



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 PM GMT

PDB ID : 4R7Y  
Title : Crystal structure of an active MCM hexamer  
Authors : Miller, J.M.; Arachea, B.T.; Epling, L.B.; Enemark, E.J.  
Deposited on : 2014-08-28  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

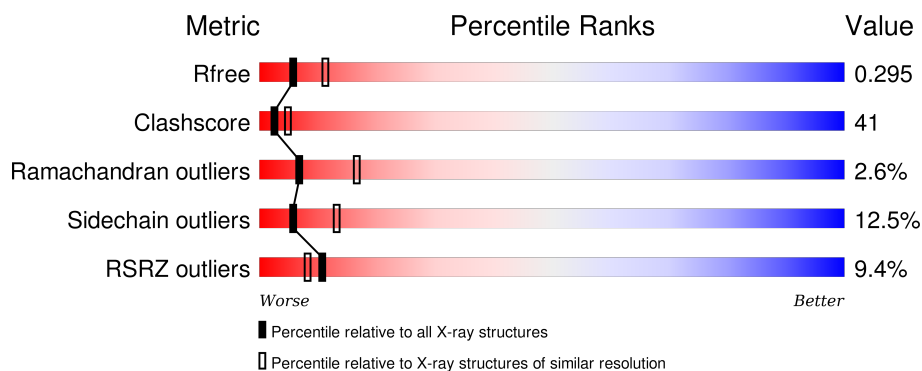
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	613	<div> <div>10%</div> <div> <div>44%</div> <div>43%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	613	<div> <div>8%</div> <div> <div>44%</div> <div>44%</div> <div>8%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	2006	-	-	X	-
5	CL	B	2006	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9494 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.

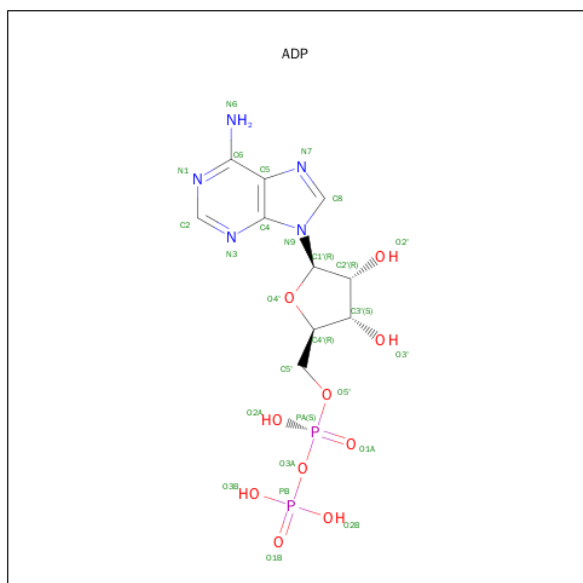
- Molecule 1 is a protein called Minichromosome maintenance protein MCM, Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			
1	B	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q9UXG1
A	1	LEU	-	EXPRESSION TAG	UNP Q9UXG1
B	0	SER	-	EXPRESSION TAG	UNP Q9UXG1
B	1	LEU	-	EXPRESSION TAG	UNP Q9UXG1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

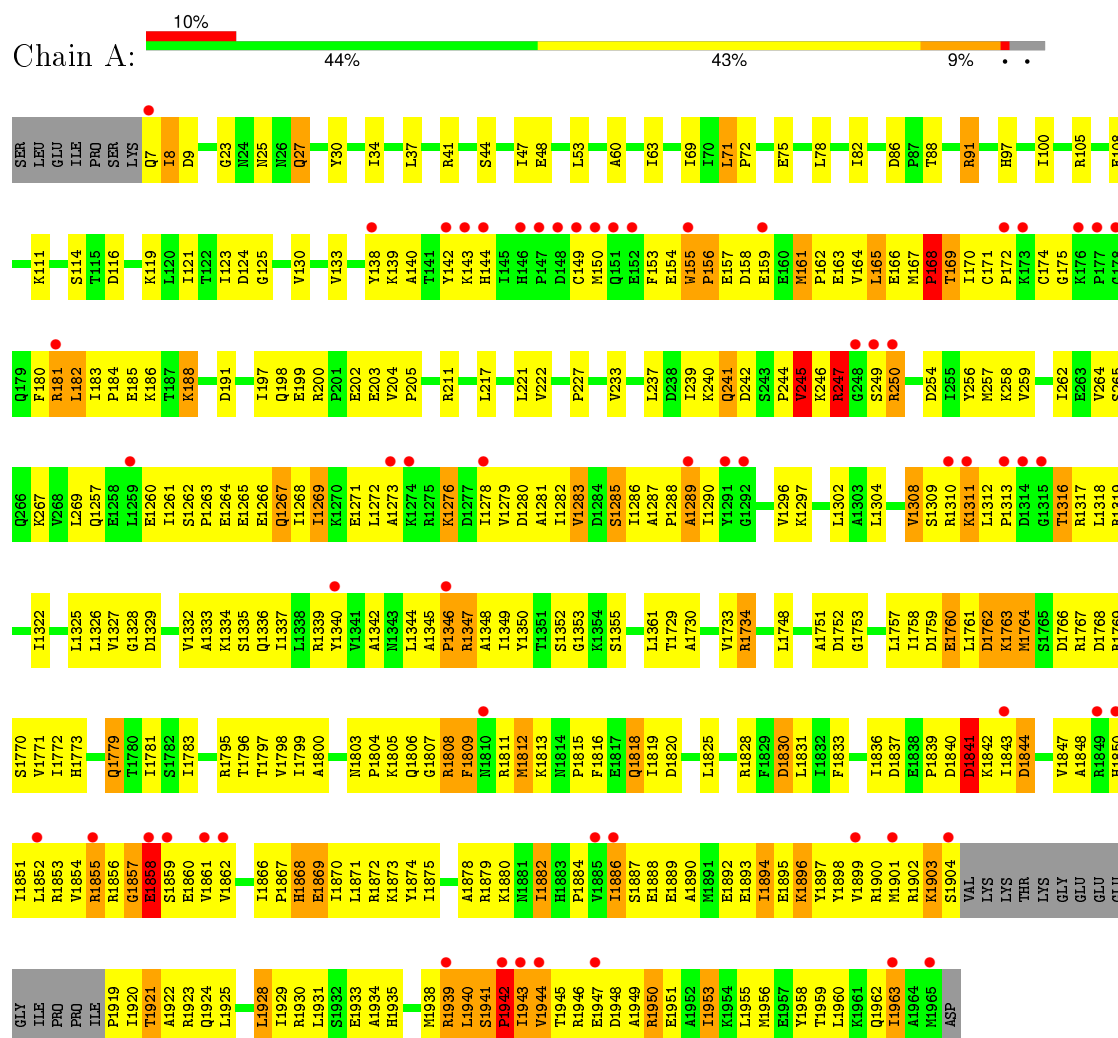
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

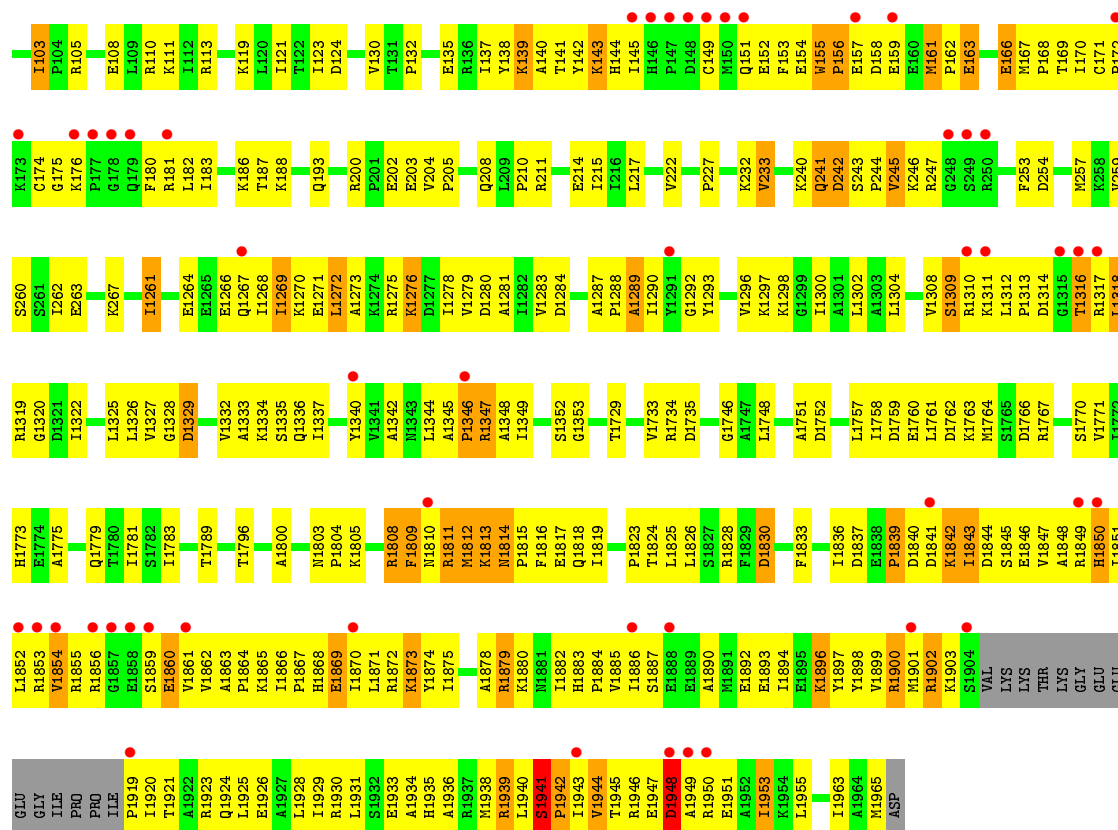
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Cl	0	0
			3	3		
5	A	3	Total	Cl	0	0
			3	3		

### 3 Residue-property plots

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

- Molecule 1: Minichromosome maintenance protein MCM, Cell division control protein 21





