



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 PM GMT

PDB ID : 4JT5  
Title : mTORdeltaN-mLST8-pp242 complex  
Authors : Pavletich, N.P.; Yang, H.  
Deposited on : 2013-03-22  
Resolution : 3.45 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

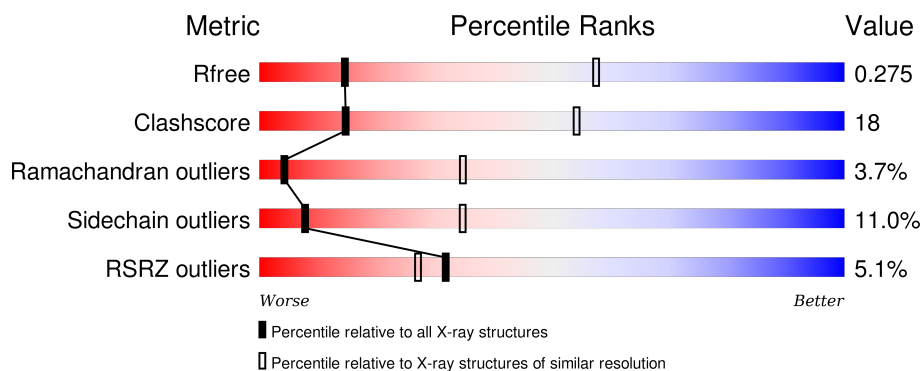
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	1174	<div> <div>7%</div> <div>56%</div> <div>29%</div> <div>10%</div> </div>
1	B	1174	<div> <div>4%</div> <div>55%</div> <div>29%</div> <div>5%</div> <div>10%</div> </div>
2	C	326	<div> <div>4%</div> <div>48%</div> <div>40%</div> <div>9%</div> <div>• •</div> </div>
2	D	326	<div> <div>%</div> <div>46%</div> <div>41%</div> <div>9%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22143 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

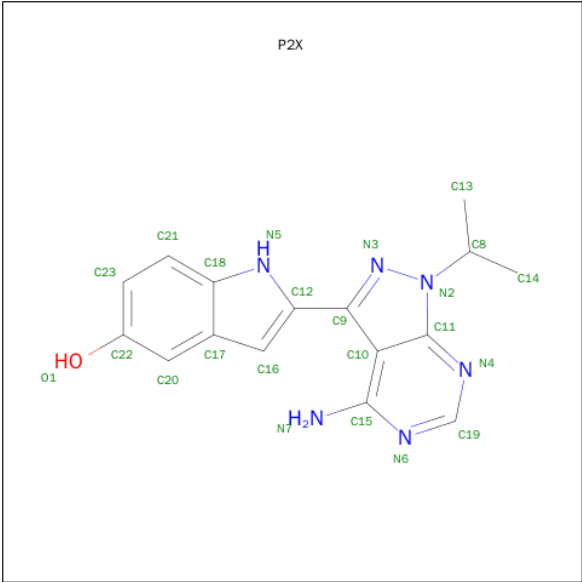
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	324	VAL	-	EXPRESSION TAG	UNP Q9BVC4
D	325	LEU	-	EXPRESSION TAG	UNP Q9BVC4
D	326	GLY	-	EXPRESSION TAG	UNP Q9BVC4
C	324	VAL	-	EXPRESSION TAG	UNP Q9BVC4
C	325	LEU	-	EXPRESSION TAG	UNP Q9BVC4
C	326	GLY	-	EXPRESSION TAG	UNP Q9BVC4

- Molecule 3 is 2-[4-AMINO-1-(PROPAN-2-YL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL]-1H-INDOL-5-OL (three-letter code: P2X) (formula: C<sub>16</sub>H<sub>16</sub>N<sub>6</sub>O).

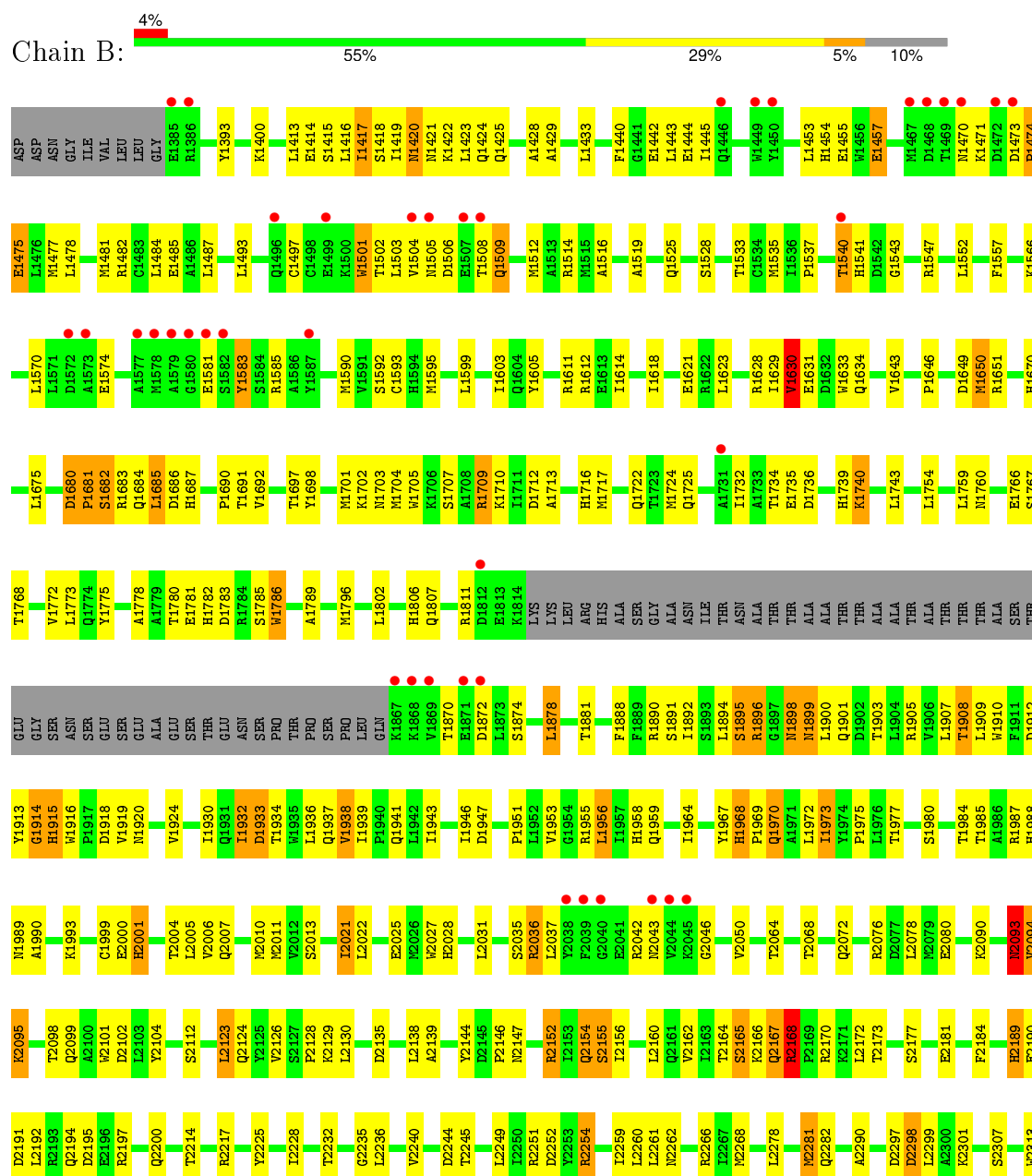


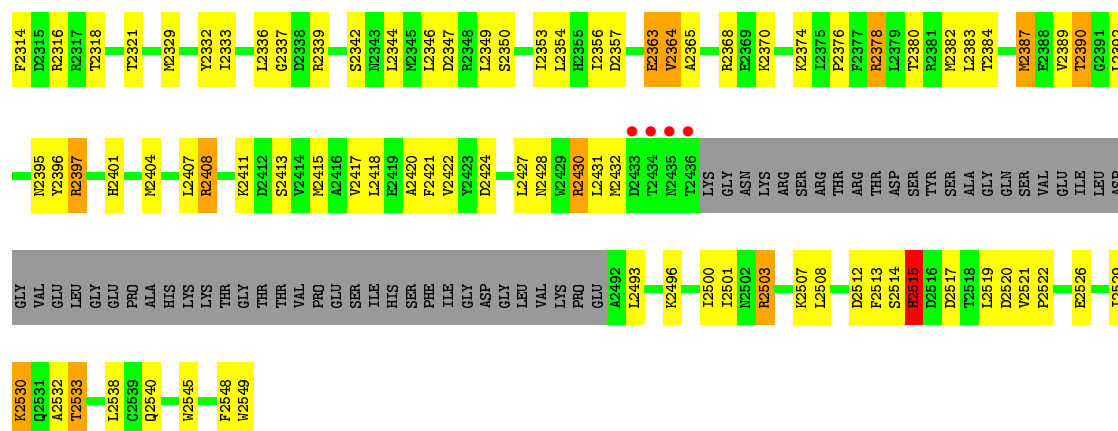
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			23	16	6	1		
3	A	1	Total	C	N	O	0	0
			23	16	6	1		

### 3 Residue-property plots

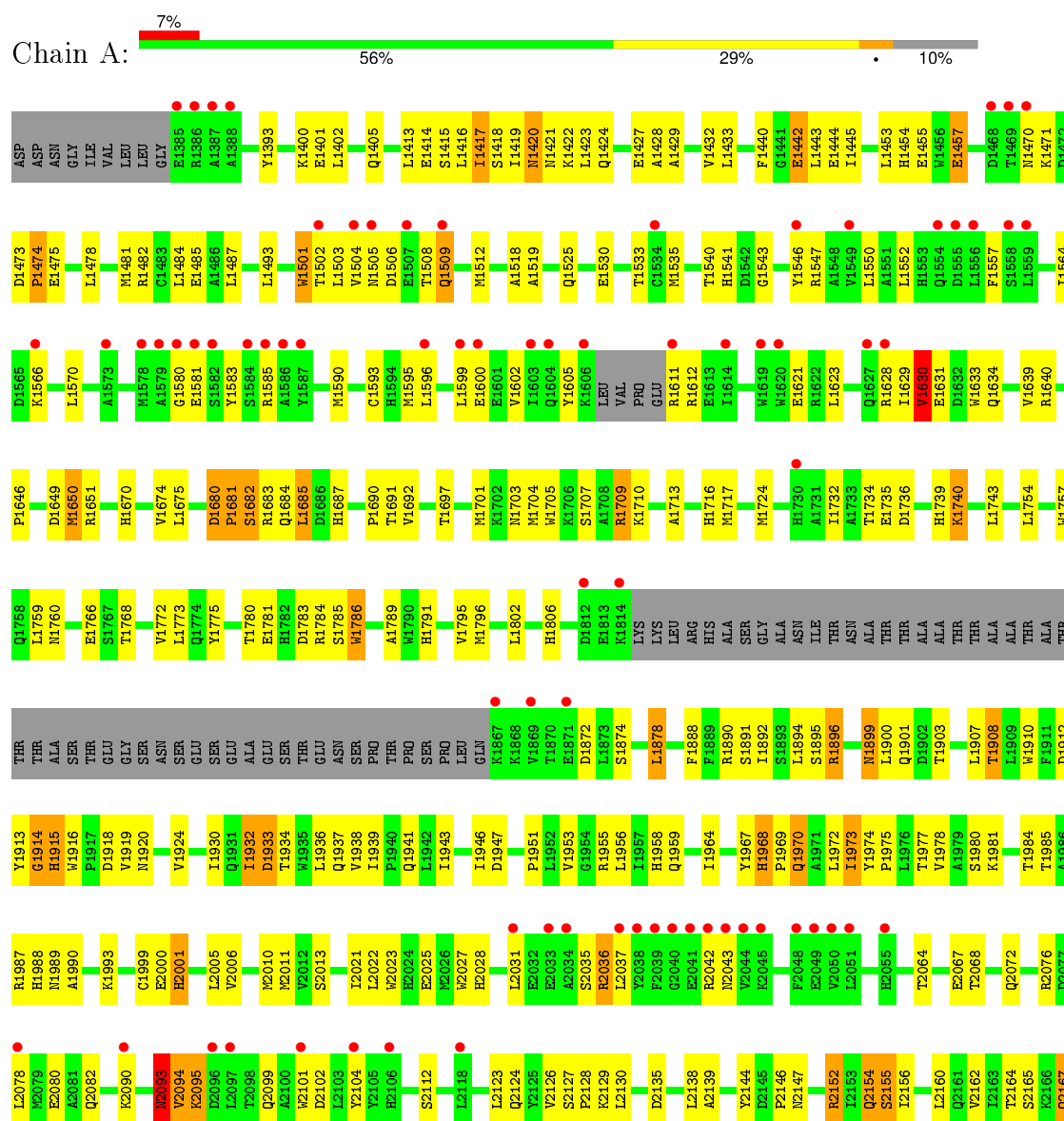
