



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 4JSV / pdb\_00004jsv  
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

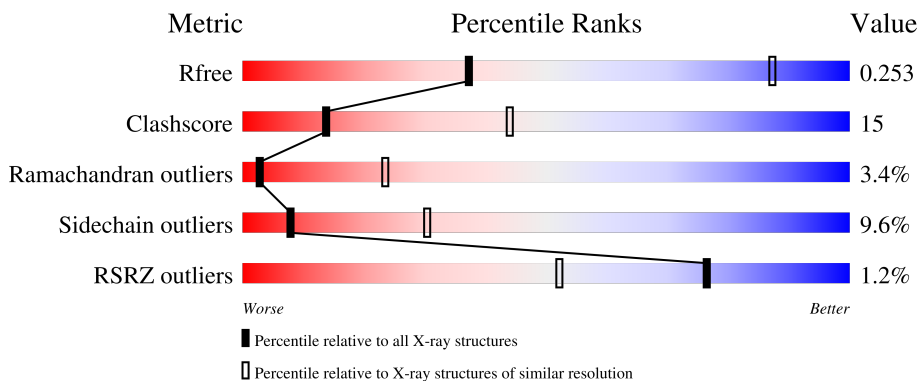
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">59%      25%      5% •      10%</p>
1	B	1174	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">60%      24%      5% •      10%</p>
2	C	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">52%      37%      8% • •</p>
2	D	326	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">52%      37%      8% • •</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22194 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.

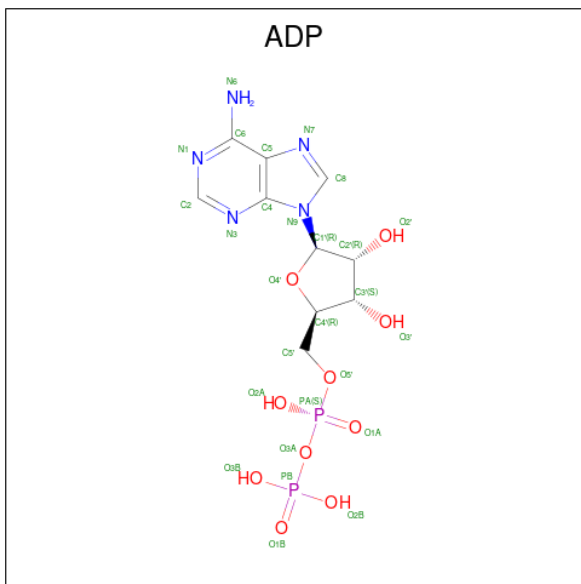
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

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

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

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

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

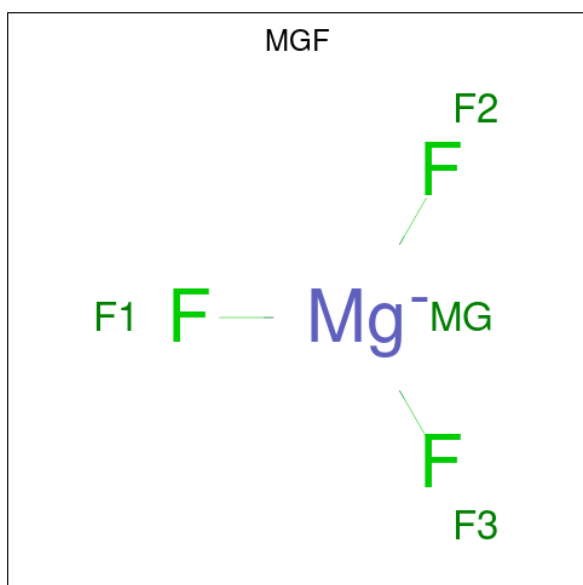


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: 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		

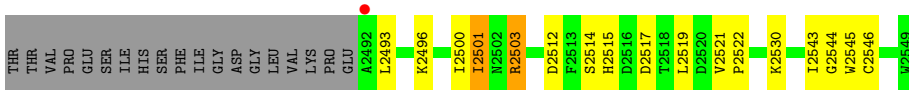
- Molecule 5 is TRIFLUOROMAGNESATE (CCD ID: MGF) (formula: F<sub>3</sub>Mg).



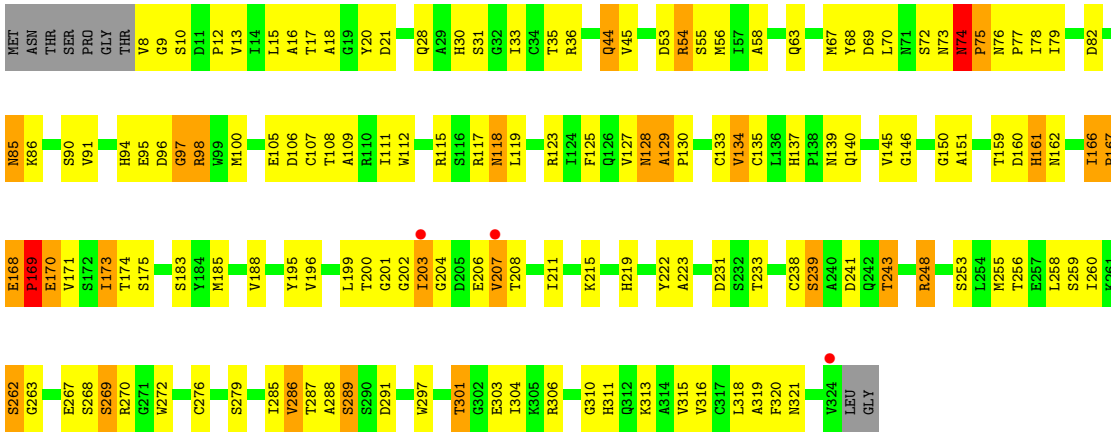
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	F	Mg	0	0
			4	3	1		
5	A	1	Total	F	Mg	0	0
			4	3	1		