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.90Å 118.90Å 199.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.83 – 2.70 49.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.7 (49.83-2.70) 89.7 (49.83-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.263 , 0.295 0.263 , 0.295	Depositor DCC
$R_{free}$ test set	1976 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 39044 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	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 49.42 % 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 7.4816e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.45	0/4793	0.69	0/6476
1	B	0.45	0/4793	0.70	0/6476
All	All	0.45	0/9586	0.70	0/12952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4715	0	4876	420	0
1	B	4715	0	4876	393	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	2	0
5	B	3	0	0	2	0
All	All	9494	0	9776	798	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1346:PRO:HB3	1:B:1872:ARG:HD3	1.29	1.10
1:A:156:PRO:HB2	1:A:159:GLU:O	1.53	1.07
1:B:1261:ILE:HA	1:B:1873:LYS:HZ1	1.17	1.05
1:A:1878:ALA:HA	1:A:1882:ILE:HD11	1.37	1.05
1:B:1261:ILE:HA	1:B:1873:LYS:NZ	1.73	1.04
1:A:1902:ARG:HB3	1:A:1903:LYS:HZ3	1.22	1.02
1:A:105:ARG:NH1	5:A:2006:CL:CL	2.32	1.00
1:A:1260:GLU:O	1:A:1873:LYS:HE2	1.62	0.99
1:A:1345:ALA:HB1	1:A:1348:ALA:HB3	1.44	0.97
1:B:105:ARG:NH1	5:B:2006:CL:CL	2.35	0.96
1:B:1949:ALA:O	1:B:1953:ILE:HG22	1.65	0.96
1:A:1809:PHE:HD1	1:A:1809:PHE:H	1.10	0.96
1:B:1311:LYS:HE2	1:B:1317:ARG:HH11	1.31	0.95
1:B:1809:PHE:HD1	1:B:1809:PHE:H	1.10	0.95
1:B:1894:ILE:HG13	1:B:1928:LEU:HD23	1.49	0.95
1:A:1920:ILE:HG23	1:A:1924:GLN:HG3	1.47	0.94
1:A:1882:ILE:HD13	1:A:1882:ILE:N	1.82	0.92
1:B:156:PRO:HB2	1:B:159:GLU:O	1.67	0.92
1:A:170:ILE:HG23	1:A:175:GLY:O	1.70	0.92
1:B:103:ILE:H	1:B:103:ILE:HD13	1.36	0.90
1:A:162:PRO:HG2	1:A:164:VAL:O	1.70	0.90
1:B:1290:ILE:HD11	1:B:1297:LYS:HE2	1.51	0.90
1:B:1261:ILE:H	1:B:1261:ILE:HD13	1.35	0.90
1:A:1889:GLU:HB3	1:A:1946:ARG:CG	2.02	0.89
1:B:214:GLU:OE2	1:B:240:LYS:HE2	1.74	0.88
1:A:143:LYS:HB2	1:A:183:ILE:HD11	1.52	0.88
1:B:1886:ILE:H	1:B:1886:ILE:HD12	1.39	0.88
1:B:1317:ARG:NH2	1:B:1779:GLN:HG3	1.88	0.87
1:A:1889:GLU:HB3	1:A:1946:ARG:HG2	1.56	0.86
1:A:161:MET:HE1	1:A:165:LEU:HD13	1.58	0.86
1:B:1863:ALA:HB1	1:B:1864:PRO:HD2	1.58	0.85
1:B:25:ASN:H	1:B:27:GLN:NE2	1.76	0.84
1:B:1317:ARG:HH21	1:B:1779:GLN:HG3	1.42	0.84
1:B:143:LYS:HG3	1:B:152:GLU:HG2	1.60	0.84
1:A:144:HIS:HB3	1:A:149:CYS:SG	2.17	0.83
1:B:1329:ASP:O	1:B:1332:VAL:HG22	1.78	0.83
1:A:1312:LEU:HB3	1:A:1313:PRO:HD2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:ASP:OD1	1:B:1808:ARG:HA	1.78	0.82
1:B:1269:ILE:HD11	1:B:1874:TYR:HA	1.62	0.82
1:A:1893:GLU:OE1	1:A:1950:ARG:HD2	1.79	0.82
1:B:1752:ASP:HA	1:B:1796:THR:HG22	1.61	0.82
1:B:1276:LYS:HE2	1:B:1276:LYS:HA	1.62	0.82
1:B:156:PRO:HG3	1:B:161:MET:HG2	1.62	0.82
1:A:1960:LEU:O	1:A:1963:ILE:HG13	1.81	0.81
1:A:41:ARG:NH2	1:A:88:THR:HG22	1.96	0.81
1:B:1281:ALA:HB1	1:B:1866:ILE:HD11	1.62	0.80
1:A:1882:ILE:HD13	1:A:1882:ILE:H	1.40	0.80
1:A:1901:MET:SD	1:A:1920:ILE:HG21	2.21	0.80
1:B:1310:ARG:O	1:B:1318:LEU:HB2	1.81	0.79
1:A:25:ASN:H	1:A:27:GLN:HE21	1.28	0.79
1:B:1317:ARG:HH22	1:B:1779:GLN:HE21	1.30	0.79
1:B:1823:PRO:HA	1:B:1826:LEU:HD12	1.65	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:CG	2.13	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:HG3	1.65	0.79
1:B:1946:ARG:HD3	1:B:1950:ARG:HH12	1.46	0.79
1:B:25:ASN:H	1:B:27:GLN:HE21	1.30	0.79
1:A:1265:GLU:O	1:A:1269:ILE:HG22	1.82	0.78
1:A:249:SER:O	1:A:250:ARG:HG3	1.83	0.78
1:B:86:ASP:OD1	1:B:88:THR:HB	1.82	0.78
1:B:1311:LYS:NZ	1:B:1317:ARG:HB2	1.99	0.78
1:A:1276:LYS:HE2	1:A:1276:LYS:HA	1.65	0.78
1:A:1901:MET:SD	1:A:1920:ILE:HG13	2.24	0.77
1:B:41:ARG:NH2	1:B:88:THR:HG22	1.99	0.77
1:B:1345:ALA:HB1	1:B:1348:ALA:HB3	1.64	0.77
1:B:1810:ASN:HD21	1:B:1836:ILE:CG2	1.97	0.77
1:B:1946:ARG:HD3	1:B:1950:ARG:NH1	1.99	0.77
1:A:1878:ALA:O	1:A:1882:ILE:HG12	1.83	0.77
1:B:1311:LYS:HZ3	1:B:1317:ARG:HB2	1.48	0.77
1:A:1779:GLN:CG	1:A:1795:ARG:HA	2.15	0.77
1:A:1902:ARG:HB3	1:A:1903:LYS:NZ	1.99	0.77
1:A:1752:ASP:HA	1:A:1796:THR:HG22	1.66	0.76
1:B:1850:HIS:O	1:B:1854:VAL:HG23	1.85	0.76
1:B:1336:GLN:HG3	1:B:1340:TYR:HE1	1.51	0.76
1:A:1729:THR:HB	1:A:1781:ILE:HD13	1.66	0.76
1:A:1264:GLU:O	1:A:1268:ILE:HG13	1.86	0.75
1:B:1332:VAL:HG23	1:B:1334:LYS:HD2	1.69	0.75
1:A:1899:VAL:O	1:A:1903:LYS:HE2	1.86	0.75
1:A:1828:ARG:HE	1:A:1923:ARG:NH2	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:ALA:HB3	1:A:1340:TYR:CE2	2.21	0.75
1:B:1327:VAL:HG13	1:B:1819:ILE:HG21	1.67	0.75
1:A:1345:ALA:CB	1:A:1348:ALA:HB3	2.17	0.75
1:B:1332:VAL:CG2	1:B:1334:LYS:HD2	2.17	0.74
1:A:1280:ASP:O	1:A:1283:VAL:HG13	1.88	0.74
1:B:1336:GLN:HG3	1:B:1340:TYR:CE1	2.23	0.73
1:B:1874:TYR:OH	1:B:1940:LEU:HD11	1.88	0.73
1:A:1278:ILE:HG23	1:A:1279:VAL:H	1.53	0.73
1:B:143:LYS:HB2	1:B:183:ILE:HD11	1.69	0.73
1:A:1839:PRO:HB3	1:B:1902:ARG:HH11	1.53	0.73
1:A:161:MET:HE1	1:A:165:LEU:HA	1.71	0.72
1:A:1278:ILE:HG23	1:A:1279:VAL:N	2.04	0.72
1:A:1332:VAL:HG12	1:A:1332:VAL:O	1.88	0.72
1:A:1878:ALA:HA	1:A:1882:ILE:CD1	2.18	0.72
1:A:1878:ALA:CA	1:A:1882:ILE:HD11	2.19	0.72
1:A:1828:ARG:NE	1:A:1923:ARG:HH22	1.87	0.72
1:A:1289:ALA:HB3	1:A:1340:TYR:HE2	1.56	0.71
1:A:1815:PRO:HG2	1:A:1963:ILE:HG22	1.72	0.71
1:A:1809:PHE:HB2	1:A:1818:GLN:OE1	1.90	0.71
1:B:1901:MET:SD	1:B:1920:ILE:HG13	2.30	0.71
1:A:1261:ILE:HA	1:A:1873:LYS:NZ	2.05	0.71
1:A:211:ARG:NH1	1:B:132:PRO:HA	2.07	0.70
1:B:1919:PRO:HG2	1:B:1920:ILE:H	1.57	0.70
1:B:1809:PHE:HD1	1:B:1809:PHE:N	1.88	0.70
1:B:1843:ILE:HA	1:B:1846:GLU:HG3	1.74	0.70
1:A:1348:ALA:C	1:A:1349:ILE:HD12	2.11	0.70
1:A:156:PRO:HG3	1:A:161:MET:HG2	1.73	0.70
1:A:1869:GLU:HA	1:A:1872:ARG:HH11	1.57	0.70
1:B:1312:LEU:O	1:B:1316:THR:HA	1.92	0.69
1:B:1809:PHE:CD1	1:B:1809:PHE:N	2.60	0.69
1:B:1810:ASN:HD21	1:B:1836:ILE:HG23	1.57	0.69
1:B:1944:VAL:HG12	1:B:1948:ASP:CB	2.22	0.69
1:A:171:CYS:HB3	1:A:174:CYS:SG	2.33	0.69
1:A:1779:GLN:HG3	1:A:1795:ARG:HA	1.74	0.69
1:A:1960:LEU:HA	1:A:1963:ILE:HD11	1.74	0.69
1:B:140:ALA:HA	1:B:187:THR:HG23	1.73	0.69
1:B:144:HIS:HB3	1:B:149:CYS:SG	2.33	0.69
1:B:1333:ALA:O	1:B:1337:ILE:HG13	1.93	0.69
1:A:1871:LEU:O	1:A:1874:TYR:HB3	1.92	0.69
1:A:1867:PRO:HG2	1:A:1870:ILE:HD12	1.75	0.69
1:A:1886:ILE:HA	1:A:1944:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1884:PRO:HA	1:B:1942:PRO:HB2	1.75	0.69
1:A:1760:GLU:HA	1:A:1760:GLU:OE2	1.92	0.68
1:A:1267:GLN:O	1:A:1271:GLU:HG2	1.92	0.68
1:B:1316:THR:OG1	1:B:1317:ARG:N	2.25	0.68
1:A:1773:HIS:HB3	1:A:1828:ARG:HH12	1.58	0.68
1:A:202:GLU:HG2	1:A:267:LYS:NZ	2.07	0.68
1:A:161:MET:CE	1:A:165:LEU:HA	2.23	0.68
1:B:170:ILE:HG23	1:B:175:GLY:O	1.93	0.68
1:B:1871:LEU:O	1:B:1874:TYR:HB3	1.94	0.68
1:A:1290:ILE:HD11	1:A:1297:LYS:HE2	1.75	0.68
1:B:155:TRP:O	1:B:157:GLU:N	2.27	0.68
1:A:1828:ARG:HE	1:A:1923:ARG:HH22	1.41	0.68
1:B:1893:GLU:HG3	1:B:1946:ARG:HG2	1.76	0.67
1:A:1929:ILE:O	1:A:1933:GLU:HG3	1.94	0.67
1:A:130:VAL:HG23	1:A:227:PRO:HG3	1.76	0.67
1:B:1936:ALA:HB2	1:B:1948:ASP:OD1	1.94	0.67
1:B:25:ASN:N	1:B:27:GLN:HE21	1.93	0.67
1:A:1287:ALA:O	1:A:1290:ILE:HG12	1.95	0.67
1:B:1899:VAL:O	1:B:1903:LYS:HE3	1.95	0.67
1:A:1342:ALA:HA	1:A:1345:ALA:HB2	1.74	0.67
1:A:1308:VAL:HB	1:A:1933:GLU:OE2	1.94	0.67
1:A:1920:ILE:CG2	1:A:1924:GLN:HG3	2.23	0.67
1:B:1312:LEU:O	1:B:1316:THR:CA	2.43	0.67
1:B:141:THR:HG22	1:B:183:ILE:HB	1.76	0.67
1:B:1311:LYS:HE2	1:B:1317:ARG:NH1	2.07	0.67
1:A:1280:ASP:HA	1:A:1283:VAL:CG1	2.25	0.66
1:A:161:MET:CE	1:A:165:LEU:HD13	2.24	0.66
1:A:1839:PRO:HB3	1:B:1902:ARG:NH1	2.10	0.66
1:B:242:ASP:O	1:B:244:PRO:HD3	1.95	0.66
1:A:155:TRP:O	1:A:157:GLU:N	2.29	0.66
1:B:1276:LYS:CE	1:B:1276:LYS:HA	2.25	0.66
1:B:1327:VAL:CG1	1:B:1819:ILE:HG21	2.26	0.66
1:B:1867:PRO:HB2	1:B:1870:ILE:HB	1.76	0.66
1:B:1280:ASP:O	1:B:1283:VAL:HG22	1.95	0.66
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.61	0.66
1:A:1809:PHE:N	1:A:1809:PHE:CD1	2.61	0.66
1:B:1943:ILE:HG22	1:B:1944:VAL:O	1.95	0.65
1:B:1812:MET:SD	1:B:1812:MET:N	2.69	0.65
1:B:1890:ALA:O	1:B:1894:ILE:HG22	1.97	0.65
1:A:165:LEU:HD12	1:A:166:GLU:N	2.12	0.65
1:B:1941:SER:CB	1:B:1943:ILE:H	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:PRO:C	1:B:1290:ILE:H	2.00	0.65
1:A:143:LYS:HE3	1:A:150:MET:HG3	1.80	0.64
1:B:1748:LEU:O	1:B:1796:THR:HG21	1.97	0.64
1:A:1848:ALA:HB2	1:B:1898:TYR:HD2	1.61	0.64
1:B:161:MET:HE1	1:B:166:GLU:H	1.61	0.64
1:A:1958:TYR:O	1:A:1962:GLN:HG3	1.98	0.64
1:A:1939:ARG:HH12	1:A:1948:ASP:CG	2.00	0.64
1:B:1311:LYS:HZ3	1:B:1317:ARG:CB	2.09	0.64
1:A:168:PRO:O	1:A:180:PHE:CE2	2.51	0.64
1:B:1317:ARG:NH2	1:B:1779:GLN:HE21	1.95	0.64
1:B:1758:ILE:O	1:B:1800:ALA:HA	1.97	0.64
1:A:1949:ALA:O	1:A:1953:ILE:HG22	1.98	0.64
1:B:1939:ARG:C	1:B:1940:LEU:HD12	2.18	0.64
1:A:30:TYR:CE1	1:A:47:ILE:HD13	2.32	0.64
1:B:1729:THR:HB	1:B:1781:ILE:HD13	1.79	0.63
1:A:1850:HIS:O	1:A:1854:VAL:HG23	1.98	0.63
1:B:1767:ARG:CZ	1:B:1767:ARG:HB3	2.26	0.63
1:B:1856:ARG:HB2	1:B:1860:GLU:OE2	1.97	0.63
1:B:1292:GLY:O	1:B:1297:LYS:HE3	1.98	0.63
1:B:1886:ILE:HA	1:B:1944:VAL:HG21	1.81	0.63
1:B:1348:ALA:C	1:B:1349:ILE:HD12	2.19	0.63
1:A:1285:SER:OG	1:A:1866:ILE:HG13	1.97	0.63
1:A:1848:ALA:O	1:A:1852:LEU:HD23	1.98	0.63
