



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:29 PM GMT

PDB ID : 4JSV
Title : mTOR kinase structure, mechanism and regulation.
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

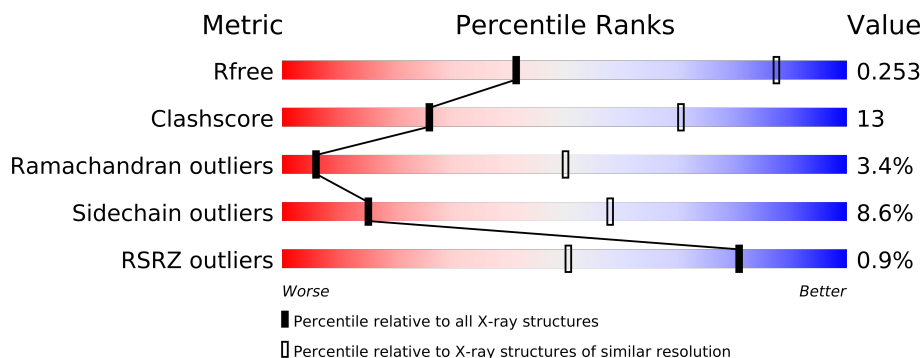
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1174	
1	B	1174	
2	C	326	
2	D	326	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MGF	A	2604	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 22194 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

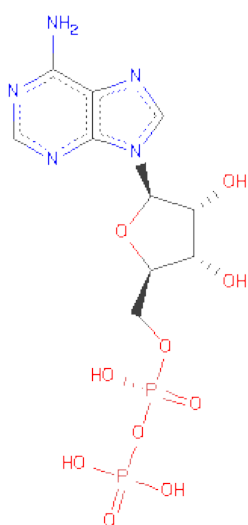
- Molecule 1 is a protein called Serine/threonine-proteinkinase mTOR.

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	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	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			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

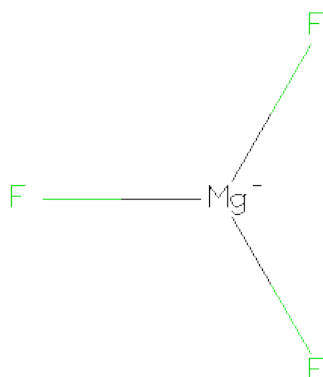


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F₃Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	F	Mg	0	0
			4	3	1		
5	A	1	Total	F	Mg	0	0
			4	3	1		



4 Data and refinement statistics i

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)	100.00 – 3.50 94.42 – 3.48	Depositor EDS
% Data completeness (in resolution range)	83.7 (100.00-3.50) 82.9 (94.42-3.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.231 , 0.251 0.233 , 0.253	Depositor DCC
R_{free} test set	1300 reflections (2.62%)	DCC
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 58045 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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 45.60 % 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 1.2913e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MGF, ADP

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	0.32	0/8805	0.56	0/11920
1	B	0.32	0/8805	0.56	0/11920
2	C	0.34	0/2514	0.61	0/3426
2	D	0.37	0/2514	0.62	0/3426
All	All	0.33	0/22638	0.57	0/30692

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.