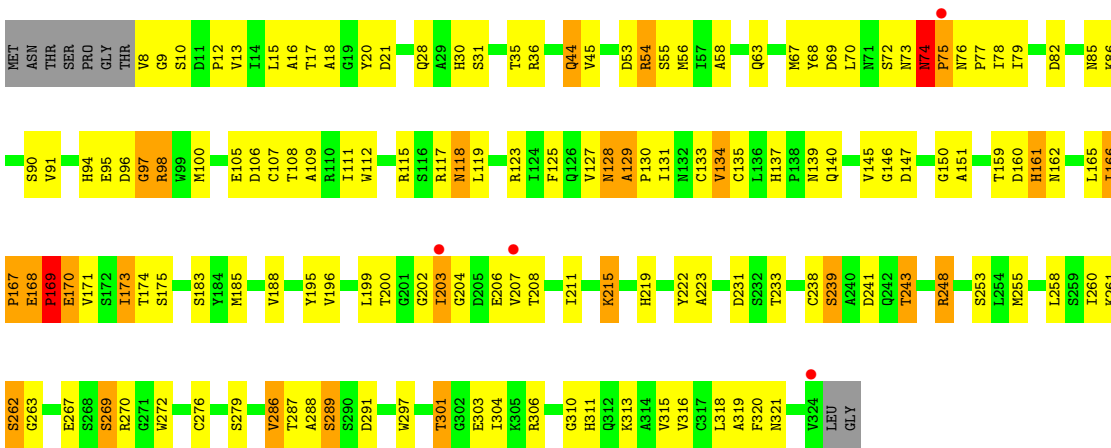




• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.50 100.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.7 (100.00-3.50) 83.7 (100.00-3.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.49Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.231 , 0.251 0.232 , 0.253	Depositor DCC
$R_{free}$ test set	1479 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtrriage
Anisotropy	0.440	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 23.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	1/8805 (0.0%)	0.92	13/11920 (0.1%)
1	B	0.43	0/8805	0.91	17/11920 (0.1%)
2	C	0.45	0/2514	0.86	4/3426 (0.1%)
2	D	0.48	0/2514	0.88	5/3426 (0.1%)
All	All	0.44	1/22638 (0.0%)	0.91	39/30692 (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	1
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1607	LEU	CA-C	5.73	1.60	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	10.61	124.43	109.15
1	B	1915	HIS	N-CA-C	10.47	124.23	109.15
2	D	170	GLU	N-CA-C	-9.55	101.31	113.72
2	C	170	GLU	N-CA-C	-9.06	102.23	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1916	TRP	CA-C-N	8.56	130.54	119.84
1	B	1916	TRP	C-N-CA	8.56	130.54	119.84
1	A	1610	GLU	N-CA-C	8.03	123.83	107.69
1	A	1916	TRP	CA-C-N	7.77	129.55	119.84
1	A	1916	TRP	C-N-CA	7.77	129.55	119.84
1	B	1913	TYR	N-CA-C	6.42	118.22	109.11
2	C	321	ASN	N-CA-C	6.08	118.36	108.26
1	A	1913	TYR	N-CA-C	6.02	117.66	109.11
2	C	98	ARG	N-CA-C	5.96	120.25	112.92
1	B	1610	GLU	N-CA-C	5.91	119.56	107.69
1	A	1968	HIS	CA-C-N	-5.88	113.48	120.13
1	A	1968	HIS	C-N-CA	-5.88	113.48	120.13
2	D	98	ARG	N-CA-C	5.78	120.03	112.92
1	B	1687	HIS	CA-C-N	5.70	126.02	119.92
1	B	1687	HIS	C-N-CA	5.70	126.02	119.92
1	B	1968	HIS	CA-C-N	-5.70	113.69	120.13
1	B	1968	HIS	C-N-CA	-5.70	113.69	120.13
1	B	1711	ILE	N-CA-C	-5.60	104.45	112.35
2	D	321	ASN	N-CA-C	5.57	118.55	108.69
1	A	1711	ILE	N-CA-C	-5.46	104.65	112.35
1	B	2422	VAL	N-CA-C	-5.46	106.38	111.45
1	B	2424	ASP	CA-C-N	5.34	124.52	118.97
1	B	2424	ASP	C-N-CA	5.34	124.52	118.97
1	A	1687	HIS	CA-C-N	5.17	125.45	119.92
1	A	1687	HIS	C-N-CA	5.17	125.45	119.92
1	A	1473	ASP	CA-C-N	5.17	125.47	119.47
1	A	1473	ASP	C-N-CA	5.17	125.47	119.47
1	A	1932	ILE	CB-CA-C	-5.13	105.14	112.22
1	B	1932	ILE	CB-CA-C	-5.09	104.01	112.26
2	D	207	VAL	N-CA-C	-5.07	107.20	111.56
2	D	74	ASN	N-CA-C	5.04	120.96	109.81
2	C	169	PRO	N-CA-C	5.04	122.85	112.47
1	B	1473	ASP	CA-C-N	5.04	125.31	119.47
1	B	1473	ASP	C-N-CA	5.04	125.31	119.47
1	B	1443	LEU	N-CA-C	-5.04	107.20	113.19