1:A:1290:ILE:HD11	1:A:1297:LYS:CE	2.29	0.63
1:B:1342:ALA:O	1:B:1345:ALA:HB3	1.98	0.63
1:A:105:ARG:HH12	1:A:119:LYS:HZ3	1.46	0.63
1:A:155:TRP:HB3	1:A:156:PRO:CD	2.29	0.63
1:B:156:PRO:CG	1:B:161:MET:HG2	2.29	0.63
1:A:1887:SER:HB3	1:A:1944:VAL:O	1.99	0.62
1:A:1290:ILE:HA	2:A:2001:ADP:N1	2.15	0.62
1:B:1729:THR:HG21	1:B:1771:VAL:HG23	1.80	0.62
1:A:1837:ASP:OD2	1:B:1902:ARG:NH2	2.32	0.62
1:A:1261:ILE:HA	1:A:1873:LYS:HZ3	1.65	0.62
1:A:1882:ILE:N	1:A:1882:ILE:CD1	2.56	0.62
1:B:1878:ALA:HA	1:B:1882:ILE:HG12	1.81	0.62
1:A:1758:ILE:O	1:A:1800:ALA:HA	1.99	0.62
1:A:1329:ASP:OD1	1:A:1808:ARG:HA	1.99	0.62
1:A:1879:ARG:HG2	1:A:1879:ARG:HH11	1.64	0.62
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.64	0.62
1:A:1959:THR:O	1:A:1962:GLN:HB2	2.00	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:ALA:HB3	1:A:1866:ILE:HD11	1.83	0.61
1:A:167:MET:HB3	1:A:168:PRO:HD2	1.82	0.61
1:A:1734:ARG:HG3	1:A:1734:ARG:HH11	1.66	0.61
1:A:119:LYS:HD2	5:A:2006:CL:CL	2.38	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:HD12	1.82	0.61
1:B:1963:ILE:O	1:B:1965:MET:HG3	2.00	0.61
1:A:1945:THR:O	1:A:1948:ASP:HB2	2.00	0.61
1:A:1840:ASP:HB3	1:A:1843:ILE:HG23	1.83	0.61
1:A:169:THR:HB	1:A:170:ILE:HD12	1.83	0.60
1:B:1903:LYS:HA	1:B:1903:LYS:HE2	1.84	0.60
1:A:1939:ARG:C	1:A:1940:LEU:HD12	2.22	0.60
1:B:1287:ALA:O	1:B:1290:ILE:HG12	2.00	0.60
1:A:1333:ALA:O	1:A:1337:ILE:HG13	2.00	0.60
1:B:1867:PRO:CB	1:B:1870:ILE:HD13	2.31	0.60
1:B:49:PHE:CZ	1:B:64:ILE:HD11	2.36	0.60
1:A:1875:ILE:O	1:A:1878:ALA:HB3	2.01	0.60
1:A:1890:ALA:O	1:A:1894:ILE:HG22	2.02	0.60
1:A:1920:ILE:HG22	1:A:1921:THR:N	2.15	0.60
1:B:1336:GLN:O	1:B:1340:TYR:HD1	1.85	0.60
1:A:1856:ARG:NH1	1:A:1860:GLU:OE1	2.34	0.60
1:A:181:ARG:O	1:A:183:ILE:HD12	2.02	0.60
1:B:1864:PRO:HB3	1:B:1868:HIS:CD2	2.37	0.60
1:B:1920:ILE:HG23	1:B:1924:GLN:HG3	1.82	0.60
1:B:1866:ILE:N	1:B:1866:ILE:HD12	2.16	0.59
1:B:88:THR:O	1:B:91:ARG:HG2	2.01	0.59
1:B:1812:MET:H	1:B:1812:MET:HE2	1.67	0.59
1:A:1329:ASP:O	1:A:1332:VAL:HG23	2.02	0.59
1:B:1311:LYS:O	1:B:1312:LEU:HD23	2.02	0.59
1:B:168:PRO:O	1:B:180:PHE:CE2	2.55	0.59
1:B:1899:VAL:O	1:B:1903:LYS:HG2	2.01	0.59
1:B:1853:ARG:O	1:B:1856:ARG:HG3	2.02	0.59
1:B:144:HIS:CE1	1:B:176:LYS:O	2.56	0.59
1:B:1760:GLU:OE2	1:B:1803:ASN:ND2	2.36	0.59
1:B:1332:VAL:HG23	1:B:1334:LYS:CD	2.32	0.59
1:B:155:TRP:O	1:B:156:PRO:C	2.41	0.59
1:A:142:TYR:OH	1:A:165:LEU:HD11	2.03	0.58
1:B:1810:ASN:HD21	1:B:1836:ILE:HG21	1.67	0.58
1:B:1290:ILE:CD1	1:B:1297:LYS:HE2	2.29	0.58
1:B:1811:ARG:CD	1:B:1813:LYS:HB2	2.32	0.58
1:B:141:THR:HG21	1:B:186:LYS:HB2	1.84	0.58
1:A:1317:ARG:NH2	1:A:1779:GLN:HE21	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:VAL:CG1	1:A:1309:SER:N	2.65	0.58
1:A:1342:ALA:O	1:A:1345:ALA:HB3	2.03	0.58
1:A:1840:ASP:O	1:A:1843:ILE:N	2.35	0.58
1:A:1860:GLU:OE1	1:A:1860:GLU:HA	2.04	0.58
1:B:1941:SER:HB2	1:B:1943:ILE:H	1.69	0.58
1:B:1311:LYS:HG2	1:B:1317:ARG:HA	1.85	0.58
1:A:246:LYS:HG2	1:A:247:ARG:N	2.18	0.58
1:B:1813:LYS:N	1:B:1813:LYS:HD2	2.18	0.58
1:B:1896:LYS:O	1:B:1899:VAL:HG12	2.03	0.58
1:A:143:LYS:CB	1:A:183:ILE:HD11	2.30	0.57
1:B:1812:MET:H	1:B:1812:MET:CE	2.16	0.57
1:A:168:PRO:HG2	1:A:180:PHE:CE2	2.39	0.57
1:B:108:GLU:OE2	1:B:111:LYS:HE3	2.04	0.57
1:B:1886:ILE:HA	1:B:1944:VAL:CG2	2.34	0.57
1:A:1769:ARG:O	1:A:1772:ILE:HG22	2.03	0.57
1:A:1332:VAL:O	1:A:1333:ALA:HB3	2.04	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG21	1.85	0.57
1:B:1900:ARG:HG3	1:B:1900:ARG:HH11	1.68	0.57
1:A:114:SER:HB3	1:B:135:GLU:OE1	2.05	0.57
1:A:1894:ILE:HG23	1:A:1895:GLU:N	2.20	0.57
1:A:1896:LYS:O	1:A:1899:VAL:HG12	2.05	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG23	1.86	0.57
1:B:1856:ARG:HB2	1:B:1860:GLU:CD	2.25	0.57
1:A:245:VAL:HG23	1:A:245:VAL:O	2.04	0.57
1:A:1748:LEU:O	1:A:1796:THR:HG21	2.05	0.57
1:B:41:ARG:HH22	1:B:88:THR:HG22	1.69	0.57
1:A:1902:ARG:O	1:A:1919:PRO:HD2	2.05	0.57
1:A:23:GLY:HA3	1:A:27:GLN:HE22	1.69	0.57
1:B:143:LYS:HB2	1:B:183:ILE:CD1	2.35	0.56
1:B:1284:ASP:O	1:B:1288:PRO:HG3	2.04	0.56
1:B:1902:ARG:HG2	1:B:1902:ARG:HH11	1.70	0.56
1:B:1941:SER:HB2	1:B:1943:ILE:N	2.19	0.56
1:B:1264:GLU:O	1:B:1268:ILE:HG13	2.05	0.56
1:B:1309:SER:HB2	1:B:1320:GLY:HA3	1.86	0.56
1:B:1304:LEU:O	1:B:1879:ARG:HD2	2.05	0.56
1:A:1811:ARG:HD3	1:A:1813:LYS:HG3	1.87	0.56
1:A:125:GLY:HA3	1:A:197:ILE:HD11	1.86	0.56
1:A:1342:ALA:HB2	1:A:1757:LEU:HD12	1.88	0.56
1:B:1773:HIS:HB3	1:B:1828:ARG:NH1	2.21	0.56
1:B:143:LYS:HD2	1:B:152:GLU:OE2	2.06	0.56
1:B:1308:VAL:HG13	1:B:1309:SER:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1311:LYS:HZ3	1:B:1317:ARG:HD2	1.71	0.56
1:B:1284:ASP:CB	1:B:1865:LYS:HG3	2.36	0.56
1:B:1929:ILE:O	1:B:1933:GLU:HG3	2.05	0.56
1:A:202:GLU:HG2	1:A:267:LYS:HZ2	1.70	0.56
1:A:1302:LEU:HD22	1:A:1934:ALA:HB3	1.87	0.56
1:B:1848:ALA:O	1:B:1852:LEU:HD23	2.05	0.56
1:A:41:ARG:HH21	1:A:88:THR:HG22	1.66	0.56
1:A:1302:LEU:HD22	1:A:1934:ALA:CB	2.35	0.56
1:B:1847:VAL:O	1:B:1851:ILE:HG13	2.06	0.56
1:A:116:ASP:HA	1:A:119:LYS:NZ	2.21	0.56
1:A:1279:VAL:O	1:A:1283:VAL:HG12	2.05	0.56
1:B:1261:ILE:CD1	1:B:1261:ILE:H	2.14	0.56
1:A:1329:ASP:OD2	1:A:1836:ILE:HG23	2.05	0.56
1:B:1278:ILE:CG2	1:B:1279:VAL:N	2.68	0.56
1:B:1815:PRO:HD3	1:B:1965:MET:HE2	1.88	0.55
1:A:1812:MET:SD	1:A:1812:MET:N	2.73	0.55
1:A:63:ILE:HD13	1:A:100:ILE:HD13	1.89	0.55
1:A:1939:ARG:NH1	1:A:1948:ASP:OD2	2.39	0.55
1:A:1308:VAL:HG13	1:A:1309:SER:N	2.19	0.55
1:A:1950:ARG:HG2	1:A:1950:ARG:NH1	2.21	0.55
1:A:1753:GLY:N	1:A:1795:ARG:O	2.38	0.55
1:B:1849:ARG:O	1:B:1853:ARG:HG3	2.07	0.55
1:A:1760:GLU:HG3	1:A:1763:LYS:HG2	1.88	0.55
1:A:1278:ILE:CG2	1:A:1279:VAL:H	2.18	0.55
1:B:1882:ILE:HG22	1:B:1884:PRO:HD3	1.89	0.55
1:A:156:PRO:CG	1:A:161:MET:HG2	2.37	0.55
1:B:1289:ALA:HB3	1:B:1340:TYR:CE2	2.41	0.55
1:B:7:GLN:HG2	1:B:8:ILE:N	2.21	0.55
1:A:1273:ALA:HB1	1:A:1940:LEU:HD13	1.89	0.55
1:B:1328:GLY:O	1:B:1804:PRO:HD3	2.07	0.55
1:A:1767:ARG:HB3	1:A:1767:ARG:CZ	2.37	0.55
1:A:1296:VAL:HG22	1:A:1833:PHE:CD2	2.42	0.54
1:B:1901:MET:HG3	1:B:1920:ILE:HG13	1.88	0.54
1:A:1946:ARG:C	1:A:1950:ARG:HE	2.11	0.54
1:A:1760:GLU:OE2	1:A:1803:ASN:ND2	2.40	0.54
1:B:202:GLU:HG2	1:B:267:LYS:NZ	2.21	0.54
1:B:63:ILE:HG21	1:B:100:ILE:HD13	1.89	0.54
1:A:1856:ARG:O	1:A:1857:GLY:O	2.26	0.54
1:A:217:LEU:CD2	1:A:259:VAL:HG21	2.37	0.54
1:B:155:TRP:CH2	1:B:168:PRO:HB3	2.43	0.54
1:A:1278:ILE:CG2	1:A:1279:VAL:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1941:SER:CB	1:A:1943:ILE:H	2.20	0.54
1:B:1325:LEU:O	1:B:1326:LEU:HD23	2.07	0.54
1:B:1261:ILE:HA	1:B:1873:LYS:HZ3	1.69	0.54
1:B:1853:ARG:HD3	1:B:1856:ARG:HH21	1.73	0.54
1:A:1894:ILE:HD11	1:A:1925:LEU:HD12	1.90	0.54
1:A:1311:LYS:C	1:A:1312:LEU:HG	2.28	0.54
1:A:1860:GLU:OE1	1:A:1860:GLU:CA	2.56	0.54
1:B:1267:GLN:O	1:B:1271:GLU:HG2	2.07	0.54
1:B:1332:VAL:O	1:B:1333:ALA:HB3	2.08	0.54
1:A:1855:ARG:HD3	1:B:1318:LEU:HD11	1.88	0.54
1:B:181:ARG:O	1:B:183:ILE:HD12	2.08	0.54
1:A:88:THR:O	1:A:91:ARG:HG3	2.08	0.54
1:A:250:ARG:NE	1:B:163:GLU:HG3	2.22	0.54
1:A:183:ILE:HG22	1:A:186:LYS:H	1.72	0.54
1:A:116:ASP:HA	1:A:119:LYS:HZ1	1.72	0.54
1:B:144:HIS:HE1	1:B:176:LYS:O	1.91	0.54
1:A:71:LEU:O	1:A:75:GLU:HG3	2.08	0.54
1:B:1288:PRO:O	1:B:1290:ILE:N	2.41	0.53
1:B:1901:MET:CG	1:B:1920:ILE:HG13	2.38	0.53
1:B:1269:ILE:HG12	1:B:1874:TYR:HD1	1.73	0.53
1:A:1853:ARG:HD3	1:A:1856:ARG:NH2	2.24	0.53
1:B:1261:ILE:HG22	1:B:1873:LYS:HZ3	1.73	0.53
1:A:1896:LYS:HE3	1:A:1900:ARG:HG3	1.90	0.53
1:A:1809:PHE:N	1:A:1809:PHE:HD1	1.89	0.53
1:A:30:TYR:O	1:A:34:ILE:HG13	2.07	0.53
1:A:1929:ILE:N	1:A:1929:ILE:HD12	2.24	0.53
1:B:1284:ASP:HB3	1:B:1865:LYS:HG3	1.88	0.53
1:B:1819:ILE:HD12	1:B:1819:ILE:O	2.07	0.53
1:B:1939:ARG:HH21	1:B:1947:GLU:HB2	1.74	0.53
1:A:1853:ARG:CD	1:A:1856:ARG:NH2	2.72	0.53
1:A:155:TRP:HB3	1:A:156:PRO:HD2	1.90	0.53
1:B:1887:SER:HG	1:B:1943:ILE:HG22	1.74	0.53
1:B:262:ILE:O	1:B:262:ILE:HG23	2.09	0.53
1:B:155:TRP:CZ3	1:B:168:PRO:HB3	2.44	0.52
1:A:108:GLU:OE2	1:A:111:LYS:HE3	2.08	0.52
1:B:1298:LYS:HG2	1:B:1955:LEU:HD22	1.91	0.52
1:A:1901:MET:O	1:A:1904:SER:HB3	2.08	0.52
1:B:143:LYS:CG	1:B:152:GLU:HG2	2.37	0.52
1:B:1884:PRO:CA	1:B:1942:PRO:HB2	2.37	0.52
1:B:1325:LEU:C	1:B:1326:LEU:HD23	2.29	0.52
1:B:1290:ILE:O	1:B:1290:ILE:HG13	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1842:LYS:O	1:B:1846:GLU:HG2	2.09	0.52
1:A:1322:ILE:HD13	1:A:1931:LEU:HD23	1.91	0.52
1:B:1302:LEU:HD22	1:B:1934:ALA:HB3	1.91	0.52
1:B:1281:ALA:CB	1:B:1866:ILE:HD11	2.37	0.52
1:A:1311:LYS:CD	1:A:1317:ARG:HB2	2.39	0.52
1:A:1779:GLN:HG2	1:A:1795:ARG:HG2	1.91	0.52
1:A:250:ARG:CZ	1:B:163:GLU:HG3	2.39	0.52
1:A:183:ILE:N	1:A:183:ILE:HD12	2.25	0.52
1:A:1950:ARG:HG2	1:A:1950:ARG:HH11	1.74	0.52
1:A:1261:ILE:HA	1:A:1873:LYS:CE	2.39	0.52
1:B:140:ALA:O	1:B:154:GLU:HA	2.10	0.52
1:A:1897:TYR:CG	1:A:1953:ILE:HD12	2.45	0.52
1:B:155:TRP:HB3	1:B:156:PRO:CD	2.39	0.52
1:A:1941:SER:HB2	1:A:1943:ILE:N	2.25	0.52
1:A:133:VAL:HG22	1:A:222:VAL:HG13	1.92	0.52
1:A:1771:VAL:HG12	1:A:1771:VAL:O	2.10	0.52
1:A:23:GLY:HA3	1:A:27:GLN:NE2	2.24	0.52
1:A:262:ILE:HG23	1:A:262:ILE:O	2.09	0.52
1:B:153:PHE:HZ	1:B:168:PRO:HG3	1.75	0.52
1:B:1903:LYS:HE2	1:B:1903:LYS:CA	2.40	0.52
1:B:1261:ILE:HG12	1:B:1261:ILE:O	2.10	0.51
1:B:1288:PRO:C	1:B:1290:ILE:N	2.63	0.51
1:A:1855:ARG:HG2	1:B:1929:ILE:HG21	1.91	0.51