There are no bond angle outliers.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8608	0	8593	215	5
1	B	8608	0	8593	203	0
2	C	2456	0	2341	91	0
2	D	2456	0	2341	94	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	22194	0	21892	589	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (589) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.23	1.14
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.21	1.14
2:C:76:ASN:HB3	2:C:77:PRO:CD	1.96	0.95
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.47	0.94
2:D:76:ASN:HB3	2:D:77:PRO:CD	1.98	0.94
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.69	0.93
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.70	0.91
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.90
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.55	0.88
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.56	0.86
2:C:279:SER:HA	2:C:320:PHE:HE2	1.43	0.84
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.77	0.83
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.59	0.82
2:D:279:SER:HA	2:D:320:PHE:HE2	1.45	0.82
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.62	0.82
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.79	0.81
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.62	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.47	0.79
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.83	0.79
2:C:137:HIS:HD2	2:C:139:ASN:H	1.31	0.78
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.64	0.78
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.84	0.78
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.63	0.77
2:D:107:CYS:HB3	2:D:127:VAL:O	1.83	0.77
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.84	0.77
2:D:137:HIS:HD2	2:D:139:ASN:H	1.34	0.76
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.86	0.76
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.65	0.76
1:A:2357:ASP:OD2	3:A:2601:ADP:O3B	2.04	0.76
2:C:107:CYS:HB3	2:C:127:VAL:O	1.84	0.76
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.51	0.76
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.16	0.75
1:B:2401:HIS:O	1:B:2405:GLU:HB2	1.86	0.75
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.70	0.75
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.68	0.74
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.68	0.74
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.69	0.74
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.70	0.74
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.71	0.74
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.69	0.74
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.67	0.74
2:D:301:THR:HB	2:D:303:GLU:HG2	1.70	0.74
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	1.70	0.73
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.18	0.73
1:A:2401:HIS:O	1:A:2405:GLU:HB2	1.86	0.73
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.70	0.73
1:A:2266:ARG:HH11	1:A:2266:ARG:HB2	1.54	0.73
1:B:1915:HIS:CD2	1:B:1953:VAL:HG22	2.24	0.73
2:D:241:ASP:OD2	2:D:243:THR:HB	1.90	0.72
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.30	0.72
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.72	0.71
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.23	0.71
2:C:117:ARG:O	2:C:118:ASN:HB2	1.90	0.71
2:C:301:THR:HB	2:C:303:GLU:HG2	1.73	0.71
1:A:1916:TRP:HD1	1:A:1916:TRP:H	1.38	0.71
1:B:2266:ARG:HH11	1:B:2266:ARG:HB2	1.56	0.70
2:C:279:SER:HA	2:C:320:PHE:CE2	2.27	0.70
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.72	0.70
1:A:2223:GLN:HE22	1:A:2352:LYS:HB2	1.57	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:117:ARG:O	2:D:118:ASN:HB2	1.91	0.69
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.73	0.69
2:C:241:ASP:OD2	2:C:243:THR:HB	1.92	0.69
1:B:2223:GLN:HE22	1:B:2352:LYS:HB2	1.56	0.69
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	0.69
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.74	0.69
2:D:279:SER:HA	2:D:320:PHE:CE2	2.28	0.69
2:C:200:THR:O	2:C:208:THR:HA	1.94	0.68
1:A:1990:ALA:HA	1:A:1993:LYS:HD2	1.74	0.68
1:B:2178:ASN:HD22	1:B:2179:GLY:N	1.91	0.68
1:A:2178:ASN:HD22	1:A:2179:GLY:N	1.91	0.68
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.58	0.68
2:D:200:THR:O	2:D:208:THR:HA	1.94	0.68
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.59	0.67
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.76	0.67
1:A:1915:HIS:CD2	1:A:1953:VAL:HG22	2.30	0.67
1:A:1680:ASP:C	1:A:1682:SER:H	1.97	0.66
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.78	0.66
2:C:137:HIS:CD2	2:C:139:ASN:H	2.12	0.66
1:A:1583:TYR:C	1:A:1585:ARG:H	1.99	0.66
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.77	0.66
1:A:1732:ILE:HD13	1:A:1740:LYS:HD2	1.78	0.66
1:A:1980:SER:O	1:A:1988:HIS:HB2	1.96	0.66
2:D:137:HIS:CD2	2:D:139:ASN:H	2.12	0.65
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.77	0.65
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.61	0.65
1:B:1583:TYR:C	1:B:1585:ARG:H	2.00	0.65
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.79	0.65
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.78	0.65
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.79	0.65
1:B:1680:ASP:C	1:B:1682:SER:H	1.99	0.65
1:B:1980:SER:O	1:B:1988:HIS:HB2	1.96	0.65
2:D:21:ASP:HB3	2:D:313:LYS:H	1.62	0.65
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.78	0.64
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.32	0.64
1:B:2281:MET:HE2	1:B:2281:MET:HA	1.79	0.64
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.33	0.64
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.98	0.64
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.98	0.63
2:C:133:CYS:SG	2:C:175:SER:HA	2.38	0.63
2:C:21:ASP:HB3	2:C:313:LYS:H	1.63	0.63
1:A:2093:ASN:HD22	1:A:2094:VAL:H	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.31	0.63
1:B:2419:GLU:HA	1:B:2501:ILE:HD11	1.80	0.63
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.80	0.63
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.81	0.63
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.81	0.63
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.31	0.62
1:B:2281:MET:HA	1:B:2281:MET:CE	2.29	0.62
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.79	0.62
1:B:2093:ASN:HD22	1:B:2094:VAL:H	1.47	0.62
1:B:1701:MET:HE1	1:B:1717:MET:N	2.14	0.62
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.81	0.62
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.65	0.62
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.81	0.62
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.63	0.62
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.34	0.62
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.82	0.62
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.81	0.61
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.83	0.61
1:B:1422:LYS:HE2	1:B:1581:GLU:HG2	1.83	0.61
1:A:1701:MET:HE1	1:A:1717:MET:N	2.16	0.61
1:B:1417:ILE:HG23	1:B:1432:VAL:HB	1.80	0.61
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.01	0.61
1:B:1990:ALA:HA	1:B:1993:LYS:HD2	1.82	0.61
1:B:1401:GLU:OE1	1:B:2317:ARG:NH1	2.33	0.61
1:B:1732:ILE:HD13	1:B:1740:LYS:HD2	1.83	0.61
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.99	0.61
1:B:1970:GLN:NE2	1:B:2139:ALA:H	1.98	0.61
1:B:1916:TRP:HD1	1:B:1916:TRP:H	1.42	0.60
1:A:1771:LYS:O	1:A:1774:GLN:HB3	2.01	0.60
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.84	0.60
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.66	0.60
1:A:2419:GLU:HA	1:A:2501:ILE:HD11	1.84	0.60
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.01	0.60
1:A:1680:ASP:C	1:A:1682:SER:N	2.55	0.60