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Serine/threonine-protein kinase mTOR

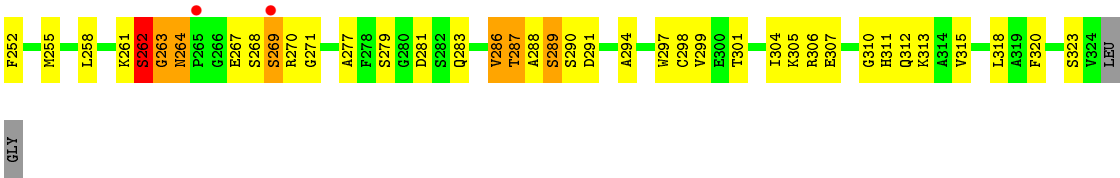




### • Molecule 1: Serine/threonine-protein kinase mTOR









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.40 Å   163.20 Å   207.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.67 – 3.45 39.64 – 3.43	Depositor EDS
% Data completeness (in resolution range)	85.8 (39.67-3.45) 85.2 (39.64-3.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.233   ,   0.271 0.235   ,   0.275	Depositor DCC
$R_{free}$ test set	1858 reflections (3.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 61679 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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 41.10 % 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 2.4826e-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, 0.375 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: P2X

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	0.35	0/8772	0.60	1/11872 (0.0%)
1	B	0.35	0/8805	0.61	1/11920 (0.0%)
2	C	0.38	0/2514	0.67	0/3426
2	D	0.41	0/2514	0.69	0/3426
All	All	0.36	0/22605	0.62	2/30644 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1915	HIS	N-CA-C	5.58	126.08	111.00
1	B	1915	HIS	N-CA-C	5.40	125.57	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1442	GLU	Peptide
1	A	1914	GLY	Peptide
1	B	1914	GLY	Peptide
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	8577	0	8559	262	0
1	B	8608	0	8593	263	0
2	C	2456	0	2341	131	0
2	D	2456	0	2341	137	0
3	A	23	0	16	3	0
3	B	23	0	16	4	0
All	All	22143	0	21866	784	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 18.