1:A:1899:VAL:HG13	1:A:1900:ARG:N	2.25	0.51
1:B:100:ILE:HG22	1:B:103:ILE:HG23	1.92	0.51
1:B:1278:ILE:HG23	1:B:1279:VAL:N	2.25	0.51
1:A:1339:ARG:HG2	1:A:1350:TYR:CE2	2.45	0.51
1:B:9:ASP:OD2	1:B:11:ARG:HB2	2.09	0.51
1:A:233:VAL:HG12	1:A:257:MET:HE3	1.93	0.51
1:B:1283:VAL:HG23	1:B:1284:ASP:N	2.26	0.51
1:B:257:MET:HE3	1:B:259:VAL:HG22	1.91	0.51
1:B:1289:ALA:CB	1:B:1340:TYR:CE2	2.94	0.51
1:A:1288:PRO:C	1:A:1290:ILE:H	2.14	0.51
1:B:1317:ARG:HH11	1:B:1317:ARG:HG3	1.76	0.51
1:B:1322:ILE:HD13	1:B:1931:LEU:HD23	1.93	0.51
1:B:14:PHE:CE2	1:B:74:LEU:HB3	2.45	0.51
1:A:1960:LEU:HA	1:A:1963:ILE:CD1	2.40	0.51
1:A:1898:TYR:CE1	1:A:1902:ARG:HD2	2.46	0.51
1:A:202:GLU:CD	1:A:202:GLU:H	2.14	0.51
1:A:1325:LEU:O	1:A:1326:LEU:HD23	2.10	0.51
1:A:240:LYS:HB3	1:A:256:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TRP:CB	1:A:156:PRO:CD	2.89	0.51
1:A:1920:ILE:CG2	1:A:1921:THR:N	2.74	0.51
1:A:1296:VAL:HA	1:A:1833:PHE:CE2	2.45	0.51
1:B:193:GLN:HB2	1:B:222:VAL:HG22	1.93	0.51
1:B:1939:ARG:HH11	1:B:1939:ARG:HG3	1.76	0.50
1:B:1317:ARG:HG3	1:B:1317:ARG:NH1	2.26	0.50
1:A:69:ILE:O	1:A:72:PRO:HD2	2.11	0.50
1:B:1864:PRO:HB2	1:B:1866:ILE:O	2.11	0.50
1:A:1852:LEU:HD11	1:B:1894:ILE:HD13	1.91	0.50
1:B:244:PRO:O	1:B:246:LYS:N	2.39	0.50
1:A:41:ARG:HH22	1:A:88:THR:HG22	1.75	0.50
1:B:1342:ALA:HB2	1:B:1757:LEU:HD12	1.92	0.50
1:B:241:GLN:NE2	1:B:253:PHE:CE2	2.80	0.50
1:A:1317:ARG:O	1:A:1317:ARG:HG3	2.11	0.50
1:A:1282:ILE:HD12	1:A:1938:MET:CE	2.41	0.50
1:A:1844:ASP:OD2	1:B:1902:ARG:HD3	2.12	0.50
1:A:1816:PHE:O	1:A:1819:ILE:HG12	2.11	0.50
1:A:1840:ASP:O	1:A:1842:LYS:N	2.45	0.50
1:B:1773:HIS:CD2	1:B:1828:ARG:NH1	2.80	0.50
1:A:1840:ASP:HB3	1:A:1843:ILE:CG2	2.42	0.50
1:A:240:LYS:HG3	1:A:241:GLN:N	2.26	0.50
1:A:1943:ILE:HG22	1:A:1944:VAL:O	2.11	0.50
1:A:1920:ILE:HG23	1:A:1924:GLN:CG	2.33	0.50
1:B:41:ARG:HH21	1:B:88:THR:HG22	1.77	0.50
1:A:1773:HIS:HB3	1:A:1828:ARG:NH1	2.24	0.50
1:A:1840:ASP:O	1:A:1841:ASP:C	2.50	0.50
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.50
1:B:1853:ARG:HD3	1:B:1856:ARG:NH2	2.27	0.50
1:A:161:MET:HE3	1:A:166:GLU:H	1.77	0.49
1:B:1293:TYR:HB3	1:B:1296:VAL:HB	1.93	0.49
1:A:1928:LEU:HD22	1:A:1956:MET:CE	2.42	0.49
1:B:181:ARG:O	1:B:183:ILE:CD1	2.59	0.49
1:B:1332:VAL:HG12	1:B:1837:ASP:HB3	1.94	0.49
1:B:1815:PRO:HD3	1:B:1965:MET:CE	2.41	0.49
1:A:1759:ASP:OD1	1:A:1760:GLU:N	2.46	0.49
1:A:1304:LEU:O	1:A:1879:ARG:HD2	2.12	0.49
1:B:156:PRO:CD	1:B:161:MET:HG2	2.43	0.49
1:B:1312:LEU:O	1:B:1316:THR:N	2.45	0.49
1:A:1848:ALA:HB2	1:B:1898:TYR:CD2	2.46	0.49
1:B:156:PRO:CB	1:B:159:GLU:O	2.52	0.49
1:A:1752:ASP:CA	1:A:1796:THR:HG22	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1869:GLU:HA	1:A:1872:ARG:NH1	2.26	0.49
1:A:1767:ARG:HG3	1:A:1767:ARG:HH11	1.77	0.49
1:B:233:VAL:HG12	1:B:257:MET:HE1	1.93	0.49
1:B:30:TYR:CE1	1:B:47:ILE:HD13	2.48	0.49
1:B:1869:GLU:HA	1:B:1872:ARG:HH11	1.78	0.49
1:B:1329:ASP:OD1	1:B:1808:ARG:CA	2.54	0.49
1:A:1290:ILE:O	1:A:1290:ILE:HG13	2.10	0.49
1:B:1939:ARG:HG3	1:B:1939:ARG:NH1	2.27	0.49
1:B:167:MET:HB2	1:B:168:PRO:HD2	1.95	0.49
1:B:1293:TYR:O	1:B:1297:LYS:HG3	2.13	0.49
1:A:246:LYS:HG2	1:A:247:ARG:H	1.75	0.49
1:B:1266:GLU:O	1:B:1269:ILE:HG22	2.12	0.49
1:B:139:LYS:NZ	1:B:156:PRO:O	2.45	0.49
1:A:1928:LEU:HD22	1:A:1956:MET:HE2	1.95	0.49
1:B:1816:PHE:O	1:B:1819:ILE:HG13	2.13	0.49
1:A:1868:HIS:O	1:A:1871:LEU:N	2.43	0.49
1:A:153:PHE:CD2	1:A:172:PRO:HG3	2.48	0.49
1:B:155:TRP:O	1:B:157:GLU:HG3	2.13	0.48
1:A:1886:ILE:H	1:A:1886:ILE:HD12	1.78	0.48
1:A:1879:ARG:NH1	1:A:1879:ARG:HG2	2.27	0.48
1:B:1867:PRO:HB3	1:B:1870:ILE:HD13	1.95	0.48
1:A:1322:ILE:O	1:A:1797:THR:HG23	2.13	0.48
1:B:1830:ASP:CG	1:B:1930:ARG:HH21	2.17	0.48
1:A:1312:LEU:O	1:A:1316:THR:HA	2.12	0.48
1:B:1938:MET:O	1:B:1940:LEU:HD12	2.14	0.48
1:A:168:PRO:HG2	1:A:180:PHE:CZ	2.49	0.48
1:A:44:SER:HA	1:A:97:HIS:O	2.13	0.48
1:A:200:ARG:O	1:A:203:GLU:HG2	2.14	0.48
1:B:1939:ARG:CG	1:B:1939:ARG:HH11	2.26	0.48
1:A:1311:LYS:HA	1:A:1317:ARG:HA	1.95	0.48
1:A:1319:ARG:O	1:A:1930:ARG:HD3	2.14	0.48
1:A:1730:ALA:CB	1:A:1783:ILE:HD11	2.43	0.48
1:A:1856:ARG:HG3	1:A:1860:GLU:OE2	2.14	0.48
1:A:1889:GLU:HB3	1:A:1946:ARG:HG3	1.90	0.48
1:A:1902:ARG:CB	1:A:1903:LYS:HZ3	2.10	0.48
1:B:119:LYS:HD3	5:B:2006:CL:CL	2.51	0.48
1:B:1809:PHE:HB2	1:B:1818:GLN:CD	2.33	0.48
1:B:1345:ALA:CB	1:B:1348:ALA:HB3	2.38	0.48
1:A:1804:PRO:CG	1:A:1807:GLY:O	2.62	0.48
1:B:1867:PRO:HB2	1:B:1870:ILE:HD13	1.95	0.48
1:A:155:TRP:HA	1:A:155:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:ILE:HD11	1:A:1880:LYS:HE2	1.96	0.48
1:B:1312:LEU:HB3	1:B:1313:PRO:HD2	1.95	0.48
1:A:1281:ALA:O	1:A:1285:SER:OG	2.23	0.48
1:B:211:ARG:NH1	1:B:211:ARG:HG3	2.26	0.48
1:B:1936:ALA:O	1:B:1939:ARG:HB2	2.14	0.48
1:B:1879:ARG:HH11	1:B:1879:ARG:HG2	1.77	0.48
1:A:1939:ARG:NH2	1:A:1945:THR:OG1	2.46	0.48
1:B:1944:VAL:HG12	1:B:1948:ASP:CG	2.33	0.48
1:B:1945:THR:O	1:B:1948:ASP:HB2	2.13	0.48
1:B:103:ILE:H	1:B:103:ILE:CD1	2.16	0.48
1:B:161:MET:HE3	1:B:162:PRO:HD2	1.96	0.47
1:B:1948:ASP:O	1:B:1949:ALA:C	2.52	0.47
1:A:171:CYS:CB	1:A:174:CYS:SG	2.99	0.47
1:A:1853:ARG:O	1:A:1856:ARG:HG2	2.13	0.47
1:A:1898:TYR:CE2	1:A:1925:LEU:HD22	2.49	0.47
1:B:1948:ASP:O	1:B:1951:GLU:N	2.46	0.47
1:A:1346:PRO:HG2	1:A:1347:ARG:HG3	1.95	0.47
1:B:202:GLU:CD	1:B:202:GLU:H	2.18	0.47
1:A:1839:PRO:HA	1:A:1844:ASP:OD1	2.13	0.47
1:B:1828:ARG:HE	1:B:1923:ARG:NH2	2.13	0.47
1:A:1311:LYS:HD3	1:A:1317:ARG:HB2	1.96	0.47
1:A:155:TRP:O	1:A:156:PRO:C	2.51	0.47
1:A:1847:VAL:O	1:A:1851:ILE:HG13	2.14	0.47
1:B:1298:LYS:HZ1	1:B:1935:HIS:CD2	2.32	0.47
1:A:8:ILE:CG1	1:A:9:ASP:N	2.76	0.47
1:A:1922:ALA:O	1:A:1925:LEU:HB3	2.15	0.47
1:A:1262:SER:HB3	1:A:1265:GLU:OE2	2.14	0.47
1:A:1263:PRO:HA	1:A:1266:GLU:HB3	1.95	0.47
1:A:171:CYS:O	1:A:175:GLY:N	2.42	0.47
1:A:170:ILE:HG23	1:A:175:GLY:C	2.35	0.47
1:A:1278:ILE:HD11	1:A:1874:TYR:OH	2.14	0.47
1:A:1332:VAL:CG1	1:A:1332:VAL:O	2.59	0.47
1:A:1346:PRO:C	1:A:1347:ARG:HG3	2.34	0.47
1:B:1853:ARG:O	1:B:1855:ARG:N	2.48	0.47
1:A:1257:GLN:HG3	1:A:1257:GLN:O	2.14	0.47
1:B:65:ASN:ND2	1:B:263:GLU:HG3	2.30	0.47
1:B:1346:PRO:HG2	1:B:1347:ARG:N	2.30	0.47
1:B:1311:LYS:HG2	1:B:1317:ARG:CA	2.44	0.47
1:A:1311:LYS:HD2	1:A:1317:ARG:NH1	2.30	0.47
1:A:1276:LYS:CE	1:A:1276:LYS:HA	2.30	0.47
1:B:1840:ASP:HB3	1:B:1843:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1882:ILE:CG2	1:B:1942:PRO:HB3	2.45	0.47
1:B:1815:PRO:HG3	1:B:1963:ILE:HG23	1.96	0.47
1:B:153:PHE:CZ	1:B:168:PRO:HG3	2.50	0.47
1:A:1853:ARG:HD3	1:A:1856:ARG:HH21	1.80	0.47
1:A:239:ILE:HG13	1:A:239:ILE:O	2.15	0.47
1:A:1925:LEU:O	1:A:1929:ILE:HD13	2.15	0.47
1:A:1856:ARG:O	1:A:1860:GLU:OE2	2.33	0.47
1:B:145:ILE:HG22	1:B:145:ILE:O	2.15	0.47
1:A:1276:LYS:HE2	1:A:1276:LYS:CA	2.40	0.46
1:B:137:ILE:HG23	1:B:187:THR:CG2	2.45	0.46
1:B:1319:ARG:O	1:B:1930:ARG:HD3	2.15	0.46
1:A:1325:LEU:C	1:A:1326:LEU:HD23	2.35	0.46
1:B:103:ILE:N	1:B:103:ILE:HD13	2.15	0.46
1:A:1310:ARG:HB3	1:A:1312:LEU:HD11	1.96	0.46
1:B:1939:ARG:O	1:B:1940:LEU:HB2	2.15	0.46
1:B:155:TRP:CG	1:B:156:PRO:N	2.82	0.46
1:A:164:VAL:CG2	1:A:244:PRO:HB2	2.46	0.46
1:A:1843:ILE:HG13	1:A:1844:ASP:N	2.30	0.46
1:A:1804:PRO:HG2	1:A:1807:GLY:O	2.15	0.46
1:B:1920:ILE:CG2	1:B:1921:THR:N	2.78	0.46
1:A:1779:GLN:HG2	1:A:1795:ARG:HA	1.97	0.46
1:B:9:ASP:OD1	1:B:9:ASP:O	2.34	0.46
1:B:155:TRP:CB	1:B:156:PRO:CD	2.94	0.46
1:A:1311:LYS:HD2	1:A:1317:ARG:HB2	1.98	0.46
1:A:1867:PRO:CG	1:A:1870:ILE:HD12	2.45	0.46
1:A:182:LEU:O	1:A:184:PRO:HD3	2.16	0.46
1:B:1317:ARG:NH2	1:B:1779:GLN:CG	2.72	0.46
1:A:1853:ARG:HA	1:A:1856:ARG:HG2	1.98	0.46
1:B:71:LEU:HB3	1:B:72:PRO:HD3	1.98	0.46
1:A:1288:PRO:O	1:A:1290:ILE:N	2.44	0.46
1:B:61:TYR:HD1	1:B:64:ILE:HD12	1.81	0.46
1:A:233:VAL:CG1	1:A:257:MET:HE3	2.45	0.46
1:B:65:ASN:OD1	1:B:232:LYS:HD2	2.16	0.46
1:B:1269:ILE:HG22	1:B:1270:LYS:N	2.31	0.45
1:A:25:ASN:H	1:A:27:GLN:NE2	2.05	0.45
1:A:1798:VAL:O	1:A:1799:ILE:HD13	2.17	0.45
1:A:1317:ARG:HH21	1:A:1779:GLN:HE21	1.62	0.45
1:B:1352:SER:OG	1:B:1353:GLY:N	2.50	0.45
1:A:1272:LEU:H	1:A:1272:LEU:HD12	1.81	0.45
1:A:1945:THR:O	1:A:1948:ASP:N	2.50	0.45
1:A:1893:GLU:HG2	1:A:1946:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLN:HG3	1:A:199:GLU:O	2.16	0.45
1:B:88:THR:O	1:B:91:ARG:CG	2.64	0.45
1:A:1946:ARG:HB3	1:A:1950:ARG:NE	2.32	0.45
1:B:1296:VAL:HG22	1:B:1833:PHE:CD2	2.51	0.45
1:B:1322:ILE:HG23	1:B:1830:ASP:CG	2.36	0.45
1:A:1951:GLU:OE1	1:A:1951:GLU:HA	2.17	0.45
1:A:258:LYS:HA	1:A:258:LYS:HD2	1.78	0.45
1:A:123:ILE:HG22	1:A:124:ASP:N	2.32	0.45
1:A:1353:GLY:N	1:A:1759:ASP:O	2.50	0.45
1:B:1760:GLU:CG	1:B:1763:LYS:HD2	2.46	0.45
1:A:217:LEU:HD23	1:A:259:VAL:HG21	1.99	0.45
1:B:1272:LEU:O	1:B:1275:ARG:HB3	2.16	0.45
1:B:123:ILE:HG22	1:B:124:ASP:N	2.31	0.45
1:A:1779:GLN:HG2	1:A:1795:ARG:CG	2.47	0.45
1:B:1946:ARG:O	1:B:1950:ARG:HB2	2.17	0.45
1:A:1752:ASP:HA	1:A:1796:THR:CG2	2.44	0.45
1:A:1729:THR:OG1	1:A:1730:ALA:N	2.48	0.45
1:A:1871:LEU:HD12	1:A:1874:TYR:HB3	1.99	0.45
1:B:1900:ARG:CG	1:B:1900:ARG:HH11	2.30	0.45
1:B:1853:ARG:C	1:B:1855:ARG:N	2.70	0.45
1:B:202:GLU:HG2	1:B:267:LYS:HZ2	1.80	0.45
1:B:1276:LYS:HE2	1:B:1276:LYS:CA	2.41	0.45
1:A:1956:MET:O	1:A:1959:THR:OG1	2.28	0.45
1:A:1866:ILE:HG22	1:A:1867:PRO:CD	2.46	0.45
1:A:1858:GLU:O	1:A:1859:SER:HB3	2.16	0.45
1:B:200:ARG:HB2	1:B:203:GLU:HG2	1.99	0.45