2:D:133:CYS:SG	2:D:175:SER:HA	2.41	0.60
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.60
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.84	0.60
1:A:2178:ASN:HD22	1:A:2179:GLY:H	1.50	0.60
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.68	0.59
1:A:2281:MET:CE	1:A:2281:MET:HA	2.32	0.59
1:B:1680:ASP:C	1:B:1682:SER:N	2.56	0.59
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.15	0.59
2:C:166:ILE:HG13	2:C:166:ILE:O	2.02	0.59
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.83	0.59
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.20	0.59
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.66	0.58
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.38	0.58
1:B:1783:ASP:O	1:B:1785:SER:N	2.37	0.58
1:A:1733:ALA:O	1:A:1735:GLU:N	2.36	0.58
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.28	0.58
2:C:151:ALA:HA	2:C:166:ILE:HG22	1.84	0.58
2:C:95:GLU:H	2:C:140:GLN:HE22	1.50	0.58
1:A:1783:ASP:O	1:A:1785:SER:N	2.37	0.58
1:A:2281:MET:HE2	1:A:2281:MET:HA	1.85	0.58
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.39	0.58
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.85	0.58
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.04	0.58
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.86	0.58
1:B:1771:LYS:O	1:B:1774:GLN:HB3	2.03	0.58
2:D:166:ILE:O	2:D:166:ILE:HG13	2.03	0.57
2:D:151:ALA:HA	2:D:166:ILE:HG22	1.85	0.57
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.20	0.57
1:A:1701:MET:HE1	1:A:1717:MET:CA	2.35	0.57
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.22	0.57
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.87	0.57
1:B:1505:ASN:HB2	1:B:1508:THR:HB	1.86	0.56
1:B:2178:ASN:HD22	1:B:2179:GLY:H	1.52	0.56
2:D:219:HIS:HE1	2:D:243:THR:HG22	1.71	0.56
1:A:1505:ASN:HB2	1:A:1508:THR:HB	1.87	0.56
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.71	0.56
2:D:95:GLU:H	2:D:140:GLN:HE22	1.51	0.56
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.38	0.56
2:C:17:THR:HB	2:C:311:HIS:HE1	1.70	0.56
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.87	0.56
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.06	0.56
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.56
1:A:2163:ILE:HB	1:A:2169:PRO:HG2	1.87	0.56
2:C:18:ALA:HB1	2:C:45:VAL:HG21	1.88	0.56
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.87	0.56
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.87	0.56
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.70	0.55
1:B:2390:THR:HG23	1:B:2390:THR:O	2.06	0.55
2:D:168:GLU:N	2:D:169:PRO:HD2	2.20	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.72	0.55
2:C:167:PRO:HB2	2:C:169:PRO:HD2	1.89	0.55
2:C:168:GLU:N	2:C:169:PRO:HD2	2.21	0.55
1:B:1680:ASP:OD2	1:B:1683:ARG:HB2	2.06	0.55
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.41	0.55
1:B:1701:MET:HE1	1:B:1717:MET:CA	2.37	0.55
1:A:2390:THR:O	1:A:2390:THR:HG23	2.06	0.55
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.71	0.55
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.38	0.55
1:B:1466:LYS:O	1:B:1470:ASN:HB2	2.07	0.55
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.07	0.55
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.32	0.54
2:D:167:PRO:HB2	2:D:169:PRO:HD2	1.89	0.54
2:D:18:ALA:HB1	2:D:45:VAL:HG21	1.89	0.54
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.04	0.54
1:A:2278:LEU:HD21	2:C:44:GLN:HG2	1.90	0.54
2:D:17:THR:HB	2:D:311:HIS:HE1	1.72	0.54
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.72	0.54
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.71	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.89	0.54
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.90	0.54
1:B:2163:ILE:HB	1:B:2169:PRO:HG2	1.90	0.54
2:D:53:ASP:C	2:D:55:SER:H	2.11	0.54
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.05	0.54
1:B:1933:ASP:O	1:B:1934:THR:C	2.47	0.54
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.89	0.54
1:B:1943:ILE:O	1:B:1946:ILE:HG13	2.08	0.54
2:C:36:ARG:NH2	2:C:69:ASP:O	2.41	0.53
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.89	0.53
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.08	0.53
2:C:8:VAL:HG11	2:C:36:ARG:HE	1.73	0.53
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.43	0.53
1:A:1916:TRP:N	1:A:1916:TRP:CD1	2.64	0.53
2:C:12:PRO:O	2:C:54:ARG:NH2	2.42	0.53
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.91	0.53
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.41	0.53
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.90	0.53
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.91	0.53
2:D:55:SER:O	2:D:56:MET:HG2	2.09	0.53
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.50	0.53
1:B:2357:ASP:OD2	3:B:2601:ADP:O3B	2.27	0.53
2:D:36:ARG:NH2	2:D:69:ASP:O	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:128:ASN:O	2:D:129:ALA:HB3	2.09	0.53
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.74	0.53
2:C:269:SER:OG	2:C:270:ARG:N	2.42	0.53
2:D:169:PRO:HA	2:D:171:VAL:H	1.74	0.52
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.90	0.52
2:D:223:ALA:HA	2:D:239:SER:HB2	1.92	0.52
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.50	0.52
2:C:223:ALA:HA	2:C:239:SER:HB2	1.91	0.52
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.91	0.52
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.45	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
1:A:1557:PHE:CE2	1:A:1606:LYS:HB3	2.44	0.52
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.91	0.52
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.92	0.52
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.10	0.52
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.92	0.52
2:C:28:GLN:O	2:C:28:GLN:HG3	2.10	0.52
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.30	0.51
2:D:12:PRO:O	2:D:54:ARG:NH2	2.44	0.51
2:C:9:GLY:HA3	2:C:70:LEU:HB3	1.93	0.51
2:D:8:VAL:HG11	2:D:36:ARG:HE	1.74	0.51
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.38	0.51
2:C:28:GLN:OE1	2:C:30:HIS:CE1	2.64	0.51
1:A:1999:CYS:HA	1:A:2003:ASN:HA	1.92	0.51
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.92	0.51
1:A:1401:GLU:OE1	1:A:2317:ARG:NH1	2.40	0.51
2:C:31:SER:C	2:C:306:ARG:HD3	2.30	0.51
1:B:1605:TYR:CD2	1:B:1643:VAL:HG11	2.46	0.51
2:C:169:PRO:HA	2:C:171:VAL:H	1.76	0.51
2:C:97:GLY:HA3	2:C:115:ARG:NH2	2.25	0.51
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.91	0.51
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.92	0.51
2:C:53:ASP:C	2:C:55:SER:H	2.14	0.51
2:D:9:GLY:HA3	2:D:70:LEU:HB3	1.93	0.51
2:D:28:GLN:OE1	2:D:30:HIS:CE1	2.64	0.51
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	1.93	0.50
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.92	0.50
1:A:1437:MET:SD	1:A:1453:LEU:HD11	2.52	0.50
2:C:238:CYS:SG	2:C:276:CYS:HB3	2.52	0.50
2:C:128:ASN:O	2:C:129:ALA:HB3	2.11	0.50
1:A:1933:ASP:O	1:A:1934:THR:C	2.50	0.50
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	1.94	0.50
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.93	0.50
1:A:1943:ILE:O	1:A:1946:ILE:HG13	2.12	0.50
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.12	0.50
2:D:31:SER:C	2:D:306:ARG:HD3	2.32	0.50
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.41	0.50
2:C:17:THR:HB	2:C:311:HIS:CE1	2.47	0.50
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.42	0.50
1:B:1752:LEU:O	1:B:1756:GLU:HB2	2.12	0.50
1:B:1936:LEU:HD23	1:B:1939:ILE:HD11	1.94	0.50
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.94	0.49
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.93	0.49
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.94	0.49
1:B:1697:THR:O	1:B:1701:MET:HG3	2.12	0.49
1:A:1497:CYS:SG	1:A:1516:ALA:HB2	2.52	0.49