All (784) 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:C:76:ASN:HB3	2:C:77:PRO:HD2	1.35	1.09
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.05
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.36	1.04
2:D:170:GLU:OE2	2:D:170:GLU:HA	1.61	0.98
2:C:170:GLU:OE2	2:C:170:GLU:HA	1.62	0.96
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.50	0.94
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.94
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.48	0.93
2:C:95:GLU:HB2	2:C:140:GLN:NE2	1.85	0.91
2:D:95:GLU:HB2	2:D:140:GLN:NE2	1.86	0.90
2:D:117:ARG:O	2:D:118:ASN:HB2	1.73	0.89
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.56	0.87
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.37	0.86
2:C:117:ARG:O	2:C:118:ASN:HB2	1.74	0.86
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.54	0.86
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.11	0.85
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.06	0.85
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.58	0.84
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.77	0.83
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.78	0.83
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.41	0.82
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.61	0.82
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.08	0.82
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.61	0.82
1:A:2390:THR:HG23	1:A:2390:THR:O	1.80	0.81
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.61	0.80
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.61	0.80
2:C:63:GLN:HE21	2:C:86:LYS:H	1.27	0.80
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.61	0.80
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.17	0.80
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.82	0.79
3:B:2601:P2X:C16	3:B:2601:P2X:H15	1.96	0.79
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.83	0.79
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.15	0.78
1:A:2387:MET:CE	1:A:2396:TYR:HB2	2.13	0.78
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.66	0.78
1:B:2387:MET:CE	1:B:2396:TYR:HB2	2.14	0.78
2:D:63:GLN:HE21	2:D:86:LYS:H	1.29	0.77
1:B:2390:THR:O	1:B:2390:THR:HG23	1.84	0.76
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.66	0.76
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.67	0.76
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.66	0.76
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	1.87	0.75
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.67	0.75
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.66	0.74
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.19	0.74
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.68	0.74
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.70	0.74
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.68	0.74
3:B:2601:P2X:H15	3:B:2601:P2X:H5	1.52	0.73
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.23	0.73
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.71	0.73
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.70	0.72
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.19	0.72
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.72	0.72
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.72	0.71
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.53	0.71
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.91	0.70
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.37	0.70
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.21	0.70
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.73	0.70
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.73	0.70
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.56	0.70
2:D:17:THR:HB	2:D:311:HIS:HE1	1.56	0.70
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.74	0.69
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.74	0.69
2:D:137:HIS:CD2	2:D:138:PRO:HD2	2.27	0.69
1:A:1415:SER:O	1:A:1419:ILE:HG22	1.93	0.69
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.74	0.69
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.26	0.69
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.76	0.68
2:D:241:ASP:OD2	2:D:243:THR:HB	1.94	0.68
1:B:1415:SER:O	1:B:1419:ILE:HG22	1.94	0.68
2:C:231:ASP:CB	2:C:233:THR:OG1	2.41	0.67
1:A:1920:ASN:O	1:A:1924:VAL:HG23	1.94	0.67
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.93	0.67
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.76	0.67
1:A:1508:THR:O	1:A:1512:MET:HB2	1.94	0.67
2:D:17:THR:HB	2:D:311:HIS:CE1	2.30	0.67
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.95	0.67
1:B:1920:ASN:O	1:B:1924:VAL:HG23	1.93	0.67
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	1.77	0.67
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.14	0.67
1:B:1508:THR:O	1:B:1512:MET:HB2	1.93	0.67
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.76	0.67
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.77	0.67
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.75	0.66
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.15	0.66
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.78	0.66
1:B:1680:ASP:O	1:B:1682:SER:N	2.28	0.66
1:B:2514:SER:OG	1:B:2517:ASP:HB2	1.96	0.66
2:D:306:ARG:HG2	2:D:307:GLU:H	1.60	0.66
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.77	0.66
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.30	0.66
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.24	0.66
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.76	0.65
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.30	0.65
1:A:1393:TYR:CZ	1:A:1422:LYS:HD2	2.32	0.65
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.96	0.65
1:A:1874:SER:O	1:A:1878:LEU:HB2	1.96	0.65
1:A:1680:ASP:O	1:A:1682:SER:N	2.29	0.65
2:D:231:ASP:CB	2:D:233:THR:OG1	2.45	0.64
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	1.97	0.64
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.45	0.64
2:C:306:ARG:HG2	2:C:307:GLU:H	1.62	0.64
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	1.78	0.64
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.97	0.64
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.28	0.64
2:D:55:SER:O	2:D:56:MET:HG2	1.97	0.64
2:C:279:SER:HA	2:C:320:PHE:HE2	1.62	0.64
1:A:1734:THR:O	1:A:1736:ASP:N	2.25	0.64
3:A:2601:P2X:H5	3:A:2601:P2X:H15	1.63	0.64
2:C:137:HIS:CD2	2:C:138:PRO:HD2	2.32	0.64
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.62	0.64
1:A:2130:LEU:HD22	1:A:2156:ILE:CD1	2.28	0.64