1:A:1260:GLU:HA	1:A:1260:GLU:OE2	2.17	0.45
1:B:1760:GLU:HA	1:B:1760:GLU:OE2	2.17	0.45
1:A:1831:LEU:HD11	1:A:1955:LEU:HD23	1.99	0.45
1:A:1897:TYR:CE1	1:A:1901:MET:HB3	2.52	0.45
1:A:1844:ASP:OD2	1:B:1902:ARG:NH1	2.50	0.45
1:B:1308:VAL:CG1	1:B:1309:SER:N	2.80	0.45
1:A:1946:ARG:CB	1:A:1950:ARG:HE	2.30	0.44
1:B:25:ASN:CA	1:B:27:GLN:HE21	2.29	0.44
1:A:86:ASP:OD1	1:A:88:THR:HB	2.17	0.44
1:B:174:CYS:SG	1:B:176:LYS:N	2.81	0.44
1:A:1950:ARG:O	1:A:1953:ILE:HG23	2.17	0.44
1:A:242:ASP:O	1:A:244:PRO:HD3	2.18	0.44
1:A:1760:GLU:OE1	1:A:1763:LYS:HE3	2.17	0.44
1:B:1897:TYR:CE1	1:B:1901:MET:HB3	2.52	0.44
1:B:1921:THR:H	1:B:1924:GLN:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1843:ILE:HG13	1:B:1844:ASP:N	2.30	0.44
1:B:1869:GLU:N	1:B:1869:GLU:OE1	2.45	0.44
1:B:1775:ALA:O	1:B:1779:GLN:HA	2.17	0.44
1:A:1346:PRO:HG2	1:A:1347:ARG:N	2.32	0.44
1:A:161:MET:HE2	1:A:161:MET:HB3	1.49	0.44
1:A:1897:TYR:CE2	1:A:1901:MET:HE3	2.53	0.44
1:B:153:PHE:CD2	1:B:172:PRO:HG3	2.53	0.44
1:B:108:GLU:HB2	1:B:111:LYS:HG3	1.99	0.44
1:A:1262:SER:HB3	1:A:1265:GLU:HB2	2.00	0.44
1:A:1730:ALA:HB3	1:A:1783:ILE:HD11	1.99	0.44
1:B:1805:LYS:N	1:B:1818:GLN:O	2.40	0.44
1:A:1282:ILE:HG12	1:A:1866:ILE:HD12	2.00	0.44
1:A:1334:LYS:HB2	2:A:2001:ADP:O2B	2.18	0.44
1:B:1810:ASN:ND2	1:B:1836:ILE:HG21	2.33	0.44
1:A:1807:GLY:O	1:A:1808:ARG:C	2.56	0.44
1:B:1840:ASP:O	1:B:1843:ILE:HG23	2.18	0.44
1:B:200:ARG:O	1:B:203:GLU:HG2	2.18	0.44
1:B:1311:LYS:HZ3	1:B:1317:ARG:CD	2.31	0.44
1:B:1804:PRO:O	1:B:1805:LYS:C	2.56	0.44
1:A:1956:MET:O	1:A:1960:LEU:HG	2.18	0.44
1:B:1853:ARG:C	1:B:1855:ARG:H	2.22	0.44
1:A:1322:ILE:HG23	1:A:1830:ASP:HB2	1.99	0.44
1:A:1894:ILE:HD11	1:A:1925:LEU:CD1	2.47	0.43
1:B:182:LEU:C	1:B:183:ILE:HD12	2.39	0.43
1:A:1960:LEU:HA	1:A:1963:ILE:CG1	2.48	0.43
1:A:237:LEU:HD23	1:A:257:MET:HB2	2.00	0.43
1:B:1269:ILE:CG2	1:B:1270:LYS:N	2.80	0.43
1:B:1902:ARG:NH1	1:B:1902:ARG:HG2	2.32	0.43
1:A:1346:PRO:HB3	1:A:1872:ARG:HD3	2.00	0.43
1:B:169:THR:HB	1:B:170:ILE:HD12	2.00	0.43
1:B:215:ILE:HD12	1:B:217:LEU:HD21	1.99	0.43
1:A:1266:GLU:O	1:A:1269:ILE:HG23	2.19	0.43
1:A:164:VAL:HG21	1:A:244:PRO:HB2	2.00	0.43
1:B:1899:VAL:HG13	1:B:1900:ARG:N	2.33	0.43
1:B:1809:PHE:HB2	1:B:1818:GLN:NE2	2.33	0.43
1:A:168:PRO:HG2	1:A:168:PRO:O	2.17	0.43
1:B:1759:ASP:OD1	1:B:1760:GLU:N	2.51	0.43
1:B:1851:ILE:HG12	2:B:2001:ADP:O2'	2.18	0.43
1:B:233:VAL:HG12	1:B:257:MET:CE	2.48	0.43
1:A:1265:GLU:OE2	1:A:1873:LYS:HE3	2.18	0.43
1:B:1311:LYS:HG2	1:B:1317:ARG:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1919:PRO:CG	1:B:1920:ILE:H	2.29	0.43
1:A:153:PHE:CD1	1:A:153:PHE:N	2.87	0.43
1:B:204:VAL:HG21	1:B:210:PRO:HB3	2.00	0.43
1:B:130:VAL:HG23	1:B:227:PRO:HG3	2.01	0.43
1:A:1308:VAL:O	1:A:1309:SER:HB3	2.19	0.43
1:A:1311:LYS:NZ	1:A:1319:ARG:HA	2.34	0.43
1:A:1353:GLY:O	1:A:1764:MET:HA	2.19	0.43
1:A:191:ASP:HB3	1:A:222:VAL:HG21	2.00	0.43
1:A:1286:ILE:HA	1:A:1286:ILE:HD13	1.91	0.43
1:B:1939:ARG:NH1	1:B:1948:ASP:OD2	2.52	0.43
1:A:1290:ILE:HA	2:A:2001:ADP:C2	2.53	0.43
1:B:1300:ILE:O	1:B:1304:LEU:HG	2.18	0.43
1:A:1350:TYR:C	1:A:1350:TYR:CD1	2.92	0.43
1:A:138:TYR:OH	1:A:188:LYS:HD2	2.18	0.43
1:A:140:ALA:O	1:A:154:GLU:HA	2.19	0.43
1:B:1885:VAL:O	1:B:1944:VAL:HG23	2.19	0.43
1:B:121:ILE:HD12	1:B:123:ILE:HD11	1.99	0.43
1:A:161:MET:HE3	1:A:165:LEU:HA	2.00	0.43
1:B:1811:ARG:HG3	1:B:1813:LYS:HB2	2.01	0.43
1:A:1328:GLY:HA3	1:A:1334:LYS:HD2	2.01	0.43
1:A:1261:ILE:HG23	1:A:1873:LYS:HZ1	1.84	0.43
1:B:162:PRO:HG2	1:B:166:GLU:OE2	2.18	0.43
1:B:1842:LYS:O	1:B:1845:SER:HB3	2.19	0.43
1:B:1308:VAL:O	1:B:1309:SER:HB3	2.18	0.43
1:B:1926:GLU:O	1:B:1930:ARG:HG3	2.19	0.43
1:B:205:PRO:O	1:B:208:GLN:HB2	2.19	0.43
1:A:165:LEU:C	1:A:165:LEU:HD12	2.39	0.42
1:A:105:ARG:NH2	1:A:116:ASP:OD1	2.50	0.42
1:A:1311:LYS:HE3	1:A:1317:ARG:NH2	2.34	0.42
1:B:1318:LEU:HA	1:B:1318:LEU:HD22	1.89	0.42
1:B:241:GLN:HE21	1:B:241:GLN:HB2	1.50	0.42
1:A:1840:ASP:HB3	1:A:1843:ILE:HG12	2.02	0.42
1:A:1860:GLU:HB2	1:A:1862:VAL:HG22	2.00	0.42
1:A:1862:VAL:HG23	1:A:1862:VAL:O	2.18	0.42
1:A:1935:HIS:CE1	1:A:1951:GLU:HG3	2.54	0.42
1:A:1894:ILE:HG23	1:A:1895:GLU:H	1.83	0.42
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.84	0.42
1:A:1947:GLU:O	1:A:1951:GLU:HG2	2.19	0.42
1:A:1762:ASP:OD1	1:A:1820:ASP:HB3	2.20	0.42
1:A:204:VAL:HA	1:A:205:PRO:HD3	1.77	0.42
1:B:245:VAL:HG22	1:B:245:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:O	1:B:113:ARG:NH2	2.52	0.42
1:B:12:ASP:O	1:B:16:GLU:HB2	2.18	0.42
1:A:1919:PRO:HG2	1:A:1920:ILE:H	1.84	0.42
1:B:143:LYS:HA	1:B:151:GLN:O	2.18	0.42
1:A:1828:ARG:NE	1:A:1923:ARG:NH2	2.51	0.42
1:B:1839:PRO:O	1:B:1843:ILE:HG23	2.18	0.42
1:B:1878:ALA:HA	1:B:1882:ILE:CG1	2.47	0.42
1:A:1733:VAL:HG12	1:A:1734:ARG:N	2.34	0.42
1:B:11:ARG:HG2	1:B:77:ALA:HB2	2.02	0.42
1:B:241:GLN:HG2	1:B:243:SER:O	2.19	0.42
1:B:1733:VAL:CG1	1:B:1734:ARG:N	2.82	0.42
1:A:78:LEU:O	1:A:82:ILE:HG13	2.20	0.42
1:B:1296:VAL:HA	1:B:1833:PHE:CE2	2.55	0.42
1:A:1751:ALA:O	1:A:1752:ASP:C	2.57	0.42
1:B:1344:LEU:O	1:B:1346:PRO:HD3	2.20	0.42
1:B:1289:ALA:CB	1:B:1340:TYR:HE2	2.32	0.42
1:B:1882:ILE:HG23	1:B:1942:PRO:HB3	2.01	0.42
1:B:1335:SER:HA	1:B:1759:ASP:OD2	2.20	0.42
1:A:1811:ARG:HH11	1:A:1813:LYS:HD2	1.84	0.42
1:A:1342:ALA:HB2	1:A:1757:LEU:CD1	2.50	0.42
1:B:1283:VAL:CG2	1:B:1284:ASP:N	2.83	0.42
1:A:1316:THR:HB	1:A:1317:ARG:H	1.62	0.42
1:B:1342:ALA:O	1:B:1345:ALA:CB	2.65	0.42
1:B:1879:ARG:NH1	1:B:1879:ARG:HG2	2.32	0.42
1:A:1811:ARG:HD3	1:A:1813:LYS:CG	2.47	0.42
1:A:1327:VAL:HG11	1:A:1819:ILE:HG21	2.02	0.42
1:B:1761:LEU:HD11	1:B:1764:MET:HE1	2.01	0.42
1:A:155:TRP:HA	1:A:155:TRP:HE3	1.83	0.42
1:A:1899:VAL:CG1	1:A:1900:ARG:N	2.83	0.42
1:A:1312:LEU:HB3	1:A:1313:PRO:CD	2.43	0.42
1:B:1814:ASN:ND2	1:B:1817:GLU:OE2	2.53	0.42
1:B:1940:LEU:O	1:B:1941:SER:C	2.58	0.41
1:A:1734:ARG:HH11	1:A:1734:ARG:CG	2.33	0.41
1:A:53:LEU:HA	1:A:60:ALA:HB2	2.01	0.41
1:A:25:ASN:N	1:A:27:GLN:HE21	2.07	0.41
1:A:1942:PRO:HG2	1:A:1942:PRO:O	2.20	0.41
1:A:155:TRP:CG	1:A:156:PRO:N	2.88	0.41
1:A:156:PRO:CD	1:A:161:MET:HG2	2.49	0.41
1:B:183:ILE:HG22	1:B:186:LYS:H	1.85	0.41
1:B:1810:ASN:O	1:B:1811:ARG:C	2.58	0.41
1:A:1941:SER:CB	1:A:1943:ILE:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:PRO:HA	1:A:1942:PRO:HB2	2.01	0.41
1:A:143:LYS:HB2	1:A:183:ILE:CD1	2.37	0.41
1:A:156:PRO:HD3	1:A:161:MET:HG2	2.02	0.41
1:A:1308:VAL:CG1	1:A:1309:SER:H	2.33	0.41
1:A:240:LYS:HB3	1:A:256:TYR:CD1	2.56	0.41
1:B:1869:GLU:HA	1:B:1872:ARG:NH1	2.35	0.41
1:A:1945:THR:O	1:A:1946:ARG:C	2.58	0.41
1:A:1851:ILE:HD12	1:B:1925:LEU:HD23	2.03	0.41
1:B:1898:TYR:CD1	1:B:1925:LEU:HD13	2.56	0.41
1:A:1928:LEU:HA	1:A:1928:LEU:HD13	1.70	0.41
1:A:1278:ILE:O	1:A:1282:ILE:HG13	2.20	0.41
1:B:1729:THR:O	1:B:1746:GLY:N	2.46	0.41
1:B:1773:HIS:HD2	1:B:1828:ARG:NH1	2.19	0.41
1:A:37:LEU:HD23	1:A:37:LEU:C	2.41	0.41
1:B:82:ILE:CD1	1:B:96:VAL:HG11	2.51	0.41
1:A:155:TRP:O	1:A:157:GLU:HG3	2.20	0.41
1:A:1882:ILE:H	1:A:1882:ILE:CD1	2.15	0.41
1:A:1772:ILE:HG23	1:A:1773:HIS:N	2.35	0.41
1:B:30:TYR:O	1:B:34:ILE:HG13	2.21	0.41
1:B:138:TYR:CZ	1:B:188:LYS:HB3	2.55	0.41
1:A:1342:ALA:C	1:A:1345:ALA:H	2.24	0.41
1:A:1335:SER:HA	1:A:1759:ASP:OD2	2.21	0.41
1:B:1760:GLU:HG2	1:B:1763:LYS:HD2	2.02	0.41
1:A:1767:ARG:CG	1:A:1767:ARG:HH11	2.33	0.41
1:B:1880:LYS:O	1:B:1883:HIS:HE1	2.03	0.41
1:A:161:MET:SD	1:A:165:LEU:HD13	2.61	0.41
1:A:1946:ARG:HB3	1:A:1950:ARG:HE	1.86	0.41
1:B:1944:VAL:HG12	1:B:1948:ASP:HB3	2.01	0.41
1:B:1287:ALA:O	1:B:1290:ILE:CG1	2.68	0.41
1:B:61:TYR:OH	1:B:260:SER:HB3	2.21	0.41
1:B:1735:ASP:C	1:B:1735:ASP:OD1	2.59	0.41
1:B:1868:HIS:O	1:B:1871:LEU:N	2.53	0.41
1:B:1863:ALA:HB1	1:B:1864:PRO:CD	2.42	0.41
1:A:1281:ALA:O	1:A:1285:SER:N	2.54	0.41
1:B:1920:ILE:HA	1:B:1920:ILE:HD13	1.87	0.41
1:A:1811:ARG:O	1:A:1813:LYS:N	2.54	0.41
1:A:121:ILE:HD12	1:A:123:ILE:HD11	2.03	0.41
1:B:1733:VAL:HG12	1:B:1734:ARG:N	2.35	0.41
1:B:1814:ASN:OD1	1:B:1814:ASN:N	2.54	0.41
1:B:1783:ILE:O	1:B:1789:THR:HA	2.21	0.41
1:B:142:TYR:HD2	1:B:155:TRP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:CE1	1:A:174:CYS:SG	3.13	0.41
1:A:142:TYR:CE1	1:A:182:LEU:HB2	2.56	0.40
1:B:1311:LYS:HZ3	1:B:1317:ARG:CG	2.34	0.40
1:A:1761:LEU:HD11	1:A:1764:MET:CE	2.51	0.40
1:A:1336:GLN:HE21	1:A:1340:TYR:HE1	1.69	0.40
1:A:1344:LEU:O	1:A:1346:PRO:HD3	2.21	0.40
1:B:1875:ILE:HG22	1:B:1879:ARG:HD3	2.03	0.40
1:A:221:LEU:O	1:A:222:VAL:C	2.60	0.40
1:A:233:VAL:HB	1:A:257:MET:HE3	2.03	0.40
1:A:185:GLU:H	1:A:185:GLU:CD	2.24	0.40
1:A:182:LEU:HG	1:A:183:ILE:N	2.34	0.40
1:B:1939:ARG:O	1:B:1940:LEU:HD12	2.20	0.40
1:B:1939:ARG:NH2	1:B:1945:THR:OG1	2.55	0.40
1:B:1751:ALA:O	1:B:1752:ASP:C	2.58	0.40
1:A:1361:LEU:HB2	1:A:1768:ASP:OD2	2.20	0.40
1:B:155:TRP:HB3	1:B:156:PRO:HD2	2.04	0.40
1:A:144:HIS:ND1	1:A:171:CYS:HB2	2.35	0.40
1:B:152:GLU:OE1	1:B:186:LYS:NZ	2.32	0.40
1:A:1843:ILE:HG13	1:A:1844:ASP:H	1.86	0.40
1:B:70:ILE:HG23	1:B:71:LEU:N	2.37	0.40
1:A:1950:ARG:CG	1:A:1950:ARG:HH11	2.35	0.40
1:B:1899:VAL:CG1	1:B:1900:ARG:N	2.84	0.40
1:B:69:ILE:O	1:B:72:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	587/613 (96%)	519 (88%)	53 (9%)	15 (3%)	7	16
1	B	587/613 (96%)	524 (89%)	47 (8%)	16 (3%)	6	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1174/1226 (96%)	1043 (89%)	100 (8%)	31 (3%)	7	16