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

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Mol	Chain	Res	Type	Group
2	C	169	PRO	Peptide
2	D	169	PRO	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8608	0	8593	239	5
1	B	8608	0	8593	226	0
2	C	2456	0	2341	94	0
2	D	2456	0	2341	98	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	640	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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
1:B:1916:TRP:H	1:B:1916:TRP:CD1	1.89	0.89
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.55	0.88
1:A:1916:TRP:CD1	1:A:1916:TRP:H	1.86	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:2357:ASP:OD2	3:A:2601:ADP:O3B	2.04	0.76
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.65	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:B:1901:GLN:HG3	1:B:2413:SER:HA	1.69	0.74
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.68	0.74
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.71	0.74
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1680:ASP:C	1:A:1682:SER:H	1.97	0.71
2:C:301:THR:HB	2:C:303:GLU:HG2	1.73	0.71
1:A:1916:TRP:H	1:A:1916:TRP:HD1	1.38	0.71
1:A:1583:TYR:C	1:A:1585:ARG:H	1.99	0.71
1:A:1796:MET:HE2	1:A:1796:MET:HA	1.73	0.70
1:B:2266:ARG:HB2	1:B:2266:ARG:HH11	1.56	0.70
1:B:1583:TYR:C	1:B:1585:ARG:H	2.00	0.70
2:C:279:SER:HA	2:C:320:PHE:CE2	2.27	0.70
1:B:1680:ASP:C	1:B:1682:SER:H	1.99	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
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
1:B:2223:GLN:HE22	1:B:2352:LYS:HB2	1.56	0.69
2:C:241:ASP:OD2	2:C:243:THR:HB	1.92	0.69
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.74	0.69
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	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:B:1796:MET:HE2	1:B:1796:MET:HA	1.74	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
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.76	0.67
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.59	0.67
1:A:1915:HIS:CD2	1:A:1953:VAL:HG22	2.30	0.67
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
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:A:2011:MET:HE2	1:A:2129:LYS:HB3	1.77	0.65
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.78	0.65
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.79	0.65
1:B:1980:SER:O	1:B:1988:HIS:HB2	1.96	0.65
1:A:1680:ASP:C	1:A:1682:SER:N	2.55	0.65
2:D:21:ASP:HB3	2:D:313:LYS:H	1.62	0.65
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.79	0.64
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:1680:ASP:C	1:B:1682:SER:N	2.56	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:21:ASP:HB3	2:C:313:LYS:H	1.63	0.63
2:C:133:CYS:SG	2:C:175:SER:HA	2.38	0.63
1:B:1704:MET:HE3	1:B:1713:ALA:HA	1.81	0.63
1:A:2093:ASN:HD22	1:A:2094:VAL:H	1.46	0.63
1:B:2419:GLU:HA	1:B:2501:ILE:HD11	1.80	0.63
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.31	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:2011:MET:HE2	1:B:2129:LYS:HB3	1.80	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:A:1701:MET:HE1	1:A:1717:MET:CA	2.28	0.62
1:B:2093:ASN:HD22	1:B:2094:VAL:H	1.47	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:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.82	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:B:1701:MET:HE1	1:B:1717:MET:CA	2.28	0.62
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.82	0.62
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.34	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: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:1401:GLU:OE1	1:B:2317:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1990:ALA:HA	1:B:1993:LYS:HD2	1.82	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:H	1:B:1916:TRP:HD1	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
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.60
2:D:133:CYS:SG	2:D:175:SER:HA	2.41	0.60
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.01	0.60
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.84	0.60
1:B:1691:THR:CG2	1:B:1724:MET:HE1	2.32	0.60
1:A:2178:ASN:HD22	1:A:2179:GLY:H	1.50	0.60
1:A:1704:MET:HE3	1:A:1713:ALA:HA	1.84	0.60
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.68	0.59
1:A:2281:MET:HA	1:A:2281:MET:CE	2.32	0.59
1:A:1691:THR:CG2	1:A:1724:MET:HE1	2.33	0.59
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.03	0.59
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.15	0.59
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.83	0.59
2:C:166:ILE:HG13	2:C:166:ILE:O	2.02	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
2:D:53:ASP:C	2:D:55:SER:H	2.11	0.58
1:B:1933:ASP:O	1:B:1934:THR:C	2.47	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
1:A:1783:ASP:O	1:A:1785:SER:N	2.37	0.58
2:C:95:GLU:H	2:C:140:GLN:HE22	1.50	0.58
2:C:151:ALA:HA	2:C:166:ILE:HG22	1.84	0.58
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.85	0.58
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.39	0.58
1:B:1771:LYS:O	1:B:1774:GLN:HB3	2.03	0.58
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.86	0.58
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.04	0.58
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.20	0.57
2:D:166:ILE:HG13	2:D:166:ILE:O	2.03	0.57
2:D:151:ALA:HA	2:D:166:ILE:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.20	0.57
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.87	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:D:95:GLU:H	2:D:140:GLN:HE22	1.51	0.56
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.71	0.56
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.38	0.56
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.87	0.56
2:C:17:THR:HB	2:C:311:HIS:HE1	1.70	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
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.40	0.56
2:C:31:SER:C	2:C:306:ARG:HD3	2.30	0.56
2:C:18:ALA:HB1	2:C:45:VAL:HG21	1.88	0.56
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.87	0.56
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	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:C:53:ASP:C	2:C:55:SER:H	2.14	0.55
2:D:168:GLU:N	2:D:169:PRO:HD2	2.20	0.55
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.72	0.55
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.41	0.55
1:B:1680:ASP:OD2	1:B:1683:ARG:HB2	2.06	0.55
1:A:2390:THR:HG23	1:A:2390:THR:O	2.06	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: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:1933:ASP:O	1:A:1934:THR:C	2.50	0.55
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.07	0.55
2:D:18:ALA:HB1	2:D:45:VAL:HG21	1.89	0.54
2:D:31:SER:C	2:D:306:ARG:HD3	2.32	0.54
2:D:167:PRO:HB2	2:D:169:PRO:HD2	1.89	0.54
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.32	0.54
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.72	0.54
2:D:17:THR:HB	2:D:311:HIS:HE1	1.72	0.54
1:A:2278:LEU:HD21	2:C:44:GLN:HG2	1.90	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.89	0.54
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.71	0.54
1:B:1701:MET:HE1	1:B:1717:MET:N	2.23	0.54
1:B:2163:ILE:HB	1:B:2169:PRO:HG2	1.90	0.54
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.90	0.54
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.89	0.54
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.05	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
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.43	0.53
2:C:8:VAL:HG11	2:C:36:ARG:HE	1.73	0.53
1:A:1916:TRP:CD1	1:A:1916:TRP:N	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:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.91	0.53
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.90	0.53
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.41	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
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.74	0.53
2:D:36:ARG:NH2	2:D:69:ASP:O	2.42	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:D:223:ALA:HA	2:D:239:SER:HB2	1.92	0.52
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.90	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:2281:MET:HA	1:A:2281:MET:HE3	1.90	0.52
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.91	0.52
1:A:1701:MET:HE1	1:A:1717:MET:HA	1.89	0.52
1:B:2281:MET:HA	1:B:2281:MET:HE3	1.89	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.45	0.52