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.28	0.63
2:C:17:THR:HB	2:C:311:HIS:HE1	1.63	0.63
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.31	0.63
1:A:1913:TYR:O	1:A:1915:HIS:HA	1.97	0.63
2:C:166:ILE:HG13	2:C:166:ILE:O	1.97	0.63
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.81	0.63
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.34	0.63
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.63	0.63
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.99	0.63
2:D:279:SER:HA	2:D:320:PHE:HE2	1.63	0.63
1:A:1783:ASP:O	1:A:1785:SER:N	2.32	0.63
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.62	0.62
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.79	0.62
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.80	0.62
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.81	0.62
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	1.97	0.62
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.81	0.62
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.47	0.62
1:B:1701:MET:HE1	1:B:1717:MET:N	2.15	0.62
1:A:2503:ARG:HH11	1:A:2507:LYS:HE3	1.64	0.62
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.32	0.62
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.63	0.62
1:B:1646:PRO:HG3	1:B:1675:LEU:HD21	1.82	0.62
1:A:2390:THR:CG2	1:A:2390:THR:O	2.47	0.62
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.35	0.62
2:C:17:THR:HB	2:C:311:HIS:CE1	2.35	0.62
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.82	0.62
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.33	0.61
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.35	0.61
2:C:241:ASP:OD2	2:C:243:THR:HB	1.99	0.61
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.33	0.61
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.35	0.61
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.47	0.61
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.29	0.61
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.81	0.61
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.81	0.61
1:B:2194:GLN:HG2	1:B:2427:LEU:HD22	1.82	0.61
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.36	0.61
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.28	0.61
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	1.97	0.61
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.30	0.61
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.35	0.61
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.82	0.61
1:B:2251:ARG:NH1	1:B:2252:ASP:OD1	2.34	0.61
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.01	0.61
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.01	0.61
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.16	0.60
1:A:1701:MET:HE1	1:A:1717:MET:N	2.17	0.60
1:B:1874:SER:O	1:B:1878:LEU:HB2	2.01	0.60
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.36	0.60
1:B:2281:MET:HA	1:B:2281:MET:CE	2.31	0.60
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.02	0.60
2:C:248:ARG:HD2	2:C:255:MET:HB2	1.84	0.60
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.83	0.60
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.34	0.60
1:B:1783:ASP:O	1:B:1785:SER:N	2.35	0.59
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.02	0.59
2:D:128:ASN:H	2:D:128:ASN:ND2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.83	0.59
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.02	0.59
1:A:2415:MET:CE	1:A:2501:ILE:HG23	2.31	0.59
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.84	0.59
2:D:21:ASP:HB3	2:D:313:LYS:H	1.67	0.59
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.67	0.59
1:B:1785:SER:O	1:B:1786:TRP:CB	2.48	0.59
2:D:133:CYS:SG	2:D:175:SER:HA	2.42	0.59
1:B:2167:GLN:O	1:B:2168:ARG:C	2.40	0.59
3:B:2601:P2X:N7	3:B:2601:P2X:H5	2.17	0.59
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.84	0.59
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.01	0.59
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.03	0.59
1:A:2515:HIS:N	1:A:2515:HIS:ND1	2.49	0.59
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.33	0.58
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.85	0.58
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.04	0.58
1:A:1680:ASP:C	1:A:1682:SER:N	2.56	0.58
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.85	0.58
2:C:21:ASP:HB3	2:C:313:LYS:H	1.68	0.58
2:D:166:ILE:HG13	2:D:166:ILE:O	2.02	0.58
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.84	0.58
1:A:1785:SER:O	1:A:1786:TRP:CB	2.49	0.58
1:A:1583:TYR:C	1:A:1585:ARG:H	2.06	0.58
1:A:2415:MET:HE2	1:A:2501:ILE:HG23	1.86	0.58
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.86	0.58
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.01	0.58
2:C:55:SER:O	2:C:56:MET:HG2	2.03	0.58
1:B:2154:GLN:HE21	1:B:2155:SER:HB3	1.68	0.58
1:B:2503:ARG:HH11	1:B:2507:LYS:HE3	1.69	0.58
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.85	0.58
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.34	0.57
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.19	0.57
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.69	0.57
2:C:133:CYS:SG	2:C:175:SER:HA	2.43	0.57
1:B:2390:THR:O	1:B:2390:THR:CG2	2.52	0.57
1:A:2240:VAL:HG23	3:A:2601:P2X:N6	2.20	0.57
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.87	0.57
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.17	0.57
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.86	0.57
2:C:128:ASN:ND2	2:C:128:ASN:H	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.86	0.57
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.86	0.57
3:A:2601:P2X:C16	3:A:2601:P2X:H15	2.17	0.57
1:B:1680:ASP:C	1:B:1682:SER:N	2.57	0.57
1:A:1475:GLU:HA	1:A:1478:LEU:HD12	1.86	0.57
1:A:2251:ARG:HA	1:A:2261:LEU:CD1	2.35	0.57
1:A:2408:ARG:HG2	1:A:2508:LEU:O	2.05	0.56
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.86	0.56
1:B:2130:LEU:HD22	1:B:2156:ILE:CD1	2.34	0.56
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.06	0.56
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.05	0.56
1:A:1414:GLU:O	1:A:1417:ILE:HG13	2.05	0.56
1:A:1646:PRO:HG3	1:A:1675:LEU:HD21	1.88	0.56
2:C:96:ASP:O	2:C:98:ARG:N	2.37	0.56
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.88	0.56
1:A:2154:GLN:HE21	1:A:2155:SER:HB3	1.70	0.56
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.05	0.56
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.86	0.56
1:B:2503:ARG:HH11	1:B:2507:LYS:CE	2.19	0.56
2:C:279:SER:HA	2:C:320:PHE:CE2	2.41	0.56
2:D:107:CYS:HB3	2:D:127:VAL:O	2.05	0.56