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	TRP
1	A	247	ARG
1	A	1841	ASP
1	A	1857	GLY
1	B	155	TRP
1	B	245	VAL
1	B	1841	ASP
1	B	1861	VAL
1	B	1948	ASP
1	A	245	VAL
1	A	1812	MET
1	A	1858	GLU
1	B	1289	ALA
1	B	1811	ARG
1	B	1839	PRO
1	A	139	LYS
1	A	156	PRO
1	A	1289	ALA
1	A	1868	HIS
1	B	156	PRO
1	B	1346	PRO
1	B	1859	SER
1	A	250	ARG
1	A	1346	PRO
1	B	1309	SER
1	B	1854	VAL
1	B	89	TYR
1	A	168	PRO
1	B	1941	SER
1	A	1942	PRO
1	B	1942	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	517/537 (96%)	444 (86%)	73 (14%)	4	10
1	B	517/537 (96%)	461 (89%)	56 (11%)	8	18
All	All	1034/1074 (96%)	905 (88%)	129 (12%)	6	13

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	8	ILE
1	A	27	GLN
1	A	48	GLU
1	A	71	LEU
1	A	91	ARG
1	A	158	ASP
1	A	161	MET
1	A	163	GLU
1	A	165	LEU
1	A	168	PRO
1	A	169	THR
1	A	181	ARG
1	A	182	LEU
1	A	188	LYS
1	A	241	GLN
1	A	245	VAL
1	A	247	ARG
1	A	254	ASP
1	A	264	VAL
1	A	265	SER
1	A	269	LEU
1	A	1267	GLN
1	A	1269	ILE
1	A	1276	LYS
1	A	1283	VAL
1	A	1285	SER
1	A	1308	VAL
1	A	1311	LYS
1	A	1316	THR
1	A	1318	LEU
1	A	1347	ARG
1	A	1352	SER