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	1.93	0.49
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.47	0.49
1:B:1797:ASN:HB3	1:B:1884:ALA:HB2	1.93	0.49
2:D:97:GLY:HA3	2:D:115:ARG:NH2	2.27	0.49
2:D:203:ILE:HA	2:D:206:GLU:HG2	1.95	0.49
1:B:2139:ALA:HA	1:B:2152:ARG:HA	1.94	0.49
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.13	0.49
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.13	0.49
1:A:2321:THR:HG23	1:A:2387:MET:HG2	1.94	0.49
1:B:2278:LEU:HD21	2:D:44:GLN:HG2	1.95	0.49
1:B:1916:TRP:N	1:B:1916:TRP:CD1	2.66	0.49
2:C:203:ILE:HA	2:C:206:GLU:HG2	1.95	0.48
1:B:2345:MET:HG3	1:B:2354:LEU:HD23	1.95	0.48
1:B:2009:ALA:HA	1:B:2138:LEU:HD11	1.94	0.48
1:B:1734:THR:O	1:B:1736:ASP:N	2.46	0.48
1:B:2281:MET:HE2	1:B:2281:MET:CA	2.41	0.48
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.13	0.48
1:A:2078:LEU:HD11	1:A:2107:VAL:HG21	1.95	0.48
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.43	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.94	0.48
1:A:2310:SER:HA	1:A:2313:TRP:HB3	1.95	0.48
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.33	0.48
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.94	0.48
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.94	0.48
1:A:2024:HIS:NE2	1:A:2118:LEU:HD11	2.29	0.48
1:A:1496:GLN:NE2	1:A:1500:LYS:HG3	2.29	0.48
1:A:1895:SER:CB	1:A:1899:ASN:HB3	2.41	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1916:TRP:HA	1:B:1917:PRO:HD2	1.62	0.48
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.47	0.48
1:B:2310:SER:HA	1:B:2313:TRP:HB3	1.96	0.48
1:B:1992:ASN:HA	1:B:1995:LEU:HD12	1.96	0.48
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.79	0.48
2:D:28:GLN:O	2:D:28:GLN:HG3	2.14	0.48
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.14	0.48
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.14	0.48
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.94	0.48
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.14	0.48
1:B:1733:ALA:O	1:B:1735:GLU:N	2.47	0.48
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.46	0.47
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.14	0.47
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.96	0.47
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.47
1:A:1734:THR:O	1:A:1736:ASP:N	2.47	0.47
1:A:1876:THR:O	1:A:1879:MET:HB3	2.14	0.47
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.39	0.47
1:A:1752:LEU:O	1:A:1756:GLU:HB2	2.14	0.47
1:B:1496:GLN:NE2	1:B:1500:LYS:HG3	2.29	0.47
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.15	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.45	0.47
1:B:1564:ILE:HG23	1:B:1596:LEU:HD22	1.95	0.47
2:C:55:SER:O	2:C:56:MET:HG2	2.14	0.47
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.80	0.47
2:D:269:SER:OG	2:D:270:ARG:N	2.47	0.47
2:D:63:GLN:HE21	2:D:86:LYS:H	1.62	0.47
1:B:1734:THR:C	1:B:1736:ASP:H	2.18	0.47
1:A:1982:SER:OG	1:A:1984:THR:HG23	2.14	0.47
2:D:109:ALA:HB3	2:D:125:PHE:HB3	1.97	0.47
1:A:2025:GLU:HG2	1:A:2168:ARG:HH21	1.80	0.47
1:A:1608:VAL:O	1:A:1608:VAL:HG23	2.15	0.47
2:C:159:THR:C	2:C:161:HIS:H	2.18	0.47
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.15	0.47
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.49	0.47
1:B:1393:TYR:CE2	1:B:1422:LYS:HD2	2.49	0.47
1:A:1508:THR:O	1:A:1512:MET:HB2	2.14	0.47
1:A:1734:THR:C	1:A:1736:ASP:H	2.18	0.47
2:D:58:ALA:HA	2:D:67:MET:HG2	1.97	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB2	2.30	0.47
1:B:1508:THR:O	1:B:1512:MET:HB2	2.13	0.47
2:C:63:GLN:NE2	2:C:86:LYS:H	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.97	0.47
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.97	0.47
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.95	0.47
2:D:202:GLY:HA3	2:D:207:VAL:H	1.80	0.46
1:A:2156:ILE:HG12	1:A:2174:LEU:HD22	1.97	0.46
1:B:2421:PHE:CD1	1:B:2430:ARG:NH2	2.84	0.46
1:A:1747:MET:O	1:A:1750:CYS:HB2	2.14	0.46
2:D:248:ARG:HG3	2:D:253:SER:OG	2.16	0.46
2:D:238:CYS:SG	2:D:276:CYS:HB3	2.56	0.46
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.30	0.46
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.14	0.46
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.97	0.46
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.46
1:A:1797:ASN:HB3	1:A:1884:ALA:HB2	1.96	0.46
2:D:117:ARG:O	2:D:118:ASN:CB	2.62	0.46
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.79	0.46
2:D:63:GLN:NE2	2:D:86:LYS:H	2.14	0.46
1:A:2281:MET:HE2	1:A:2281:MET:CA	2.45	0.46
1:B:2360:ASP:N	1:B:2360:ASP:OD1	2.49	0.46
1:B:1939:ILE:N	1:B:1940:PRO:HD2	2.31	0.46
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.81	0.46
1:B:1895:SER:O	1:B:1896:ARG:C	2.54	0.46
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.98	0.46
1:B:2363:GLU:O	1:B:2366:MET:N	2.45	0.46
2:C:117:ARG:O	2:C:118:ASN:CB	2.62	0.46
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.98	0.46
1:B:1415:SER:O	1:B:1419:ILE:HG22	2.15	0.46
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.15	0.46
1:B:2154:GLN:NE2	1:B:2155:SER:HB2	2.31	0.46
2:D:56:MET:HB2	2:D:68:TYR:O	2.15	0.46
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.16	0.45
1:A:2322:ARG:O	1:A:2326:VAL:HG23	2.17	0.45
1:A:2363:GLU:OE2	1:A:2503:ARG:NH1	2.49	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.98	0.45
1:A:1649:ASP:HB3	1:A:1653:TRP:HD1	1.81	0.45
1:A:2208:LEU:HD22	1:A:2410:HIS:CD2	2.51	0.45
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.85	0.45
1:B:2078:LEU:HD11	1:B:2107:VAL:HG21	1.98	0.45
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.81	0.45
1:A:2123:LEU:HB2	1:A:2158:PRO:O	2.17	0.45
1:A:2329:MET:HB3	1:A:2404:MET:HE2	1.99	0.45
2:C:20:TYR:HD2	2:C:44:GLN:HB3	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2336:LEU:HG	1:B:2339:ARG:NH1	2.31	0.45
1:A:2363:GLU:O	1:A:2366:MET:N	2.47	0.45
1:B:1943:ILE:CD1	1:B:1975:PRO:HB2	2.46	0.45
1:A:1433:LEU:HD21	1:A:1452:LYS:HB3	1.98	0.45
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.32	0.45
1:B:2004:THR:HA	1:B:2007:GLN:HB2	1.99	0.45
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.65	0.45
1:B:1437:MET:SD	1:B:1453:LEU:HD11	2.57	0.45
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.97	0.45
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.99	0.45
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.52	0.45
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.45
2:D:17:THR:HB	2:D:311:HIS:CE1	2.49	0.45
1:A:1936:LEU:HD23	1:A:1939:ILE:HD11	1.98	0.45
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.17	0.45
1:A:1415:SER:O	1:A:1419:ILE:HG22	2.16	0.45
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.98	0.45
1:B:1982:SER:OG	1:B:1984:THR:HG23	2.16	0.45
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.99	0.45
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.45
1:A:1701:MET:HE1	1:A:1717:MET:HA	1.98	0.45
2:D:72:SER:O	2:D:74:ASN:N	2.50	0.45
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.20	0.45
1:B:1895:SER:CB	1:B:1899:ASN:HB3	2.44	0.44
1:B:1574:GLU:HG2	1:B:1585:ARG:HH22	1.81	0.44
1:B:1876:THR:O	1:B:1879:MET:HB3	2.17	0.44
1:A:1744:HIS:O	1:A:1782:HIS:HB3	2.18	0.44
1:A:2167:GLN:CG	1:A:2189:HIS:CD2	3.00	0.44
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.32	0.44
1:B:2167:GLN:CG	1:B:2189:HIS:CD2	3.00	0.44
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.53	0.44
1:A:2004:THR:HA	1:A:2007:GLN:HB2	1.99	0.44
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.82	0.44
1:B:1649:ASP:HB3	1:B:1653:TRP:HD1	1.83	0.44
1:B:1583:TYR:C	1:B:1585:ARG:N	2.68	0.44
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.52	0.44
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.52	0.44
1:B:1796:MET:HA	1:B:1796:MET:CE	2.48	0.44