1:A:2152:ARG:HG2	1:A:2177:SER:OG	2.06	0.56
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.88	0.56
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	1.87	0.56
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.88	0.56
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.87	0.56
1:B:1583:TYR:C	1:B:1585:ARG:H	2.08	0.56
1:A:2167:GLN:O	1:A:2168:ARG:C	2.43	0.56
1:B:1802:LEU:HD22	1:B:1806:HIS:NE2	2.20	0.56
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.88	0.55
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.36	0.55
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.53	0.55
1:B:2251:ARG:HA	1:B:2261:LEU:CD1	2.36	0.55
2:D:268:SER:O	2:D:269:SER:HB3	2.07	0.55
1:B:1703:ASN:O	1:B:1707:SER:HB2	2.05	0.55
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.89	0.55
2:C:36:ARG:NH2	2:C:69:ASP:O	2.39	0.55
1:B:2415:MET:CE	1:B:2501:ILE:HG23	2.36	0.55
1:B:2387:MET:HE1	1:B:2396:TYR:HB2	1.87	0.55
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.88	0.55
1:B:1475:GLU:HA	1:B:1478:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.42	0.55
2:C:268:SER:O	2:C:269:SER:HB3	2.07	0.55
1:A:1951:PRO:HB2	1:A:1955:ARG:HH21	1.72	0.55
2:C:286:VAL:HB	2:C:318:LEU:HD13	1.89	0.55
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.05	0.54
2:D:196:VAL:HG11	2:D:252:PHE:CZ	2.42	0.54
2:D:279:SER:HA	2:D:320:PHE:CE2	2.43	0.54
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.42	0.54
2:C:65:ILE:HD11	2:C:88:ILE:HD13	1.89	0.54
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.89	0.54
1:A:1552:LEU:HD22	1:A:1602:VAL:HG12	1.89	0.54
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.89	0.54
2:D:96:ASP:O	2:D:98:ARG:N	2.35	0.54
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.07	0.54
1:A:2298:ASP:HB2	1:A:2382:MET:HE1	1.89	0.54
2:D:65:ILE:HD11	2:D:88:ILE:HD13	1.89	0.54
2:C:246:ILE:HD13	2:C:299:VAL:HG13	1.88	0.54
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.07	0.53
2:D:246:ILE:HD13	2:D:299:VAL:HG13	1.90	0.53
1:B:1781:GLU:HA	1:B:1781:GLU:OE1	2.07	0.53
1:B:1414:GLU:O	1:B:1417:ILE:HG13	2.07	0.53
1:B:1766:GLU:N	1:B:1766:GLU:OE1	2.42	0.53
1:A:1422:LYS:C	1:A:1424:GLN:H	2.12	0.53
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.89	0.53
1:A:2251:ARG:NH1	1:A:2252:ASP:OD1	2.42	0.53
1:B:1773:LEU:HG	1:B:1796:MET:HG3	1.91	0.53
2:D:128:ASN:O	2:D:129:ALA:HB3	2.08	0.53
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.09	0.53
2:C:168:GLU:N	2:C:169:PRO:HD2	2.24	0.53
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.89	0.53
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.91	0.53
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.38	0.53
1:A:1401:GLU:HG2	1:A:2389:VAL:HG22	1.90	0.53
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.09	0.53
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.91	0.53
2:D:267:GLU:HG3	2:D:267:GLU:O	2.09	0.53
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.09	0.53
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.44	0.52
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.09	0.52
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.37	0.52
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:GLY:O	2:C:203:ILE:O	2.28	0.52
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.91	0.52
1:A:2192:LEU:HD12	1:A:2235:GLY:CA	2.37	0.52
2:C:128:ASN:O	2:C:129:ALA:HB3	2.09	0.52
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.74	0.52
1:A:2512:ASP:N	1:A:2512:ASP:OD1	2.43	0.52
1:B:1422:LYS:C	1:B:1424:GLN:H	2.13	0.52
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.74	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.92	0.52
2:C:267:GLU:O	2:C:267:GLU:HG3	2.10	0.52
1:B:1552:LEU:HD11	1:B:1603:ILE:HG13	1.90	0.52
1:B:2417:VAL:O	1:B:2420:ALA:HB3	2.09	0.52
2:C:60:ALA:HB1	2:C:88:ILE:HG22	1.91	0.52
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.43	0.52
2:C:137:HIS:CD2	2:C:139:ASN:H	2.28	0.52
2:C:74:ASN:H	2:C:75:PRO:HD3	1.75	0.52
1:A:1999:CYS:C	1:A:2001:HIS:H	2.12	0.52
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.13	0.52
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.26	0.52
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.92	0.52
2:D:36:ARG:NH2	2:D:69:ASP:O	2.43	0.51
1:A:1649:ASP:O	1:A:1651:ARG:N	2.44	0.51
2:C:200:THR:O	2:C:208:THR:HA	2.11	0.51
1:A:2281:MET:CE	1:A:2281:MET:HA	2.40	0.51
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.45	0.51
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.93	0.51
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.92	0.51
1:A:1754:LEU:HD13	1:A:1775:TYR:CE2	2.45	0.51
2:D:137:HIS:CD2	2:D:139:ASN:H	2.28	0.51
2:C:202:GLY:HA3	2:C:208:THR:H	1.76	0.51
1:A:2152:ARG:HG2	1:A:2177:SER:CB	2.41	0.51
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.11	0.51
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.14	0.51
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.92	0.51
2:C:95:GLU:CB	2:C:140:GLN:HE22	2.15	0.51
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.46	0.51
1:B:2281:MET:HE2	1:B:2281:MET:HA	1.93	0.51
1:A:1802:LEU:HD22	1:A:1806:HIS:NE2	2.25	0.51
2:C:128:ASN:O	2:C:129:ALA:CB	2.59	0.51
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2417:VAL:O	1:A:2420:ALA:HB3	2.11	0.51
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.92	0.51
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.93	0.51
2:D:82:ASP:H	2:D:119:LEU:HD22	1.76	0.51
1:B:2408:ARG:HG2	1:B:2508:LEU:O	2.10	0.51
2:D:168:GLU:N	2:D:169:PRO:HD2	2.26	0.51
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.11	0.51
2:D:137:HIS:CD2	2:D:138:PRO:CD	2.94	0.51
2:D:202:GLY:O	2:D:203:ILE:O	2.29	0.51
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.93	0.51
2:C:262:SER:OG	2:C:267:GLU:HG2	2.11	0.51
1:A:1999:CYS:C	1:A:2001:HIS:N	2.64	0.51
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.91	0.51
2:C:14:ILE:HD13	2:C:70:LEU:HD13	1.92	0.50
1:B:1951:PRO:HB2	1:B:1955:ARG:HH21	1.76	0.50
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.93	0.50
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.93	0.50
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.92	0.50
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.75	0.50
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	1.94	0.50
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.12	0.50
2:C:107:CYS:HB3	2:C:127:VAL:O	2.11	0.50
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.92	0.50
2:C:72:SER:O	2:C:74:ASN:N	2.45	0.50
2:C:207:VAL:HG12	2:C:209:GLN:HG2	1.94	0.50
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.92	0.50