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Mol	Chain	Res	Type
1	A	1355	SER
1	A	1734	ARG
1	A	1760	GLU
1	A	1762	ASP
1	A	1763	LYS
1	A	1764	MET
1	A	1766	ASP
1	A	1770	SER
1	A	1779	GLN
1	A	1805	LYS
1	A	1806	GLN
1	A	1808	ARG
1	A	1809	PHE
1	A	1818	GLN
1	A	1825	LEU
1	A	1830	ASP
1	A	1841	ASP
1	A	1844	ASP
1	A	1855	ARG
1	A	1858	GLU
1	A	1861	VAL
1	A	1869	GLU
1	A	1882	ILE
1	A	1886	ILE
1	A	1888	GLU
1	A	1892	GLU
1	A	1894	ILE
1	A	1896	LYS
1	A	1903	LYS
1	A	1921	THR
1	A	1928	LEU
1	A	1939	ARG
1	A	1940	LEU
1	A	1941	SER
1	A	1942	PRO
1	A	1943	ILE
1	A	1944	VAL
1	A	1950	ARG
1	A	1953	ILE
1	A	1963	ILE
1	B	9	ASP
1	B	27	GLN

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Mol	Chain	Res	Type
1	B	48	GLU
1	B	68	LYS
1	B	91	ARG
1	B	96	VAL
1	B	103	ILE
1	B	139	LYS
1	B	143	LYS
1	B	158	ASP
1	B	161	MET
1	B	163	GLU
1	B	166	GLU
1	B	171	CYS
1	B	233	VAL
1	B	241	GLN
1	B	242	ASP
1	B	247	ARG
1	B	254	ASP
1	B	1261	ILE
1	B	1269	ILE
1	B	1272	LEU
1	B	1276	LYS
1	B	1314	ASP
1	B	1316	THR
1	B	1318	LEU
1	B	1329	ASP
1	B	1347	ARG
1	B	1762	ASP
1	B	1766	ASP
1	B	1770	SER
1	B	1808	ARG
1	B	1809	PHE
1	B	1812	MET
1	B	1813	LYS
1	B	1814	ASN
1	B	1824	THR
1	B	1825	LEU
1	B	1830	ASP
1	B	1842	LYS
1	B	1843	ILE
1	B	1850	HIS
1	B	1860	GLU
1	B	1862	VAL