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1557:PHE:CE2	1:A:1606:LYS:HB3	2.44	0.52
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.91	0.52
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.90	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
1:A:1701:MET:HE1	1:A:1717:MET:N	2.25	0.52
2:C:28:GLN:O	2:C:28:GLN:HG3	2.10	0.52
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.92	0.52
1:B:1734:THR:C	1:B:1736:ASP:H	2.18	0.51
2:D:12:PRO:O	2:D:54:ARG:NH2	2.44	0.51
2:C:159:THR:C	2:C:161:HIS:H	2.18	0.51
1:A:1734:THR:C	1:A:1736:ASP:H	2.18	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
1:A:1401:GLU:OE1	1:A:2317:ARG:NH1	2.40	0.51
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.92	0.51
1:A:1999:CYS:HA	1:A:2003:ASN:HA	1.92	0.51
2:C:28:GLN:OE1	2:C:30:HIS:CE1	2.64	0.51
1:B:1605:TYR:CD2	1:B:1643:VAL:HG11	2.46	0.51
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.51
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.92	0.51
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.91	0.51
1:A:1583:TYR:C	1:A:1585:ARG:N	2.67	0.51
2:C:97:GLY:HA3	2:C:115:ARG:NH2	2.25	0.51
2:C:169:PRO:HA	2:C:171:VAL:H	1.76	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
2:D:128:ASN:O	2:D:129:ALA:HB3	2.09	0.51
1:B:1895:SER:O	1:B:1896:ARG:C	2.54	0.50
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:B:1759:LEU:HD11	1:B:1796:MET:HE3	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
1:B:1701:MET:HE1	1:B:1717:MET:HA	1.91	0.50
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	1.94	0.50
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.41	0.50
1:B:1477:MET:HE1	1:B:1512:MET:HE1	1.94	0.50
1:B:1752:LEU:O	1:B:1756:GLU:HB2	2.12	0.50
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.42	0.50
1:B:1936:LEU:HD23	1:B:1939:ILE:HD11	1.94	0.50
2:C:17:THR:HB	2:C:311:HIS:CE1	2.47	0.50
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.94	0.49
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.94	0.49
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.93	0.49
1:B:1697:THR:O	1:B:1701:MET:HG3	2.12	0.49
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	1.93	0.49
1:A:1497:CYS:SG	1:A:1516:ALA:HB2	2.52	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
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.47	0.49
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.20	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:2321:THR:HG23	1:A:2387:MET:HG2	1.94	0.49
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.13	0.49
1:B:1916:TRP:CD1	1:B:1916:TRP:N	2.66	0.49
1:B:2278:LEU:HD21	2:D:44:GLN:HG2	1.95	0.49
1:B:1734:THR:O	1:B:1736:ASP:N	2.46	0.48
1:B:2009:ALA:HA	1:B:2138:LEU:HD11	1.94	0.48
1:B:2345:MET:HG3	1:B:2354:LEU:HD23	1.95	0.48
2:C:128:ASN:O	2:C:129:ALA:HB3	2.11	0.48
2:C:203:ILE:HA	2:C:206:GLU:HG2	1.95	0.48
1:A:2078:LEU:HD11	1:A:2107:VAL:HG21	1.95	0.48
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.13	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: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:1496:GLN:NE2	1:A:1500:LYS:HG3	2.29	0.48
1:A:2024:HIS:NE2	1:A:2118:LEU:HD11	2.29	0.48
1:B:1916:TRP:HA	1:B:1917:PRO:HD2	1.62	0.48
1:B:1992:ASN:HA	1:B:1995:LEU:HD12	1.96	0.48
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.48	0.48
1:B:2310:SER:HA	1:B:2313:TRP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:SER:CB	1:A:1899:ASN:HB3	2.41	0.48
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.47	0.48
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.79	0.48
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.14	0.48
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.14	0.48
2:D:28:GLN:HG3	2:D:28:GLN:O	2.14	0.48
1:B:1733:ALA:O	1:B:1735:GLU:N	2.47	0.48
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.14	0.48
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.94	0.48
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.14	0.47
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.47
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.46	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
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.96	0.47
1:A:1752:LEU:O	1:A:1756:GLU:HB2	2.14	0.47
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.39	0.47
1:B:1496:GLN:NE2	1:B:1500:LYS:HG3	2.29	0.47
1:A:1701:MET:HE2	1:A:1717:MET:HE2	1.95	0.47
1:B:1564:ILE:HG23	1:B:1596:LEU:HD22	1.95	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.45	0.47
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.15	0.47
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.80	0.47
1:B:1701:MET:HE2	1:B:1701:MET:HB3	1.60	0.47
2:D:269:SER:OG	2:D:270:ARG:N	2.47	0.47
1:A:1701:MET:HE2	1:A:1701:MET:HB3	1.60	0.47
2:C:55:SER:O	2:C:56:MET:HG2	2.14	0.47
2:D:63:GLN:HE21	2:D:86:LYS:H	1.62	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:1608:VAL:O	1:A:1608:VAL:HG23	2.15	0.47
1:A:2025:GLU:HG2	1:A:2168:ARG:HH21	1.80	0.47
2:C:159:THR:C	2:C:161:HIS:N	2.71	0.47
1:B:1393:TYR:CE2	1:B:1422:LYS:HD2	2.49	0.47
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.49	0.47
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.15	0.47
2:D:58:ALA:HA	2:D:67:MET:HG2	1.97	0.47
1:A:1508:THR:O	1:A:1512:MET:HB2	2.14	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
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
2:C:63:GLN:NE2	2:C:86:LYS:H	2.13	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:1631:GLU:CD	1:B:1631:GLU:H	2.23	0.46
1:B:2421:PHE:CD1	1:B:2430:ARG:NH2	2.84	0.46
2:D:238:CYS:SG	2:D:276:CYS:HB3	2.56	0.46
2:D:248:ARG:HG3	2:D:253:SER:OG	2.16	0.46
1:A:1747:MET:O	1:A:1750:CYS:HB2	2.14	0.46
2:D:159:THR:C	2:D:161:HIS:N	2.72	0.46
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.97	0.46
1:A:1797:ASN:HB3	1:A:1884:ALA:HB2	1.96	0.46
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.14	0.46
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.30	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
2:D:117:ARG:O	2:D:118:ASN:CB	2.62	0.46
1:B:2360:ASP:OD1	1:B:2360:ASP:N	2.49	0.46
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.81	0.46
1:B:1939:ILE:N	1:B:1940:PRO:HD2	2.31	0.46
2:D:58:ALA:HB2	2:D:67:MET:HE3	1.96	0.46
1:A:1895:SER:O	1:A:1896:ARG:C	2.59	0.46
1:A:2281:MET:HE1	2:C:222:TYR:CE2	2.51	0.46
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	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:2019:VAL:HG22	1:B:2126:VAL:HG12	1.98	0.46
1:B:2154:GLN:NE2	1:B:2155:SER:HB2	2.31	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
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: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:2363:GLU:OE2	1:A:2503:ARG:NH1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.24	0.45
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.85	0.45
1:B:2336:LEU:HG	1:B:2339:ARG:NH1	2.31	0.45
2:D:255:MET:HE3	2:D:256:THR:OG1	2.16	0.45
1:A:1734:THR:C	1:A:1736:ASP:N	2.74	0.45
2:C:20:TYR:HD2	2:C:44:GLN:HB3	1.81	0.45
1:B:1943:ILE:CD1	1:B:1975:PRO:HB2	2.46	0.45
1:B:2004:THR:HA	1:B:2007:GLN:HB2	1.99	0.45
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.32	0.45
1:A:1433:LEU:HD21	1:A:1452:LYS:HB3	1.98	0.45
1:A:2363:GLU:O	1:A:2366:MET:N	2.47	0.45
1:B:1437:MET:SD	1:B:1453:LEU:HD11	2.57	0.45
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.52	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:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.45
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.65	0.45
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.25	0.45
2:D:17:THR:HB	2:D:311:HIS:CE1	2.49	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
1:A:1936:LEU:HD23	1:A:1939:ILE:HD11	1.98	0.45
1:B:1982:SER:OG	1:B:1984:THR:HG23	2.16	0.45
2:C:58:ALA:HB2	2:C:67:MET:HE3	1.98	0.45
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.98	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
2:D:72:SER:O	2:D:74:ASN:N	2.50	0.45
1:A:1970:GLN:C	1:A:1972:LEU:H	2.25	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:B:1649:ASP:HB3	1:B:1653:TRP:HD1	1.83	0.44
1:B:2167:GLN:CG	1:B:2189:HIS:CD2	3.00	0.44
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.82	0.44
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.32	0.44
1:A:1744:HIS:O	1:A:1782:HIS:HB3	2.18	0.44
1:A:2004:THR:HA	1:A:2007:GLN:HB2	1.99	0.44
1:A:2167:GLN:CG	1:A:2189:HIS:CD2	3.00	0.44
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.52	0.44