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.94	0.50
1:A:1781:GLU:OE1	1:A:1781:GLU:HA	2.11	0.50
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.76	0.50
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.22	0.50
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.93	0.50
2:D:207:VAL:HG12	2:D:209:GLN:HG2	1.94	0.50
2:D:137:HIS:HD2	2:D:138:PRO:N	2.10	0.50
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.93	0.50
1:B:2027:TRP:O	1:B:2031:LEU:HG	2.11	0.50
1:B:2512:ASP:N	1:B:2512:ASP:OD1	2.41	0.50
1:A:1766:GLU:N	1:A:1766:GLU:OE1	2.45	0.50
2:C:63:GLN:NE2	2:C:86:LYS:H	2.04	0.49
1:B:1605:TYR:CZ	1:B:1612:ARG:HG2	2.46	0.49
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.46	0.49
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:THR:O	2:D:208:THR:HA	2.12	0.49
2:D:277:ALA:O	2:D:286:VAL:HG23	2.12	0.49
2:D:74:ASN:H	2:D:75:PRO:HD3	1.78	0.49
1:B:1649:ASP:O	1:B:1651:ARG:N	2.45	0.49
1:B:2298:ASP:HB2	1:B:2382:MET:HE1	1.92	0.49
2:C:277:ALA:O	2:C:286:VAL:HG23	2.12	0.49
2:D:202:GLY:HA3	2:D:208:THR:H	1.78	0.49
1:A:2006:VAL:O	1:A:2010:MET:HB2	2.12	0.49
2:D:63:GLN:NE2	2:D:86:LYS:H	2.05	0.49
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.48	0.49
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.47	0.49
2:C:248:ARG:O	2:C:252:PHE:N	2.44	0.49
1:A:1605:TYR:CZ	1:A:1612:ARG:HG2	2.47	0.49
1:B:1754:LEU:HD13	1:B:1775:TYR:CE2	2.47	0.49
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.95	0.49
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.13	0.49
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.10	0.49
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.49
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.96	0.49
1:B:2415:MET:HE2	1:B:2501:ILE:HG23	1.95	0.49
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.13	0.49
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	1.94	0.49
2:D:72:SER:O	2:D:74:ASN:N	2.46	0.48
1:A:1786:TRP:CE3	1:A:1789:ALA:HB2	2.48	0.48
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.48	0.48
1:B:2374:LYS:HE3	1:B:2540:GLN:OE1	2.13	0.48
2:D:128:ASN:O	2:D:129:ALA:CB	2.62	0.48
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.13	0.48
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.95	0.48
2:C:82:ASP:H	2:C:119:LEU:HD22	1.79	0.48
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.48	0.48
1:B:1543:GLY:O	1:B:1547:ARG:HD2	2.13	0.48
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.28	0.48
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	1.94	0.48
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.48	0.48
1:B:1999:CYS:C	1:B:2001:HIS:H	2.16	0.48
2:C:287:THR:O	2:C:294:ALA:HA	2.14	0.48
1:A:1681:PRO:O	1:A:1682:SER:C	2.52	0.48
1:B:1999:CYS:C	1:B:2001:HIS:N	2.67	0.48
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.14	0.48
1:B:1958:HIS:HE1	1:B:1990:ALA:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2520:ASP:OD2	1:B:2522:PRO:HD2	2.13	0.48
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.79	0.48
1:A:1972:LEU:O	1:A:1975:PRO:HG2	2.14	0.48
1:A:1543:GLY:O	1:A:1547:ARG:HD2	2.13	0.48
1:B:2152:ARG:HG2	1:B:2177:SER:OG	2.14	0.48
2:D:130:PRO:HD2	2:D:148:GLN:HB2	1.95	0.47
1:B:1418:SER:HB2	1:B:1581:GLU:HG2	1.96	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.95	0.47
1:A:2281:MET:HE2	1:A:2281:MET:HA	1.95	0.47
1:B:2154:GLN:NE2	1:B:2155:SER:HB3	2.28	0.47
1:B:1417:ILE:O	1:B:1421:ASN:ND2	2.47	0.47
1:B:2382:MET:SD	1:B:2549:TRP:HA	2.54	0.47
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.97	0.47
2:C:159:THR:C	2:C:161:HIS:H	2.16	0.47
2:C:68:TYR:HE2	2:C:77:PRO:HD3	1.79	0.47
2:C:69:ASP:HB3	2:C:72:SER:OG	2.14	0.47
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.15	0.47
1:A:1773:LEU:HG	1:A:1796:MET:HG3	1.96	0.47
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.15	0.47
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.96	0.47
1:B:1973:ILE:HG13	1:B:1973:ILE:H	1.47	0.47
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.79	0.47
1:B:1416:LEU:O	1:B:1420:ASN:HB2	2.14	0.47
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.96	0.47
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.14	0.47
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	1.97	0.47
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.79	0.47
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.78	0.47
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.79	0.47
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.49	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB3	2.29	0.47
1:B:1915:HIS:HE1	1:B:1919:VAL:CG1	2.28	0.47
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.97	0.47
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.15	0.47
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.97	0.47
1:A:1691:THR:HG22	1:A:1691:THR:O	2.15	0.47
1:A:2411:LYS:O	1:A:2415:MET:HG3	2.15	0.47
1:B:2347:ASP:OD1	1:B:2350:SER:OG	2.27	0.47
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.49	0.47
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.79	0.47
1:B:1932:ILE:HD12	1:B:1933:ASP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.97	0.46
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.97	0.46
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.96	0.46
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.79	0.46
1:A:2245:THR:O	1:A:2249:LEU:HD12	2.15	0.46
2:D:154:ILE:HD11	2:D:210:LEU:HD11	1.97	0.46
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.30	0.46
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.50	0.46
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.46
1:B:1566:LYS:O	1:B:1570:LEU:HG	2.14	0.46
2:C:168:GLU:HG2	2:C:169:PRO:N	2.30	0.46
1:B:1691:THR:O	1:B:1691:THR:HG22	2.15	0.46
1:A:2382:MET:SD	1:A:2549:TRP:HA	2.56	0.46
2:D:167:PRO:HD2	2:D:169:PRO:CG	2.43	0.46
1:A:1401:GLU:HG2	1:A:2389:VAL:CG2	2.46	0.46
1:B:1786:TRP:CE3	1:B:1789:ALA:HB2	2.50	0.46
2:C:225:GLN:HG2	2:C:226:CYS:N	2.30	0.46
1:A:1482:ARG:HA	1:A:1485:GLU:HG2	1.97	0.46
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.97	0.46
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.98	0.46
1:B:1734:THR:O	1:B:1736:ASP:N	2.40	0.46
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.36	0.46
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.77	0.46
1:B:1477:MET:HE2	1:B:1477:MET:HB3	1.89	0.46
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.81	0.46
1:B:1537:PRO:O	1:B:1543:GLY:HA3	2.15	0.46
1:B:2006:VAL:O	1:B:2010:MET:HB2	2.15	0.46
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.79	0.46