2:C:202:GLY:HA3	2:C:207:VAL:H	1.82	0.44
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.52	0.44
1:B:2366:MET:HG2	1:B:2373:GLU:O	2.17	0.44
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:72:SER:O	2:C:74:ASN:N	2.51	0.44
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.17	0.44
1:A:1796:MET:HA	1:A:1796:MET:CE	2.48	0.44
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.82	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.61	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.48	0.44
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.85	0.44
2:C:248:ARG:HD2	2:C:255:MET:HB2	2.00	0.44
1:B:2130:LEU:HD22	1:B:2156:ILE:HD13	2.00	0.43
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	1.99	0.43
2:D:16:ALA:HB3	2:D:319:ALA:HB3	2.00	0.43
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.18	0.43
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.17	0.43
1:B:2123:LEU:HB2	1:B:2158:PRO:O	2.18	0.43
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.43
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	2.00	0.43
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.18	0.43
1:A:1899:ASN:ND2	1:A:1937:GLN:HE22	2.17	0.43
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.52	0.43
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	2.01	0.43
2:C:109:ALA:HB3	2:C:125:PHE:HB3	2.01	0.43
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.53	0.43
2:D:100:MET:HB3	2:D:112:TRP:HB2	2.01	0.43
1:A:1992:ASN:HA	1:A:1995:LEU:HD12	2.00	0.43
1:B:1913:TYR:O	1:B:1915:HIS:HA	2.18	0.43
1:B:2363:GLU:OE2	1:B:2503:ARG:NH1	2.51	0.43
1:B:1785:SER:O	1:B:1786:TRP:CB	2.65	0.43
1:A:1710:LYS:HZ1	1:A:1760:ASN:HD21	1.65	0.43
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.87	0.43
2:C:56:MET:HB2	2:C:68:TYR:O	2.18	0.43
2:D:74:ASN:H	2:D:75:PRO:HD3	1.83	0.43
2:D:20:TYR:HD2	2:D:44:GLN:HB3	1.83	0.43
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.88	0.43
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	2.00	0.43
1:B:2024:HIS:NE2	1:B:2118:LEU:HD11	2.34	0.43
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.39	0.43
1:A:1697:THR:O	1:A:1701:MET:HG3	2.18	0.43
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	2.00	0.43
2:C:159:THR:C	2:C:161:HIS:N	2.71	0.43
2:D:159:THR:C	2:D:161:HIS:N	2.72	0.43
1:A:2297:ASP:O	1:A:2299:LEU:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.54	0.43
1:A:1505:ASN:O	1:A:1509:GLN:HB2	2.19	0.43
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	2.00	0.43
1:A:2009:ALA:HA	1:A:2138:LEU:HD11	2.01	0.43
1:B:2322:ARG:O	1:B:2326:VAL:HG23	2.19	0.43
1:B:1505:ASN:O	1:B:1509:GLN:HB2	2.19	0.42
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.83	0.42
1:B:2297:ASP:O	1:B:2299:LEU:N	2.52	0.42
1:A:2129:LYS:O	1:A:2132:MET:HB3	2.19	0.42
1:B:1717:MET:HG3	1:B:1754:LEU:HG	2.00	0.42
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.49	0.42
1:A:1939:ILE:N	1:A:1940:PRO:HD2	2.35	0.42
1:A:1418:SER:HB2	1:A:1581:GLU:CG	2.39	0.42
2:D:28:GLN:HE21	2:D:31:SER:HG	1.66	0.42
1:B:2321:THR:HG23	1:B:2387:MET:HG2	2.01	0.42
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.53	0.42
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	2.02	0.42
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.72	0.42
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.49	0.42
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.42
2:C:231:ASP:HB3	2:C:233:THR:H	1.84	0.42
2:C:248:ARG:HG3	2:C:253:SER:OG	2.20	0.42
2:D:96:ASP:O	2:D:98:ARG:N	2.52	0.42
2:C:74:ASN:H	2:C:75:PRO:CD	2.32	0.42
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.48	0.42
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.72	0.42
2:D:231:ASP:HB3	2:D:233:THR:H	1.84	0.42
2:C:63:GLN:HE21	2:C:86:LYS:H	1.66	0.42
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	2.02	0.42
1:A:2362:PHE:O	1:A:2364:VAL:N	2.52	0.42
1:A:1727:GLN:O	1:A:1731:ALA:HB3	2.19	0.42
1:A:1777:SER:O	1:A:1781:GLU:HG2	2.20	0.42
2:D:85:ASN:HD22	2:D:85:ASN:H	1.66	0.42
2:C:74:ASN:H	2:C:75:PRO:HD3	1.84	0.42
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.00	0.42
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.89	0.42
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.20	0.42
1:A:1532:TYR:O	1:A:1536:ILE:HG13	2.20	0.42
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	2.01	0.42
1:B:1899:ASN:ND2	1:B:1937:GLN:HE22	2.18	0.42
1:B:1701:MET:HE1	1:B:1717:MET:HA	2.02	0.42
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:74:ASN:H	2:D:75:PRO:CD	2.33	0.42
1:B:1722:GLN:HA	1:B:1725:GLN:NE2	2.35	0.42
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.23	0.42
1:B:2319:ASN:HD22	1:B:2352:LYS:HG3	1.85	0.41
2:C:96:ASP:O	2:C:98:ARG:N	2.53	0.41
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.21	0.41
1:B:2223:GLN:HE22	1:B:2352:LYS:CB	2.28	0.41
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.49	0.41
1:A:2360:ASP:OD1	1:A:2360:ASP:N	2.54	0.41
1:A:2319:ASN:ND2	1:A:2352:LYS:HE3	2.35	0.41
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.85	0.41
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.68	0.41
1:A:1410:PRO:HA	1:A:1413:LEU:HB2	2.02	0.41
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.85	0.41
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.41
2:D:248:ARG:H	2:D:248:ARG:HG2	1.67	0.41
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.41
1:B:1410:PRO:HA	1:B:1413:LEU:HB2	2.02	0.41
2:C:262:SER:OG	2:C:267:GLU:HG2	2.20	0.41
2:C:75:PRO:HB2	2:C:76:ASN:H	1.62	0.41
1:A:1895:SER:O	1:A:1896:ARG:C	2.59	0.41
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.56	0.41
2:D:31:SER:HG	2:D:33:ILE:HG13	1.86	0.41
1:B:1938:VAL:O	1:B:1938:VAL:HG13	2.21	0.41
1:A:2154:GLN:HE21	1:A:2155:SER:HB2	1.85	0.41
1:B:2362:PHE:O	1:B:2364:VAL:N	2.53	0.41
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.56	0.41
1:A:2363:GLU:O	1:A:2365:ALA:N	2.53	0.41
1:B:2080:GLU:O	1:B:2083:GLU:HB3	2.21	0.41
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.20	0.41
1:B:1892:ILE:CG2	1:B:1930:ILE:HD11	2.42	0.41
1:A:2093:ASN:HD22	1:A:2094:VAL:N	2.13	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.03	0.41
1:A:1423:LEU:HA	1:A:1423:LEU:HD12	1.89	0.41
2:D:285:ILE:HG23	2:D:297:TRP:HB2	2.02	0.41
1:A:2285:GLU:HB2	2:C:272:TRP:CZ3	2.56	0.41
2:D:262:SER:OG	2:D:267:GLU:HG2	2.21	0.41
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.85	0.41
1:B:2178:ASN:ND2	1:B:2180:HIS:H	2.18	0.41
1:A:2423:TYR:CE1	1:A:2501:ILE:HD13	2.56	0.41
1:A:1427:GLU:HG2	1:A:1427:GLU:H	1.64	0.41
2:C:100:MET:HB3	2:C:112:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.24	0.41
1:A:1734:THR:C	1:A:1736:ASP:N	2.74	0.41
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.56	0.41
1:B:1532:TYR:O	1:B:1536:ILE:HG13	2.20	0.41
1:B:1955:ARG:HE	1:B:1955:ARG:HB2	1.77	0.41
2:C:202:GLY:HA3	2:C:208:THR:H	1.86	0.40
1:B:1759:LEU:HD21	1:B:1772:VAL:HG21	2.03	0.40
1:B:2154:GLN:HE21	1:B:2155:SER:HB2	1.86	0.40
1:B:1777:SER:O	1:B:1781:GLU:HG2	2.22	0.40
1:B:2292:ASN:HB3	2:D:268:SER:HB2	2.02	0.40
1:A:2408:ARG:O	1:A:2411:LYS:HG2	2.21	0.40
1:B:2032:GLU:O	1:B:2036:ARG:HG2	2.19	0.40
1:A:2252:ASP:O	1:A:2255:GLU:HG2	2.21	0.40
1:A:2152:ARG:HG2	1:A:2177:SER:HB3	2.03	0.40
1:A:2378:ARG:HB2	1:A:2378:ARG:HE	1.67	0.40
1:B:2093:ASN:HD22	1:B:2094:VAL:N	2.14	0.40
1:A:2095:LYS:HA	1:A:2098:THR:HG22	2.03	0.40
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.51	0.40
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.49	0.40
2:C:131:ILE:HA	2:C:147:ASP:HA	2.03	0.40
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.21	0.40
1:B:1688:PRO:HB3	1:A:2270:ARG:NH2	2.37	0.40
2:D:202:GLY:HA3	2:D:208:THR:H	1.86	0.40
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.25	0.40
2:C:58:ALA:HA	2:C:67:MET:HG2	2.04	0.40