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2268:MET:HG2	1:B:2286:VAL:HG12	2.00	0.44
1:B:2329:MET:HE3	1:B:2400:CYS:SG	2.58	0.44
1:B:2366:MET:HG2	1:B:2373:GLU:O	2.17	0.44
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.17	0.44
2:C:72:SER:O	2:C:74:ASN:N	2.51	0.44
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.61	0.44
1:B:1734:THR:C	1:B:1736:ASP:N	2.76	0.44
2:D:270:ARG:HD2	2:D:270:ARG:HA	1.85	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.48	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.82	0.44
1:A:1603:ILE:C	1:A:1605:TYR:H	2.26	0.44
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.42	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:B:2281:MET:HE1	2:D:222:TYR:CG	2.53	0.43
2:D:16:ALA:HB3	2:D:319:ALA:HB3	2.00	0.43
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	1.99	0.43
1:B:1701:MET:HE2	1:B:1717:MET:HE2	1.99	0.43
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.18	0.43
1:B:1440:PHE:C	1:B:1442:GLU:H	2.26	0.43
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.43
1:B:2123:LEU:HB2	1:B:2158:PRO:O	2.18	0.43
1:A:1440:PHE:C	1:A:1442:GLU:H	2.26	0.43
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.17	0.43
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	2.00	0.43
1:A:2329:MET:HE3	1:A:2400:CYS:SG	2.58	0.43
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.18	0.43
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	2.01	0.43
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.52	0.43
1:A:1899:ASN:ND2	1:A:1937:GLN:HE22	2.17	0.43
2:C:109:ALA:HB3	2:C:125:PHE:HB3	2.01	0.43
2:D:100:MET:HB3	2:D:112:TRP:HB2	2.01	0.43
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.53	0.43
1:A:1992:ASN:HA	1:A:1995:LEU:HD12	2.00	0.43
1:A:2544:GLY:C	1:A:2546:CYS:H	2.26	0.43
1:B:1785:SER:O	1:B:1786:TRP:CB	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ASN:H	2:D:75:PRO:HD3	1.83	0.43
2:C:56:MET:HB2	2:C:68:TYR:O	2.18	0.43
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.87	0.43
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.88	0.43
1:B:2544:GLY:C	1:B:2546:CYS:H	2.26	0.43
2:D:20:TYR:HD2	2:D:44:GLN:HB3	1.83	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:1477:MET:HE1	1:A:1512:MET:HE1	2.00	0.43
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.54	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
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.39	0.43
1:A:2297:ASP:O	1:A:2299:LEU:N	2.51	0.43
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	2.00	0.43
1:B:2322:ARG:O	1:B:2326:VAL:HG23	2.19	0.43
1:A:1505:ASN:O	1:A:1509:GLN:HB2	2.19	0.43
1:A:2009:ALA:HA	1:A:2138:LEU:HD11	2.01	0.43
1:B:1505:ASN:O	1:B:1509:GLN:HB2	2.19	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:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.83	0.42
1:B:1717:MET:HG3	1:B:1754:LEU:HG	2.00	0.42
1:A:1939:ILE:N	1:A:1940:PRO:HD2	2.35	0.42
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.49	0.42
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	2.02	0.42
1:B:2321:THR:HG23	1:B:2387:MET:HG2	2.01	0.42
2:D:28:GLN:HE21	2:D:31:SER:HG	1.66	0.42
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.53	0.42
1:A:1418:SER:HB2	1:A:1581:GLU:CG	2.39	0.42
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.72	0.42
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.42
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.49	0.42
1:B:1980:SER:C	1:B:1988:HIS:HB2	2.44	0.42
2:D:96:ASP:O	2:D:98:ARG:N	2.52	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
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	2.02	0.42
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.48	0.42
2:D:85:ASN:H	2:D:85:ASN:HD22	1.66	0.42
2:D:231:ASP:HB3	2:D:233:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.72	0.42
1:A:2362:PHE:O	1:A:2364:VAL:N	2.52	0.42
2:C:63:GLN:HE21	2:C:86:LYS:H	1.66	0.42
2:C:74:ASN:H	2:C:75:PRO:CD	2.32	0.42
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.89	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:A:1532:TYR:O	1:A:1536:ILE:HG13	2.20	0.42
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.20	0.42
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.55	0.42
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	2.01	0.42
1:B:1629:ILE:O	1:B:1630:VAL:C	2.63	0.42
1:B:1722:GLN:HA	1:B:1725:GLN:NE2	2.35	0.42
1:B:1899:ASN:ND2	1:B:1937:GLN:HE22	2.18	0.42
2:D:74:ASN:H	2:D:75:PRO:CD	2.33	0.42
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.01	0.42
1:A:2329:MET:SD	1:A:2404:MET:HE2	2.60	0.42
1:B:1477:MET:HE2	1:B:1477:MET:HB3	1.89	0.41
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:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.49	0.41
1:B:2223:GLN:HE22	1:B:2352:LYS:CB	2.28	0.41
2:D:167:PRO:C	2:D:169:PRO:HD2	2.45	0.41
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.21	0.41
1:A:2360:ASP:OD1	1:A:2360:ASP:N	2.54	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:2319:ASN:ND2	1:A:2352:LYS:HE3	2.35	0.41
1:B:1410:PRO:HA	1:B:1413:LEU:HB2	2.02	0.41
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.41
2:D:248:ARG:H	2:D:248:ARG:HG2	1.67	0.41
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.41
1:A:1524:GLY:O	1:A:1525:GLN:C	2.64	0.41
1:A:1621:GLU:C	1:A:1623:LEU:H	2.28	0.41
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.85	0.41
2:C:262:SER:OG	2:C:267:GLU:HG2	2.20	0.41
1:B:1524:GLY:O	1:B:1525:GLN:C	2.64	0.41
1:B:1938:VAL:HG13	1:B:1938:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2362:PHE:O	1:B:2364:VAL:N	2.53	0.41
1:B:2363:GLU:O	1:B:2364:VAL:C	2.63	0.41
2:D:31:SER:HG	2:D:33:ILE:HG13	1.86	0.41
1:A:2154:GLN:HE21	1:A:2155:SER:HB2	1.85	0.41
2:C:75:PRO:HB2	2:C:76:ASN:H	1.62	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:A:1477:MET:HE2	1:A:1477:MET:HB3	1.89	0.41
1:A:2363:GLU:O	1:A:2365:ALA:N	2.53	0.41
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.56	0.41
1:B:1892:ILE:CG2	1:B:1930:ILE:HD11	2.42	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.03	0.41
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.89	0.41
1:A:2093:ASN:HD22	1:A:2094:VAL:N	2.13	0.41
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.85	0.41
2:D:262:SER:OG	2:D:267:GLU:HG2	2.21	0.41
2:D:285:ILE:HG23	2:D:297:TRP:HB2	2.02	0.41
1:A:1796:MET:HA	1:A:1796:MET:CE	2.48	0.41
1:A:1980:SER:C	1:A:1988:HIS:HB2	2.44	0.41
1:A:2285:GLU:HB2	2:C:272:TRP:CZ3	2.56	0.41
1:B:1621:GLU:C	1:B:1623:LEU:H	2.28	0.41
1:B:2178:ASN:ND2	1:B:2180:HIS:H	2.18	0.41
1:A:1427:GLU:H	1:A:1427:GLU:HG2	1.64	0.41
1:A:2423:TYR:CE1	1:A:2501:ILE:HD13	2.56	0.41
2:C:100:MET:HB3	2:C:112:TRP:HB2	2.03	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
1:B:2281:MET:HA	1:B:2281:MET:HE2	2.03	0.41
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.56	0.41
1:A:2363:GLU:O	1:A:2364:VAL:C	2.64	0.41
1:B:1603:ILE:C	1:B:1605:TYR:H	2.29	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
2:C:202:GLY:HA3	2:C:208:THR:H	1.86	0.40
1:B:1777:SER:O	1:B:1781:GLU:HG2	2.22	0.40
1:B:2032:GLU:O	1:B:2036:ARG:HG2	2.19	0.40
1:B:2292:ASN:HB3	2:D:268:SER:HB2	2.02	0.40
1:A:1725:GLN:HB3	1:A:1747:MET:HE1	2.02	0.40
1:A:2252:ASP:O	1:A:2255:GLU:HG2	2.21	0.40
1:A:2408:ARG:O	1:A:2411:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1970:GLN:C	1:B:1972:LEU:H	2.28	0.40
1:B:2093:ASN:HD22	1:B:2094:VAL:N	2.14	0.40
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.51	0.40
1:A:2095:LYS:HA	1:A:2098:THR:HG22	2.03	0.40
1:A:2152:ARG:HG2	1:A:2177:SER:HB3	2.03	0.40
1:A:2378:ARG:HE	1:A:2378:ARG:HB2	1.67	0.40
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.49	0.40
1:B:1688:PRO:HB3	1:A:2270:ARG:NH2	2.37	0.40
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.21	0.40
2:C:131:ILE:HA	2:C:147:ASP:HA	2.03	0.40
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.46	0.40
1:B:2546:CYS:C	1:B:2548:PHE:H	2.30	0.40
2:D:202:GLY:HA3	2:D:208:THR:H	1.86	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	Interatomic distance (Å)	Clash overlap (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 [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	1052/1174 (90%)	939 (89%)	84 (8%)	29 (3%)	<b>4</b> 26
1	B	1052/1174 (90%)	938 (89%)	85 (8%)	29 (3%)	<b>4</b> 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	315/326 (97%)	265 (84%)	32 (10%)	18 (6%)	1	13
2	D	315/326 (97%)	264 (84%)	33 (10%)	18 (6%)	1	13
All	All	2734/3000 (91%)	2406 (88%)	234 (9%)	94 (3%)	3	23