1:A:2333:ILE:CD1	1:A:2407:LEU:HD13	2.46	0.46
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	1.98	0.46
1:A:2214:THR:O	1:A:2217:ARG:HB3	2.16	0.46
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.56	0.46
2:C:255:MET:HE1	2:C:299:VAL:HG12	1.96	0.46
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	1.97	0.46
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.16	0.46
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.81	0.46
2:C:159:THR:HB	2:C:161:HIS:HB2	1.97	0.46
2:D:225:GLN:HG2	2:D:226:CYS:N	2.30	0.46
1:A:2201:LEU:O	1:A:2205:VAL:HG23	2.15	0.46
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.31	0.45
2:D:95:GLU:CB	2:D:140:GLN:HE22	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.69	0.45
1:B:1482:ARG:HA	1:B:1485:GLU:HG2	1.97	0.45
2:D:262:SER:OG	2:D:267:GLU:HG2	2.16	0.45
1:B:2152:ARG:HE	1:B:2152:ARG:HB3	1.61	0.45
1:B:2152:ARG:HG2	1:B:2177:SER:CB	2.46	0.45
1:A:2184:PHE:HB3	1:A:2236:LEU:HD22	1.98	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.99	0.45
2:D:17:THR:HG1	2:D:27:TRP:HE1	1.63	0.45
1:B:1915:HIS:CE1	1:B:1919:VAL:CG1	2.99	0.45
1:A:1697:THR:O	1:A:1701:MET:HG3	2.16	0.45
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.79	0.45
2:D:115:ARG:O	2:D:116:SER:HB3	2.17	0.45
2:C:137:HIS:CD2	2:C:138:PRO:CD	2.99	0.45
1:A:2333:ILE:HD12	1:A:2407:LEU:HD13	1.98	0.45
1:B:2214:THR:O	1:B:2217:ARG:HB3	2.16	0.45
1:A:1964:ILE:O	1:A:1967:TYR:O	2.35	0.45
2:C:63:GLN:HE21	2:C:86:LYS:N	2.05	0.45
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.81	0.45
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.70	0.45
1:A:1910:TRP:C	1:A:1910:TRP:CD1	2.90	0.45
1:A:1413:LEU:O	1:A:1417:ILE:HG12	2.16	0.45
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.32	0.45
1:B:2418:LEU:O	1:B:2422:VAL:HG23	2.17	0.45
2:D:248:ARG:O	2:D:252:PHE:HA	2.17	0.45
1:B:1932:ILE:O	1:B:1933:ASP:C	2.55	0.45
1:A:2027:TRP:O	1:A:2031:LEU:HG	2.16	0.45
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.17	0.45
2:D:306:ARG:HG2	2:D:307:GLU:N	2.29	0.45
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.17	0.45
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.37	0.45
2:D:287:THR:O	2:D:294:ALA:HA	2.17	0.45
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	3.00	0.45
2:C:16:ALA:O	2:C:318:LEU:HA	2.17	0.45
2:D:16:ALA:O	2:D:318:LEU:HA	2.17	0.45
1:B:1697:THR:O	1:B:1701:MET:HG3	2.17	0.45
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.47	0.45
2:C:159:THR:C	2:C:161:HIS:N	2.70	0.45
1:B:1629:ILE:O	1:B:1630:VAL:C	2.56	0.45
2:D:231:ASP:HB2	2:D:233:THR:H	1.82	0.44
2:C:137:HIS:HD2	2:C:138:PRO:N	2.16	0.44
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.81	0.44
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.17	0.44
1:B:1506:ASP:HA	1:B:1509:GLN:HB2	1.99	0.44
1:A:2210:ALA:O	1:A:2216:LEU:HD22	2.17	0.44
2:D:69:ASP:HB3	2:D:72:SER:OG	2.17	0.44
1:B:2316:ARG:NH2	1:B:2349:LEU:HD23	2.32	0.44
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.99	0.44
1:A:2192:LEU:HD21	1:A:2237:ILE:HD11	1.99	0.44
1:A:1674:VAL:HG11	1:A:1681:PRO:HD3	1.99	0.44
1:A:2260:LEU:HD12	1:A:2261:LEU:N	2.32	0.44
1:B:1605:TYR:CE2	1:B:1612:ARG:HG2	2.53	0.44
1:B:1881:THR:HG23	1:B:1909:LEU:HD22	2.00	0.44
2:D:239:SER:OG	2:D:240:ALA:N	2.50	0.44
1:A:2363:GLU:OE1	1:A:2363:GLU:HA	2.18	0.44
1:B:2281:MET:HE2	1:B:2281:MET:CA	2.48	0.44
2:D:21:ASP:HB3	2:D:313:LYS:HB2	1.99	0.44
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.50	0.44
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.99	0.44
1:A:1629:ILE:O	1:A:1630:VAL:C	2.55	0.44
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.57	0.44
2:C:28:GLN:HG3	2:C:28:GLN:O	2.17	0.44
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.52	0.44
1:B:1621:GLU:C	1:B:1623:LEU:H	2.20	0.44
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.53	0.44
1:A:1970:GLN:HA	1:A:1973:ILE:HD11	2.00	0.44
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.98	0.44
1:B:1681:PRO:O	1:B:1682:SER:C	2.56	0.44
1:A:2401:HIS:CD2	1:A:2522:PRO:HA	2.52	0.44
1:A:2261:LEU:HD23	1:A:2262:ASN:ND2	2.32	0.44
1:A:1506:ASP:HA	1:A:1509:GLN:HB2	1.99	0.44
1:B:1712:ASP:OD1	1:A:2266:ARG:NH2	2.50	0.44
2:D:159:THR:HB	2:D:161:HIS:HB2	1.99	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.98	0.44
1:A:2021:ILE:HG22	1:A:2025:GLU:HB2	1.99	0.44
1:B:1964:ILE:O	1:B:1967:TYR:O	2.35	0.44
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.34	0.44
2:D:255:MET:HE1	2:D:299:VAL:HG12	1.99	0.44
1:A:1621:GLU:C	1:A:1623:LEU:H	2.20	0.44
2:D:102:THR:O	2:D:109:ALA:HA	2.17	0.44
2:D:159:THR:C	2:D:161:HIS:N	2.71	0.44
1:B:2316:ARG:HH21	1:B:2349:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.99	0.44
1:A:2281:MET:HE2	1:A:2281:MET:CA	2.48	0.43
1:B:1413:LEU:O	1:B:1417:ILE:HG12	2.17	0.43
2:C:263:GLY:O	2:C:264:ASN:HB3	2.18	0.43
2:D:14:ILE:HD13	2:D:70:LEU:HD13	1.99	0.43
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.18	0.43
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.43
1:A:1505:ASN:CB	1:A:1508:THR:HB	2.49	0.43
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.53	0.43
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	1.99	0.43
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.82	0.43
1:B:1453:LEU:O	1:B:1455:GLU:N	2.52	0.43
1:B:1605:TYR:HD2	1:B:1605:TYR:O	2.01	0.43
1:B:1899:ASN:O	1:B:1900:LEU:C	2.55	0.43
1:A:1416:LEU:O	1:A:1420:ASN:HB2	2.18	0.43
1:A:2332:TYR:O	1:A:2507:LYS:NZ	2.36	0.43
1:B:1691:THR:HG23	1:B:1724:MET:HE1	2.00	0.43
2:C:115:ARG:O	2:C:116:SER:HB3	2.19	0.43
1:A:1682:SER:O	1:A:1685:LEU:HD12	2.19	0.43
1:B:1705:TRP:CZ2	1:B:1710:LYS:HD2	2.54	0.43
2:C:231:ASP:HB2	2:C:233:THR:H	1.84	0.43
1:A:2042:ARG:HA	1:A:2042:ARG:HD3	1.87	0.43
2:C:151:ALA:HA	2:C:166:ILE:HG22	2.01	0.43
1:B:1878:LEU:HD21	1:B:1918:ASP:CB	2.47	0.43
1:B:2401:HIS:CD2	1:B:2522:PRO:HA	2.53	0.43
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.18	0.43
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	2.01	0.43
1:B:2036:ARG:HD3	1:B:2036:ARG:HA	1.62	0.43
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.53	0.43
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.83	0.43
1:B:2387:MET:HE1	1:B:2396:TYR:CB	2.49	0.43
1:A:1415:SER:O	1:A:1419:ILE:CG2	2.65	0.43
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.19	0.43
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.99	0.43
2:C:262:SER:HB2	2:C:263:GLY:H	1.65	0.43
1:A:2374:LYS:HE3	1:A:2540:GLN:OE1	2.19	0.43
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.43
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.54	0.43
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.60	0.43