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Mol	Chain	Res	Type
1	B	1869	GLU
1	B	1873	LYS
1	B	1879	ARG
1	B	1892	GLU
1	B	1896	LYS
1	B	1900	ARG
1	B	1902	ARG
1	B	1939	ARG
1	B	1941	SER
1	B	1944	VAL
1	B	1948	ASP
1	B	1953	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	27	GLN
1	A	212	GLN
1	A	241	GLN
1	A	1267	GLN
1	A	1779	GLN
1	A	1814	ASN
1	A	1962	GLN
1	B	27	GLN
1	B	241	GLN
1	B	1336	GLN
1	B	1779	GLN
1	B	1810	ASN
1	B	1850	HIS
1	B	1962	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	$\# Z  > 2$
2	ADP	A	2001	3	22,29,29	1.36	2 (9%)	27,45,45	2.45	2 (7%)
2	ADP	B	2001	3	22,29,29	1.51	3 (13%)	27,45,45	2.30	3 (11%)

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
2	ADP	A	2001	3	-	0/12/32/32	0/3/3/3
2	ADP	B	2001	3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ADP	C8-N7	-2.56	1.29	1.34
2	A	2001	ADP	PB-O1B	2.88	1.60	1.51
2	B	2001	ADP	PB-O1B	3.05	1.61	1.51
2	A	2001	ADP	O4'-C1'	3.41	1.45	1.41
2	B	2001	ADP	O4'-C1'	3.96	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ADP	N3-C2-N1	-9.68	121.48	128.89
2	B	2001	ADP	N3-C2-N1	-8.72	122.22	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ADP	PA-O3A-PB	-6.70	110.20	132.67
2	B	2001	ADP	PA-O3A-PB	-6.53	110.77	132.67
2	B	2001	ADP	C4-C5-N7	-2.13	107.52	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	ADP	3	0
2	B	2001	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	591/613 (96%)	0.58	59 (9%) 9 7	10, 63, 109, 125	0
1	B	591/613 (96%)	0.51	52 (8%) 12 10	9, 61, 110, 128	0
All	All	1182/1226 (96%)	0.55	111 (9%) 11 8	9, 62, 110, 128	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	GLY	8.1
1	B	249	SER	7.8
1	A	249	SER	7.7
1	B	1315	GLY	6.7
1	B	146	HIS	6.5
1	A	1886	ILE	5.9
1	A	1315	GLY	5.4
1	A	177	PRO	5.4
1	B	179	GLN	5.4
1	B	147	PRO	5.1
1	A	1859	SER	4.9
1	B	1861	VAL	4.4
1	A	248	GLY	4.4
1	A	1810	ASN	4.4
1	A	147	PRO	4.3
1	A	176	LYS	4.3
1	A	1855	ARG	4.2
1	B	145	ILE	4.2
1	B	1291	TYR	4.2
1	B	181	ARG	4.1
1	A	155	TRP	4.1
1	A	1901	MET	4.1
1	B	150	MET	4.0
1	B	177	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	151	GLN	3.9
1	B	151	GLN	3.8
1	B	1901	MET	3.7
1	B	1849	ARG	3.7
1	A	1311	LYS	3.7
1	B	1317	ARG	3.7
1	B	178	GLY	3.6
1	B	1858	GLU	3.6
1	B	1311	LYS	3.6
1	B	1886	ILE	3.6
1	B	1857	GLY	3.6
1	B	1949	ALA	3.5
1	A	149	CYS	3.5
1	B	1852	LEU	3.5
1	A	159	GLU	3.5
1	B	148	ASP	3.4
1	A	1862	VAL	3.4
1	B	1850	HIS	3.2
1	B	149	CYS	3.2
1	A	143	LYS	3.2
1	B	1316	THR	3.2
1	B	1919	PRO	3.2
1	A	152	GLU	3.2
1	A	1852	LEU	3.1
1	A	1310	ARG	3.1
1	A	148	ASP	3.1
1	B	176	LYS	3.0
1	A	1843	ILE	3.0
1	A	1885	VAL	3.0
1	B	7	GLN	2.9
1	B	1853	ARG	2.9
1	A	1943	ILE	2.9
1	A	173	LYS	2.9
1	B	1859	SER	2.8
1	B	250	ARG	2.7
1	A	178	GLY	2.7
1	B	1346	PRO	2.7
1	B	1943	ILE	2.7
1	A	1346	PRO	2.7
1	A	1944	VAL	2.6
1	A	1289	ALA	2.6
1	A	1899	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1291	TYR	2.6
1	B	1310	ARG	2.5
1	A	7	GLN	2.5
1	A	1858	GLU	2.5
1	A	150	MET	2.5
1	B	172	PRO	2.5
1	B	1810	ASN	2.5
1	B	1904	SER	2.4
1	A	1273	ALA	2.4
1	B	157	GLU	2.4
1	B	1856	ARG	2.4
1	A	146	HIS	2.4
1	B	1841	ASP	2.4
1	A	172	PRO	2.4
1	A	1942	PRO	2.4
1	A	1850	HIS	2.4
1	A	1904	SER	2.4
1	A	181	ARG	2.3
1	A	1963	ILE	2.3
1	A	1340	TYR	2.3
1	B	1950	ARG	2.3
1	A	142	TYR	2.3
1	A	138	TYR	2.2
1	B	8	ILE	2.2
1	A	1274	LYS	2.2
1	A	1314	ASP	2.2
1	A	250	ARG	2.2
1	A	1939	ARG	2.2
1	B	1870	ILE	2.2
1	A	1292	GLY	2.1
1	B	1340	TYR	2.1
1	A	1313	PRO	2.1
1	B	159	GLU	2.1
1	B	1888	GLU	2.1
1	A	1947	GLU	2.1
1	B	173	LYS	2.1
1	B	1854	VAL	2.1
1	B	1267	GLN	2.1
1	A	144	HIS	2.1
1	A	1861	VAL	2.1
1	A	1965	MET	2.1
1	A	1278	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1849	ARG	2.0
1	A	1259	LEU	2.0
1	B	1948	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	A	2001	27/27	0.80	0.27	0.52	113,114,115,115	0
2	ADP	B	2001	27/27	0.81	0.27	0.35	118,121,127,128	0
4	ZN	A	2003	1/1	0.93	0.09	-1.80	163,163,163,163	0
4	ZN	B	2003	1/1	0.89	0.05	-2.28	169,169,169,169	0
5	CL	A	2006	1/1	0.99	0.22	-	41,41,41,41	0
5	CL	B	2004	1/1	0.96	0.23	-	48,48,48,48	0
5	CL	A	2004	1/1	0.97	0.25	-	48,48,48,48	0
5	CL	B	2006	1/1	0.92	0.09	-	39,39,39,39	0
5	CL	B	2005	1/1	0.96	0.17	-	53,53,53,53	0
3	MG	A	2002	1/1	0.95	0.13	-	64,64,64,64	0
5	CL	A	2005	1/1	0.96	0.21	-	59,59,59,59	0
3	MG	B	2002	1/1	0.93	0.19	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.