1	A	1807	GLN
1	A	1920	ASN
1	A	1968	HIS
1	A	2082	GLN
1	A	2124	GLN
1	A	2161	GLN
1	A	2167	GLN
1	A	2178	ASN
1	A	2200	GLN
1	A	2265	HIS
1	A	2319	ASN
1	A	2343	ASN
1	A	2395	ASN
1	A	2428	ASN
1	A	2435	ASN
1	A	2494	ASN
1	A	2502	ASN
2	C	22	HIS
2	C	41	GLN
2	C	63	GLN

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Mol	Chain	Res	Type
2	C	73	ASN
2	C	94	HIS
2	C	128	ASN
2	C	132	ASN
2	C	140	GLN
2	C	251	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1054/1174 (89%)	0.19	48 (4%)	37 23	38, 86, 178, 243	0
1	B	1058/1174 (90%)	-0.16	15 (1%)	73 54	28, 72, 150, 238	0
2	C	317/326 (97%)	-0.10	5 (1%)	70 51	40, 77, 147, 222	0
2	D	317/326 (97%)	-0.40	5 (1%)	70 51	27, 52, 116, 192	0
All	All	2746/3000 (91%)	-0.05	73 (2%)	56 36	27, 74, 170, 243	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1619	TRP	4.8
1	B	1582	SER	4.5
1	A	1599	LEU	4.2
1	A	1559	LEU	4.1
1	A	1582	SER	4.0
1	A	1596	LEU	3.8
1	A	1604	GLN	3.7
1	A	1443	LEU	3.6
2	C	8	VAL	3.4
1	B	1506	ASP	3.4
1	B	1501	TRP	3.3
1	B	1443	LEU	3.2
1	A	1453	LEU	3.2
2	D	207	VAL	3.2
2	C	203	ILE	3.2
1	A	2514	SER	3.0
1	A	1501	TRP	3.0
1	A	1614	ILE	3.0
2	C	324	VAL	3.0
1	A	2038	TYR	2.9
1	A	2094	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2031	LEU	2.9
1	B	2436	THR	2.9
1	A	1603	ILE	2.9
1	B	2493	LEU	2.8
1	A	1630	VAL	2.8
1	A	1595	MET	2.8
1	A	1552	LEU	2.8
1	A	1546	TYR	2.7
2	D	8	VAL	2.7
1	A	1629	ILE	2.6
1	A	1602	VAL	2.6
2	D	203	ILE	2.6
1	A	1563	CYS	2.6
2	C	207	VAL	2.6
1	A	1584	SER	2.5
2	C	202	GLY	2.5
1	A	1549	VAL	2.5
1	A	2044	VAL	2.5
2	D	202	GLY	2.5
1	A	1387	ALA	2.5
1	A	1633	TRP	2.5
1	A	1611	ARG	2.4
1	A	2492	ALA	2.4
1	A	1606	LYS	2.4
1	A	1469	THR	2.4
1	B	1732	ILE	2.4
1	A	1503	LEU	2.3
2	D	324	VAL	2.3
1	B	2094	VAL	2.3
1	A	1548	ALA	2.3
1	A	1543	GLY	2.2
1	A	2429	TRP	2.2
1	A	2436	THR	2.2
1	A	1656	TYR	2.2
1	A	1532	TYR	2.2
1	A	1618	ILE	2.2
1	A	1733	ALA	2.2
1	A	1635	LYS	2.1
1	A	2066	LYS	2.1
1	A	1732	ILE	2.1
1	B	1591	VAL	2.1
1	A	1575	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2493	LEU	2.1
1	B	1427	GLU	2.1
1	B	2434	THR	2.1
1	B	2492	ALA	2.1
1	A	1692	VAL	2.1
1	B	1503	LEU	2.0
1	B	1497	CYS	2.0
1	B	1733	ALA	2.0
1	A	1583	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.