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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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 [i](#)

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%)	848 (91%)	83 (9%)	9	32
1	B	931/1024 (91%)	851 (91%)	80 (9%)	10	33
2	C	269/276 (98%)	235 (87%)	34 (13%)	4	21
2	D	269/276 (98%)	235 (87%)	34 (13%)	4	21
All	All	2400/2600 (92%)	2169 (90%)	231 (10%)	8	30

All (231) 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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1457	GLU
1	B	1471	LYS
1	B	1509	GLN
1	B	1540	THR
1	B	1541	HIS
1	B	1590	MET
1	B	1598	GLU
1	B	1611	ARG
1	B	1630	VAL
1	B	1685	LEU
1	B	1724	MET
1	B	1736	ASP
1	B	1740	LYS
1	B	1746	LEU
1	B	1752	LEU
1	B	1780	THR
1	B	1870	THR
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	1985	THR
1	B	1997	ASN
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2080	GLU
1	B	2093	ASN
1	B	2095	LYS
1	B	2124	GLN
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	2164	THR
1	B	2167	GLN
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2185	LEU
1	B	2189	HIS
1	B	2214	THR
1	B	2228	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2262	ASN
1	B	2263	ILE
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	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2401	HIS
1	B	2408	ARG
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2501	ILE
1	B	2503	ARG
1	B	2515	HIS
1	B	2519	LEU
1	B	2530	LYS
1	B	2543	ILE
2	D	10	SER
2	D	13	VAL
2	D	44	GLN
2	D	74	ASN
2	D	79	ILE
2	D	85	ASN
2	D	90	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	91	VAL
2	D	128	ASN
2	D	134	VAL
2	D	135	CYS
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	188	VAL
2	D	196	VAL
2	D	211	ILE
2	D	215	LYS
2	D	239	SER
2	D	243	THR
2	D	248	ARG
2	D	259	SER
2	D	260	ILE
2	D	286	VAL
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	1471	LYS
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1590	MET
1	A	1603	ILE
1	A	1611	ARG
1	A	1630	VAL
1	A	1685	LEU
1	A	1724	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1736	ASP
1	A	1740	LYS
1	A	1746	LEU
1	A	1752	LEU
1	A	1780	THR
1	A	1896	ARG
1	A	1899	ASN
1	A	1912	ASP
1	A	1916	TRP
1	A	1918	ASP
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	1997	ASN
1	A	2005	LEU
1	A	2011	MET
1	A	2021	ILE
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2080	GLU
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	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2185	LEU
1	A	2189	HIS
1	A	2214	THR
1	A	2223	GLN
1	A	2228	ILE
1	A	2232	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2262	ASN
1	A	2263	ILE
1	A	2266	ARG
1	A	2281	MET
1	A	2297	ASP
1	A	2311	GLU
1	A	2360	ASP
1	A	2363	GLU
1	A	2378	ARG
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2401	HIS
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2501	ILE
1	A	2503	ARG
1	A	2515	HIS
1	A	2519	LEU
1	A	2530	LYS
1	A	2543	ILE
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	134	VAL
2	C	135	CYS
2	C	161	HIS
2	C	162	ASN
2	C	165	LEU
2	C	166	ILE
2	C	168	GLU

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Mol	Chain	Res	Type
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	183	SER
2	C	188	VAL
2	C	196	VAL
2	C	211	ILE
2	C	215	LYS
2	C	239	SER
2	C	243	THR
2	C	248	ARG
2	C	260	ILE
2	C	286	VAL
2	C	287	THR
2	C	289	SER
2	C	301	THR
2	C	304	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1398	HIS
1	B	1496	GLN
1	B	1594	HIS
1	B	1624	GLN
1	B	1670	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1727	GLN
1	B	1730	HIS
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	1992	ASN
1	B	2001	HIS
1	B	2043	ASN
1	B	2082	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	2093	ASN
1	B	2154	GLN
1	B	2178	ASN
1	B	2189	HIS
1	B	2223	GLN
1	B	2247	HIS
1	B	2262	ASN
1	B	2277	HIS
1	B	2319	ASN
1	B	2395	ASN
1	B	2410	HIS
1	B	2428	ASN
1	B	2502	ASN
2	D	28	GLN
2	D	30	HIS
2	D	44	GLN
2	D	85	ASN
2	D	118	ASN
2	D	128	ASN
2	D	137	HIS
2	D	139	ASN
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	311	HIS
2	D	312	GLN
2	D	321	ASN
1	A	1398	HIS
1	A	1496	GLN
1	A	1594	HIS
1	A	1624	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	GLN
1	A	1727	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1803	HIS
1	A	1898	ASN
1	A	1899	ASN
1	A	1941	GLN
1	A	1958	HIS

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Mol	Chain	Res	Type
1	A	1970	GLN
1	A	1992	ASN
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	2247	HIS
1	A	2277	HIS
1	A	2319	ASN
1	A	2340	HIS
1	A	2395	ASN
1	A	2410	HIS
1	A	2428	ASN
1	A	2502	ASN
1	A	2531	GLN
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	128	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 [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](#)

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	B	2601	4,5	28,29,29	1.67	5 (17%)	43,45,45	1.84	8 (18%)
3	ADP	A	2601	4,5	28,29,29	1.65	5 (17%)	43,45,45	1.87	10 (23%)
5	MGF	B	2604	3	0,3,3	-	-	-	-	-
5	MGF	A	2604	3	0,3,3	-	-	-	-	-

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	B	2601	4,5	-	2/16/32/32	0/3/3/3
3	ADP	A	2601	4,5	-	8/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	ADP	C5-C4	5.20	1.48	1.39
3	B	2601	ADP	C5-C4	4.91	1.47	1.39
3	B	2601	ADP	PA-O3A	4.54	1.64	1.59
3	A	2601	ADP	PA-O3A	4.08	1.63	1.59
3	A	2601	ADP	C5-C6	2.87	1.49	1.41
3	B	2601	ADP	C5-C6	2.70	1.48	1.41
3	A	2601	ADP	C8-N7	2.54	1.36	1.31
3	B	2601	ADP	C8-N7	2.39	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	ADP	C5-N7	-2.29	1.34	1.39
3	A	2601	ADP	C5-N7	-2.09	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	ADP	C5-C4-N3	-6.34	117.99	126.72
3	B	2601	ADP	C5-C4-N3	-6.06	118.37	126.72
3	A	2601	ADP	N3-C4-N9	5.15	135.92	127.17
3	B	2601	ADP	N3-C4-N9	4.91	135.51	127.17
3	A	2601	ADP	C2-N3-C4	4.13	121.92	111.83
3	B	2601	ADP	C2-N3-C4	3.79	121.08	111.83
3	A	2601	ADP	N3-C2-N1	-3.69	122.99	128.58
3	B	2601	ADP	N3-C2-N1	-3.30	123.59	128.58
3	B	2601	ADP	C4-C5-N7	-3.18	106.95	110.58
3	A	2601	ADP	C4-C5-N7	-3.03	107.11	110.58
3	B	2601	ADP	C5-N7-C8	2.49	107.37	103.45
3	B	2601	ADP	O4'-C1'-N9	2.37	112.64	108.09
3	A	2601	ADP	C5-N7-C8	2.30	107.06	103.45
3	A	2601	ADP	O4'-C1'-N9	2.27	112.45	108.09
3	B	2601	ADP	C4-N9-C8	2.26	108.11	105.74
3	A	2601	ADP	O3B-PB-O2B	2.07	115.57	107.80
3	A	2601	ADP	C4-N9-C8	2.03	107.87	105.74
3	A	2601	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