All (5) 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	Distance(Å)	Clash(Å)
1:A:1607:LEU:N	1:A:1609:PRO:O[2.554]	1.45	0.75
1:A:1608:VAL:O	1:A:1608:VAL:O[2.554]	1.62	0.58
1:A:1607:LEU:CA	1:A:1609:PRO:O[2.554]	1.83	0.37
1:A:1606:LYS:C	1:A:1609:PRO:O[2.554]	1.99	0.21
1:A:1607:LEU:C	1:A:1609:PRO:O[2.554]	2.01	0.19

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	1052/1174 (90%)	939 (89%)	84 (8%)	29 (3%)	8	55
1	B	1052/1174 (90%)	938 (89%)	85 (8%)	29 (3%)	8	55
2	C	315/326 (97%)	265 (84%)	32 (10%)	18 (6%)	3	33
2	D	315/326 (97%)	264 (84%)	33 (10%)	18 (6%)	3	33
All	All	2734/3000 (91%)	2406 (88%)	234 (9%)	94 (3%)	6	50

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1611	ARG
1	B	1630	VAL
1	B	1650	MET
1	B	1734	THR
1	B	2298	ASP
1	B	2364	VAL
2	D	74	ASN
2	D	97	GLY
2	D	169	PRO
2	D	269	SER
1	A	1525	GLN
1	A	1611	ARG
1	A	1630	VAL
1	A	1650	MET
1	A	1734	THR
1	A	1970	GLN
1	A	2298	ASP
1	A	2364	VAL
2	C	74	ASN
2	C	97	GLY
2	C	169	PRO
2	C	269	SER
1	B	1444	GLU