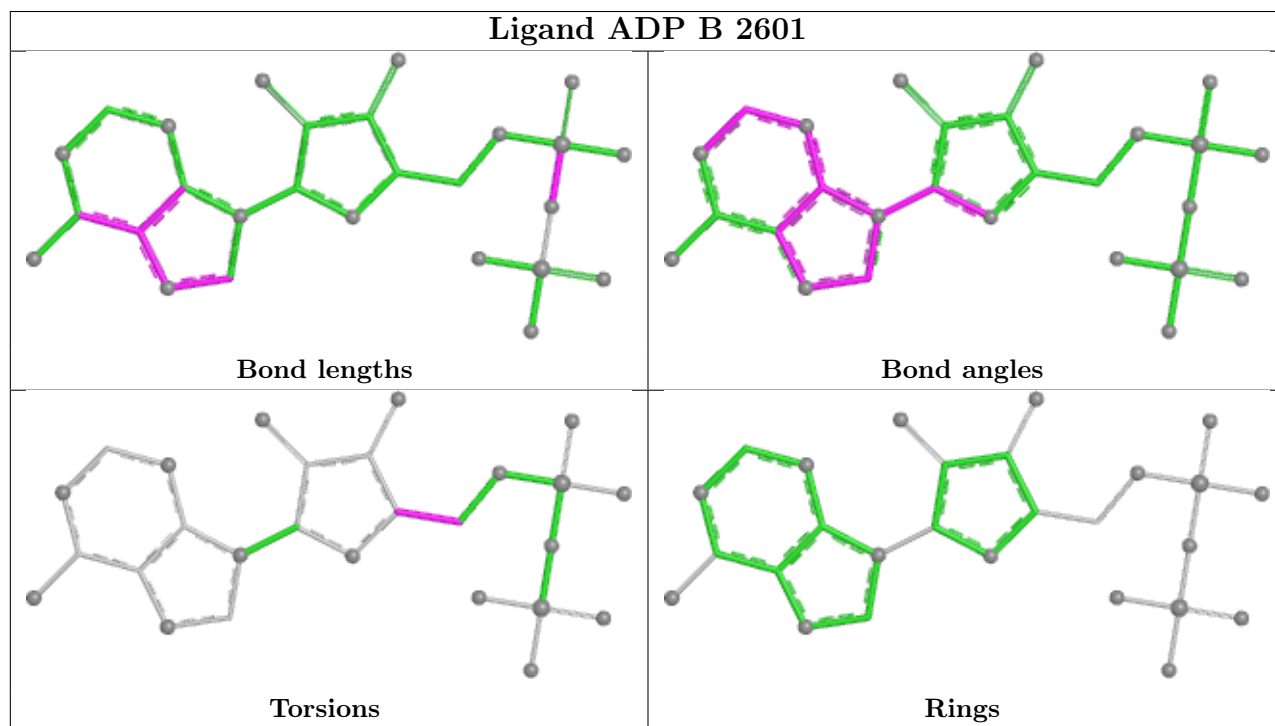
Mol	Chain	Res	Type	Atoms
3	A	2601	ADP	C5'-O5'-PA-O1A
3	A	2601	ADP	C5'-O5'-PA-O3A
3	A	2601	ADP	O4'-C4'-C5'-O5'
3	B	2601	ADP	O4'-C4'-C5'-O5'
3	A	2601	ADP	C4'-C5'-O5'-PA
3	A	2601	ADP	PB-O3A-PA-O1A
3	A	2601	ADP	C3'-C4'-C5'-O5'
3	A	2601	ADP	C5'-O5'-PA-O2A
3	A	2601	ADP	PB-O3A-PA-O2A
3	B	2601	ADP	C3'-C4'-C5'-O5'

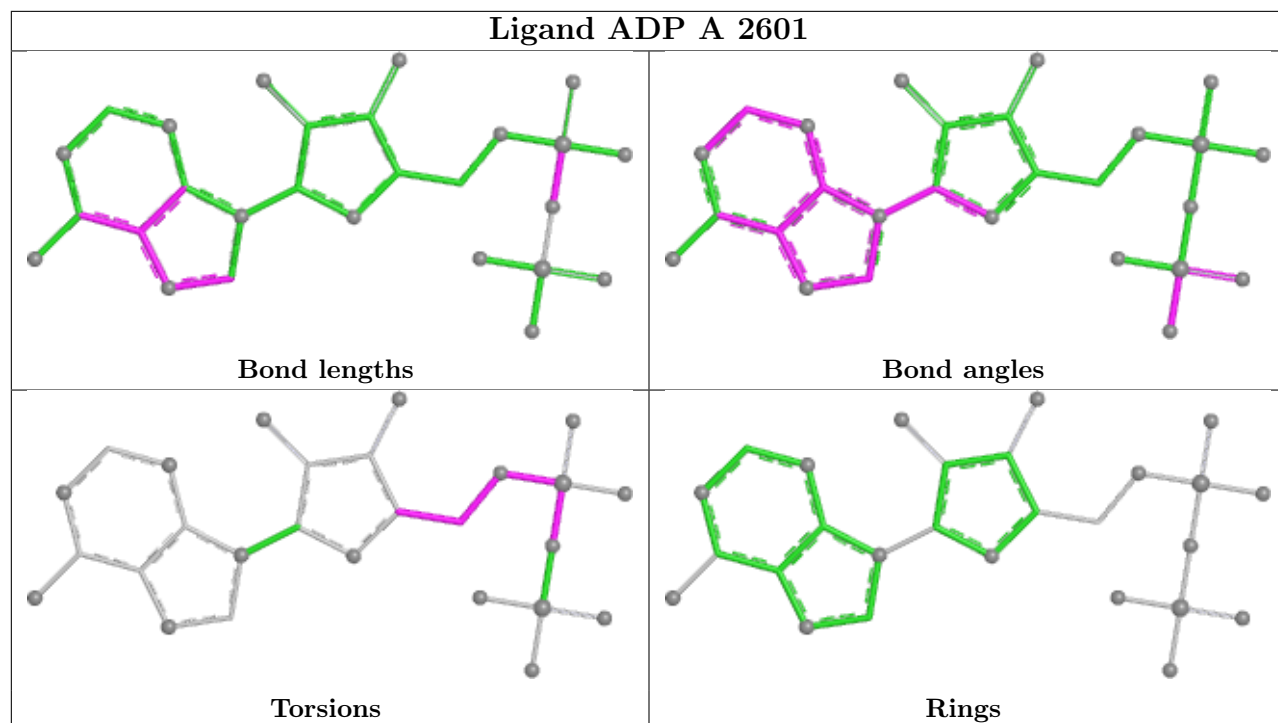
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1058/1174 (90%)	0.13	14 (1%) 75 50	37, 70, 159, 271	0
1	B	1058/1174 (90%)	-0.00	13 (1%) 76 52	29, 59, 136, 174	0
2	C	317/326 (97%)	-0.03	4 (1%) 75 50	39, 68, 116, 153	0
2	D	317/326 (97%)	-0.17	3 (0%) 81 58	30, 46, 92, 130	0
All	All	2750/3000 (91%)	0.03	34 (1%) 76 52	29, 62, 144, 271	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1504	VAL	3.7
2	C	203	ILE	3.3
2	D	203	ILE	3.3
1	B	2492	ALA	3.2
2	D	207	VAL	3.1
2	C	207	VAL	3.1
1	A	1504	VAL	3.0
1	A	1730	HIS	3.0
1	A	1614	ILE	3.0
1	B	1469	THR	2.8
1	B	1607	LEU	2.7
1	A	1457	GLU	2.7
1	B	2436	THR	2.7
1	B	1580	GLY	2.5
1	A	1619	TRP	2.4
2	C	75	PRO	2.4
1	A	2492	ALA	2.4
1	A	1443	LEU	2.4
2	C	324	VAL	2.3
1	A	1629	ILE	2.3
1	A	1444	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1608	VAL	2.3
1	A	1610	GLU	2.2
1	A	2118	LEU	2.2
1	A	1469	THR	2.2
1	B	1731	ALA	2.1
1	A	1623	LEU	2.1
2	D	324	VAL	2.1
1	B	2430	ARG	2.1
1	B	1680	ASP	2.1
1	B	2045	LYS	2.1
1	B	2429	TRP	2.1
1	B	2434	THR	2.1
1	A	1586	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 oligosaccharides in this entry.