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Mol	Chain	Res	Type
1	B	1445	ILE
1	B	1735	GLU
1	B	1896	ARG
1	B	1914	GLY
1	B	1970	GLN
1	B	2094	VAL
2	D	35	THR
2	D	54	ARG
2	D	73	ASN
2	D	75	PRO
2	D	160	ASP
2	D	203	ILE
1	A	1445	ILE
1	A	1735	GLU
1	A	1896	ARG
1	A	1914	GLY
1	A	2094	VAL
2	C	35	THR
2	C	73	ASN
2	C	75	PRO
2	C	167	PRO
2	C	203	ILE
1	B	1709	ARG
1	B	1917	PRO
2	D	118	ASN
2	D	167	PRO
1	A	1444	GLU
1	A	1784	ARG
1	A	1917	PRO
1	A	2363	GLU
2	C	54	ARG
2	C	118	ASN
2	C	160	ASP
1	B	1583	TYR
1	B	1784	ARG
1	B	1786	TRP
1	B	1934	THR
1	B	2093	ASN
1	B	2363	GLU
1	A	1583	TYR
1	A	1709	ARG
1	A	1786	TRP

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Mol	Chain	Res	Type
1	A	1934	THR
1	A	2093	ASN
1	B	1584	SER
2	D	129	ALA
1	A	1584	SER
2	C	129	ALA
1	B	1681	PRO
2	D	262	SER
1	A	1681	PRO
2	C	261	LYS
2	C	262	SER
1	B	1473	ASP
1	B	2040	GLY
2	D	263	GLY
1	A	1473	ASP
1	A	2040	GLY
2	C	263	GLY
1	B	1680	ASP
1	B	2391	GLY
2	D	204	GLY
2	D	310	GLY
2	C	204	GLY
1	A	1680	ASP
2	D	201	GLY
1	A	2391	GLY
2	C	310	GLY
1	B	2376	PRO
1	A	2376	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	931/1024 (91%)	855 (92%)	76 (8%)	17	60
1	B	931/1024 (91%)	856 (92%)	75 (8%)	17	61
2	C	269/276 (98%)	242 (90%)	27 (10%)	11	49
2	D	269/276 (98%)	241 (90%)	28 (10%)	10	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2400/2600 (92%)	2194 (91%)	206 (9%)	15 58

All (206) 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	1457	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1540	THR
1	B	1541	HIS
1	B	1590	MET
1	B	1605	TYR
1	B	1611	ARG
1	B	1630	VAL
1	B	1685	LEU
1	B	1724	MET
1	B	1736	ASP
1	B	1746	LEU
1	B	1780	THR
1	B	1872	ASP
1	B	1896	ARG
1	B	1899	ASN
1	B	1912	ASP
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL
1	B	1956	LEU
1	B	1973	ILE
1	B	1984	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS

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Mol	Chain	Res	Type
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2164	THR
1	B	2167	GLN
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2185	LEU
1	B	2189	HIS
1	B	2195	ASP
1	B	2214	THR
1	B	2224	ARG
1	B	2228	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2262	ASN
1	B	2266	ARG
1	B	2281	MET
1	B	2297	ASP
1	B	2311	GLU
1	B	2360	ASP
1	B	2363	GLU
1	B	2378	ARG
1	B	2390	THR
1	B	2397	ARG
1	B	2401	HIS
1	B	2408	ARG
1	B	2412	ASP
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2501	ILE
1	B	2503	ARG
1	B	2515	HIS
1	B	2530	LYS
2	D	10	SER
2	D	13	VAL
2	D	44	GLN
2	D	74	ASN

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Mol	Chain	Res	Type
2	D	79	ILE
2	D	85	ASN
2	D	90	SER
2	D	91	VAL
2	D	128	ASN
2	D	135	CYS
2	D	160	ASP
2	D	161	HIS
2	D	162	ASN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	173	ILE
2	D	174	THR
2	D	183	SER
2	D	239	SER
2	D	248	ARG
2	D	259	SER
2	D	260	ILE
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	304	ILE
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1590	MET
1	A	1605	TYR
1	A	1611	ARG
1	A	1630	VAL
1	A	1685	LEU
1	A	1724	MET
1	A	1736	ASP
1	A	1746	LEU
1	A	1780	THR
1	A	1872	ASP

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Mol	Chain	Res	Type
1	A	1896	ARG
1	A	1899	ASN
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1938	VAL
1	A	1956	LEU
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2077	ASP
1	A	2078	LEU
1	A	2090	LYS
1	A	2093	ASN
1	A	2095	LYS
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2164	THR
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2214	THR
1	A	2224	ARG
1	A	2228	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2262	ASN
1	A	2266	ARG
1	A	2281	MET

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Mol	Chain	Res	Type
1	A	2297	ASP
1	A	2311	GLU
1	A	2360	ASP
1	A	2363	GLU
1	A	2378	ARG
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	2501	ILE
1	A	2503	ARG
1	A	2519	LEU
1	A	2530	LYS
2	C	10	SER
2	C	13	VAL
2	C	44	GLN
2	C	74	ASN
2	C	79	ILE
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
2	C	128	ASN
2	C	135	CYS
2	C	160	ASP
2	C	161	HIS
2	C	162	ASN
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	239	SER
2	C	248	ARG
2	C	259	SER
2	C	260	ILE
2	C	287	THR
2	C	289	SER
2	C	301	THR

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Mol	Chain	Res	Type
2	C	304	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1496	GLN
1	B	1594	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1898	ASN
1	B	1899	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2043	ASN
1	B	2082	GLN
1	B	2093	ASN
1	B	2154	GLN
1	B	2178	ASN
1	B	2189	HIS
1	B	2211	ASN
1	B	2223	GLN
1	B	2277	HIS
1	B	2319	ASN
1	B	2385	ASN
1	B	2395	ASN
1	B	2410	HIS
1	B	2502	ASN
2	D	28	GLN
2	D	30	HIS
2	D	63	GLN
2	D	71	ASN
2	D	85	ASN
2	D	118	ASN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	311	HIS

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Mol	Chain	Res	Type
2	D	312	GLN
1	A	1496	GLN
1	A	1594	HIS
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	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	1970	GLN
1	A	2028	HIS
1	A	2043	ASN
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2211	ASN
1	A	2223	GLN
1	A	2277	HIS
1	A	2319	ASN
1	A	2340	HIS
1	A	2385	ASN
1	A	2395	ASN
1	A	2410	HIS
1	A	2502	ASN
2	C	28	GLN
2	C	30	HIS
2	C	44	GLN
2	C	63	GLN
2	C	71	ASN
2	C	85	ASN
2	C	118	ASN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	161	HIS
2	C	311	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	ADP	A	2601	5,4	29,29,29	1.22	4 (13%)	45,45,45	1.86	7 (15%)
5	MGF	A	2604	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	B	2601	5,4	29,29,29	1.26	4 (13%)	45,45,45	1.81	6 (13%)
5	MGF	B	2604	3	0,3,3	0.00	-	0,3,3	0.00	-

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	ADP	A	2601	5,4	-	0/16/32/32	0/1/3/3
5	MGF	A	2604	3	-	0/0/0/0	0/0/0/0
3	ADP	B	2601	5,4	-	0/16/32/32	0/1/3/3
5	MGF	B	2604	3	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	ADP	C5-C4	3.48	1.48	1.40
3	B	2601	ADP	C5-C4	3.26	1.47	1.40
3	B	2601	ADP	O4'-C1'	2.51	1.45	1.41
3	B	2601	ADP	PA-O3A	2.50	1.64	1.59
3	B	2601	ADP	PB-O3A	2.46	1.64	1.60
3	A	2601	ADP	O4'-C1'	2.31	1.44	1.41
3	A	2601	ADP	PA-O3A	2.23	1.63	1.59
3	A	2601	ADP	PB-O3A	2.14	1.63	1.60

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	ADP	N3-C2-N1	-6.84	122.99	128.71
3	B	2601	ADP	N3-C2-N1	-6.12	123.59	128.71
3	A	2601	ADP	N3-C4-N9	5.81	135.92	125.43
3	B	2601	ADP	N3-C4-N9	5.58	135.51	125.43
3	B	2601	ADP	O4'-C1'-N9	4.52	112.64	108.44
3	A	2601	ADP	O4'-C1'-N9	4.31	112.45	108.44
3	A	2601	ADP	C5-C4-N3	-3.54	117.99	125.70
3	B	2601	ADP	C5-C4-N3	-3.37	118.37	125.70
3	B	2601	ADP	C4-C5-N7	-3.00	106.95	109.52
3	A	2601	ADP	C4-C5-N7	-2.81	107.11	109.52
3	A	2601	ADP	C2-N3-C4	2.78	121.92	114.01
3	B	2601	ADP	C2-N3-C4	2.48	121.08	114.01
3	A	2601	ADP	O3B-PB-O2B	2.04	115.57	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	1058/1174 (90%)	0.11	14 (1%) 74 40	37, 70, 159, 271	0
1	B	1058/1174 (90%)	0.04	11 (1%) 79 47	29, 59, 136, 174	0
2	C	317/326 (97%)	0.16	0 100 100	39, 68, 116, 153	0
2	D	317/326 (97%)	0.08	0 100 100	30, 46, 92, 130	0
All	All	2750/3000 (91%)	0.09	25 (0%) 81 51	29, 62, 144, 271	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1581	GLU	4.0
1	B	2436	THR	3.2
1	B	1578	MET	3.0
1	A	1580	GLY	3.0
1	B	1580	GLY	2.9
1	A	1610	GLU	2.8
1	A	1581	GLU	2.8
1	A	1578	MET	2.7
1	A	2045	LYS	2.6
1	B	2435	ASN	2.4
1	A	2436	THR	2.4
1	A	1599	LEU	2.4
1	A	2097	LEU	2.3
1	B	1607	LEU	2.3
1	A	2435	ASN	2.3
1	A	2042	ARG	2.3
1	B	1469	THR	2.2
1	A	1469	THR	2.2
1	A	2044	VAL	2.2
1	A	2038	TYR	2.1
1	B	1499	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2434	THR	2.1
1	B	2432	MET	2.1
1	B	2045	LYS	2.0
1	A	2090	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MGF	A	2604	4/4	0.34	2.89	75,76,78,79	0
5	MGF	B	2604	4/4	0.18	-0.45	57,59,59,60	0
4	MG	A	2603	1/1	0.17	-0.50	72,72,72,72	0
3	ADP	A	2601	27/27	0.18	-1.29	64,69,81,82	0
4	MG	B	2603	1/1	0.13	-1.89	57,57,57,57	0
3	ADP	B	2601	27/27	0.15	-1.92	50,54,62,62	0
4	MG	A	2602	1/1	0.13	-1.94	74,74,74,74	0
4	MG	B	2602	1/1	0.10	-2.72	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.