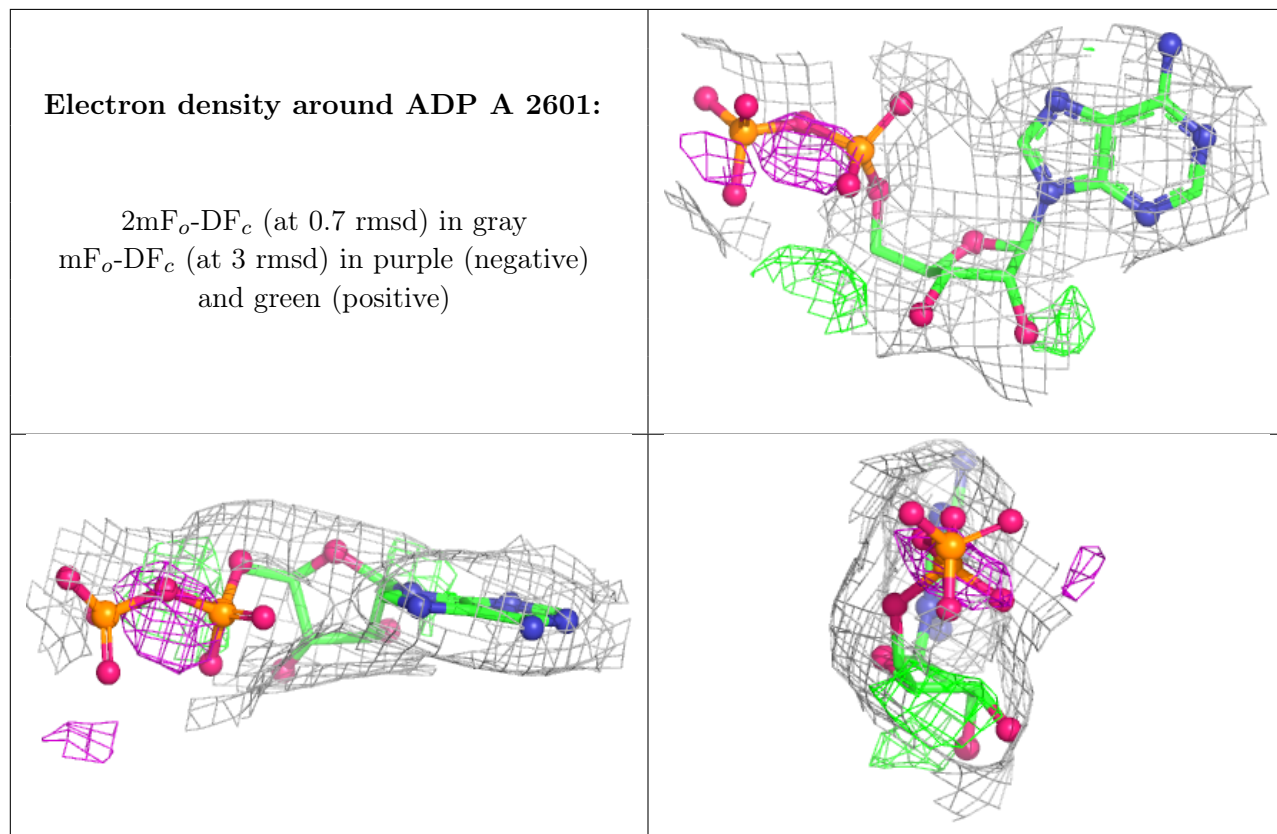
## 6.4 Ligands [i](#)

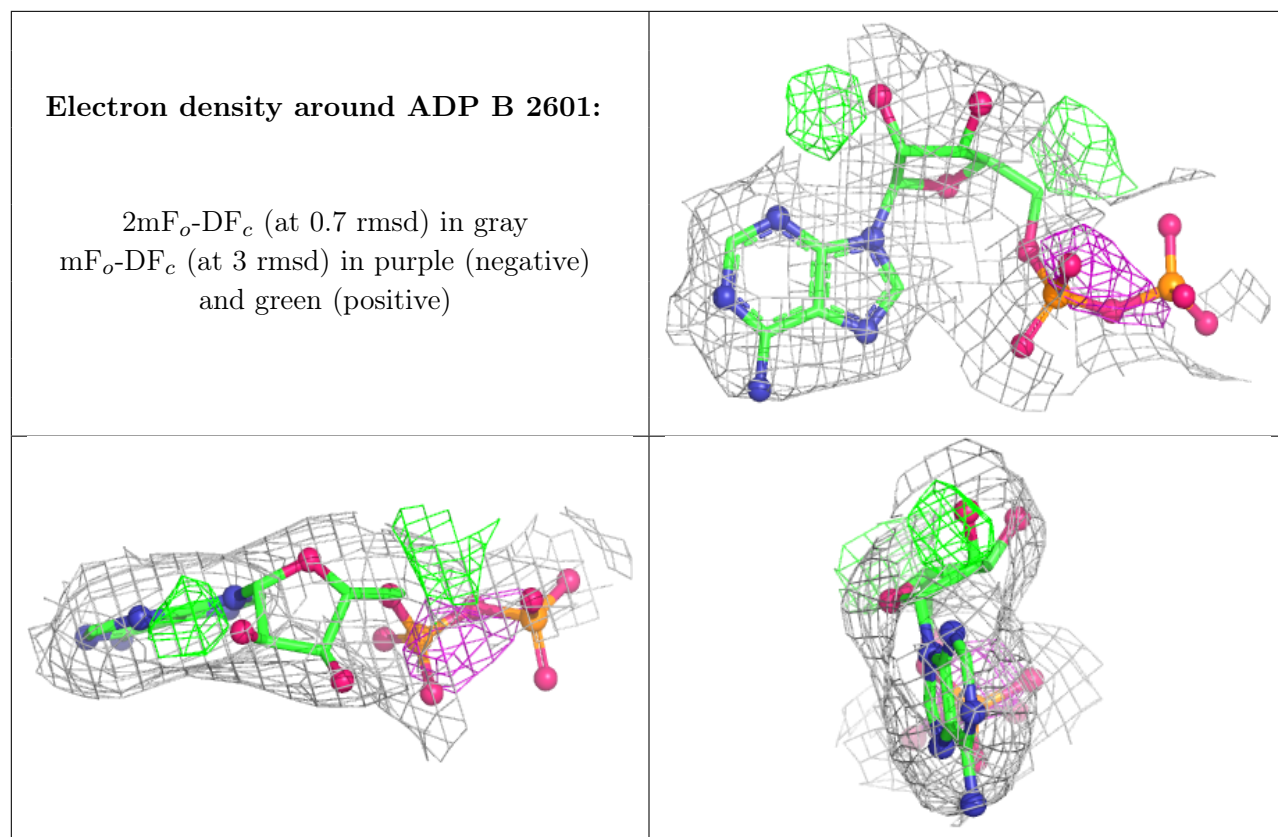
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MGF	B	2604	4/4	0.80	0.13	57,59,59,60	0
4	MG	A	2603	1/1	0.83	0.09	72,72,72,72	0
5	MGF	A	2604	4/4	0.84	0.14	75,76,78,79	0
3	ADP	A	2601	27/27	0.86	0.12	64,69,81,82	0
3	ADP	B	2601	27/27	0.89	0.11	50,54,62,62	0
4	MG	B	2603	1/1	0.92	0.08	57,57,57,57	0
4	MG	A	2602	1/1	0.93	0.14	74,74,74,74	0
4	MG	B	2602	1/1	0.97	0.09	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.