1:A:2387:MET:HE1	1:A:2396:TYR:HB2	1.98	0.42
1:B:2424:ASP:O	1:B:2428:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:THR:O	2:C:109:ALA:HA	2.18	0.42
1:A:2064:THR:CG2	1:A:2128:PRO:HD3	2.40	0.42
1:B:1505:ASN:CB	1:B:1508:THR:HB	2.50	0.42
2:C:17:THR:HG1	2:C:27:TRP:HE1	1.63	0.42
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	2.01	0.42
1:A:1900:LEU:HD23	1:A:2204:LEU:HD22	2.00	0.42
1:B:2021:ILE:HG22	1:B:2025:GLU:HB2	2.01	0.42
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.61	0.42
1:B:2184:PHE:HB3	1:B:2236:LEU:HD22	2.01	0.42
1:B:1910:TRP:CZ2	1:B:1956:LEU:HB3	2.54	0.42
2:D:169:PRO:HA	2:D:171:VAL:HG22	2.00	0.42
2:C:306:ARG:HG2	2:C:307:GLU:N	2.31	0.42
2:D:213:LYS:HD3	2:D:252:PHE:HE1	1.84	0.42
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.42
2:C:150:GLY:HA3	2:C:169:PRO:CB	2.44	0.42
2:C:248:ARG:O	2:C:252:PHE:HA	2.20	0.42
2:D:248:ARG:O	2:D:252:PHE:N	2.50	0.42
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.42
1:A:1453:LEU:O	1:A:1455:GLU:N	2.53	0.42
1:B:1710:LYS:NZ	1:B:1760:ASN:HD21	2.17	0.42
1:B:1778:ALA:O	1:B:1782:HIS:HD2	2.01	0.42
2:D:150:GLY:HA3	2:D:169:PRO:CB	2.43	0.42
2:C:203:ILE:HG22	2:C:204:GLY:N	2.34	0.42
1:A:2503:ARG:NH1	1:A:2507:LYS:CE	2.82	0.42
1:A:2037:LEU:HD22	1:A:2043:ASN:ND2	2.33	0.42
1:A:1691:THR:HG23	1:A:1724:MET:HE1	2.01	0.42
1:A:1910:TRP:O	1:A:1910:TRP:HD1	2.03	0.42
1:B:2165:SER:OG	1:B:2166:LYS:N	2.52	0.42
2:C:298:CYS:HB2	2:C:305:LYS:HE3	2.02	0.42
2:C:219:HIS:CE1	2:C:245:LYS:HD2	2.55	0.42
1:B:2042:ARG:HD3	1:B:2042:ARG:HA	1.87	0.42
1:A:1915:HIS:HE1	1:A:1919:VAL:CG1	2.33	0.42
2:C:21:ASP:HB3	2:C:313:LYS:HB2	2.02	0.42
2:D:297:TRP:CZ3	2:D:304:ILE:HG12	2.54	0.42
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	2.00	0.42
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.20	0.42
2:D:28:GLN:HG2	2:D:31:SER:OG	2.20	0.42
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.20	0.42
1:B:2123:LEU:HA	1:B:2123:LEU:HD12	1.97	0.42
1:B:2321:THR:HG23	1:B:2387:MET:HE3	2.02	0.42
1:A:1936:LEU:C	1:A:1938:VAL:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1910:TRP:CD1	1:B:1910:TRP:C	2.93	0.42
1:B:2333:ILE:HD12	1:B:2407:LEU:HD13	2.01	0.42
1:B:1614:ILE:O	1:B:1618:ILE:HG13	2.19	0.42
1:A:2101:TRP:HA	1:A:2104:TYR:HB2	2.01	0.42
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	2.01	0.42
2:D:63:GLN:HE21	2:D:86:LYS:N	2.07	0.42
1:A:2421:PHE:HD1	1:A:2430:ARG:HH22	1.65	0.42
1:B:2022:LEU:HA	1:B:2022:LEU:HD23	1.91	0.42
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.20	0.42
1:B:2329:MET:SD	1:B:2404:MET:HE2	2.60	0.42
2:D:75:PRO:HB2	2:D:76:ASN:H	1.48	0.42
1:A:2424:ASP:O	1:A:2428:ASN:ND2	2.53	0.42
2:D:203:ILE:HG22	2:D:204:GLY:N	2.35	0.42
2:D:53:ASP:C	2:D:55:SER:H	2.23	0.42
1:A:2281:MET:CE	2:C:222:TYR:CE2	3.03	0.42
1:B:2364:VAL:HG12	1:B:2365:ALA:N	2.33	0.42
1:A:2128:PRO:HD2	1:A:2129:LYS:H	1.85	0.41
1:A:1493:LEU:CD2	1:A:1519:ALA:HB2	2.46	0.41
1:B:1903:THR:HG22	1:B:1938:VAL:HG21	2.02	0.41
2:C:213:LYS:HD3	2:C:252:PHE:HE1	1.85	0.41
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	2.01	0.41
1:A:1623:LEU:HD13	1:A:1640:ARG:HH12	1.84	0.41
1:A:2184:PHE:CB	1:A:2236:LEU:HD22	2.50	0.41
2:C:281:ASP:OD1	2:C:283:GLN:HG3	2.20	0.41
1:B:2376:PRO:HG2	1:B:2532:ALA:HB2	2.02	0.41
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.20	0.41
1:B:1533:THR:C	1:B:1535:MET:H	2.22	0.41
1:A:1932:ILE:O	1:A:1933:ASP:C	2.58	0.41
1:B:1970:GLN:C	1:B:1972:LEU:N	2.73	0.41
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.01	0.41
1:B:1415:SER:O	1:B:1419:ILE:CG2	2.66	0.41
1:B:2261:LEU:HD23	1:B:2262:ASN:ND2	2.35	0.41
1:B:2004:THR:HA	1:B:2007:GLN:HB2	2.01	0.41
1:A:1481:MET:HA	1:A:1484:LEU:HD12	2.01	0.41
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.20	0.41
1:A:1915:HIS:CE1	1:A:1919:VAL:CG1	3.03	0.41
1:A:1605:TYR:O	1:A:1605:TYR:HD2	2.03	0.41
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.08	0.41
1:A:1566:LYS:O	1:A:1570:LEU:HG	2.19	0.41
1:A:2082:GLN:HE21	1:A:2082:GLN:HB3	1.64	0.41
1:A:2382:MET:HG3	1:A:2549:TRP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:HIS:CD2	2:D:138:PRO:N	2.87	0.41
2:C:203:ILE:HA	2:C:206:GLU:HG2	2.02	0.41
2:C:127:VAL:HG12	2:C:128:ASN:N	2.34	0.41
1:B:2529:ILE:O	1:B:2533:THR:HB	2.20	0.41
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.83	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
1:B:1701:MET:HE2	1:B:1701:MET:HB3	1.84	0.41
2:C:137:HIS:HD2	2:C:139:ASN:H	1.67	0.41
2:D:298:CYS:HB2	2:D:305:LYS:HE3	2.03	0.41
1:B:2225:TYR:CD1	3:B:2601:P2X:H2	2.55	0.41
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.36	0.41
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	2.03	0.41
1:A:1899:ASN:O	1:A:1900:LEU:C	2.58	0.41
2:D:28:GLN:O	2:D:28:GLN:HG3	2.20	0.41
1:B:1895:SER:HB3	1:B:1898:ASN:O	2.20	0.41
2:C:18:ALA:HB1	2:C:45:VAL:HG21	2.03	0.41
1:A:2347:ASP:OD1	1:A:2350:SER:OG	2.25	0.41
2:D:281:ASP:OD1	2:D:283:GLN:HG3	2.20	0.41
1:A:2127:SER:HA	1:A:2128:PRO:HD3	1.93	0.41
2:C:297:TRP:CZ3	2:C:304:ILE:HG12	2.55	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.02	0.41
1:A:1518:ALA:HB2	1:A:1546:TYR:OH	2.20	0.41
1:B:1425:GLN:HG2	1:B:2314:PHE:HZ	1.84	0.41
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.21	0.41
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.56	0.41
2:C:85:ASN:ND2	2:C:85:ASN:H	2.18	0.41
2:D:150:GLY:HA2	2:D:173:ILE:HG23	2.03	0.41
1:B:2128:PRO:HD2	1:B:2129:LYS:H	1.86	0.41
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	2.03	0.41
1:B:1936:LEU:C	1:B:1938:VAL:H	2.24	0.41
2:D:151:ALA:HA	2:D:166:ILE:HG22	2.03	0.41
2:D:248:ARG:CZ	2:D:248:ARG:HB3	2.51	0.41
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.02	0.41
1:B:1910:TRP:HZ2	1:B:1956:LEU:HB3	1.85	0.41
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.03	0.41
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.86	0.41
1:A:2275:TYR:HE1	1:A:2286:VAL:HB	1.85	0.41
1:B:1807:GLN:NE2	1:B:1811:ARG:HH21	2.19	0.41
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.20	0.41
1:A:1533:THR:C	1:A:1535:MET:H	2.23	0.41
2:D:263:GLY:O	2:D:264:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1681:PRO:HG2	1:A:1683:ARG:HG3	2.03	0.40
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	3.05	0.40
1:B:2189:HIS:CD2	1:B:2189:HIS:N	2.89	0.40
2:D:127:VAL:HG12	2:D:128:ASN:N	2.35	0.40
1:A:1417:ILE:O	1:A:1421:ASN:ND2	2.54	0.40
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.02	0.40
1:A:1605:TYR:CE2	1:A:1612:ARG:HG2	2.57	0.40
1:B:2530:LYS:HA	1:B:2530:LYS:HE2	2.02	0.40
1:A:1903:THR:HG22	1:A:1938:VAL:HG21	2.02	0.40
2:D:258:LEU:HD11	2:D:285:ILE:HG21	2.02	0.40
1:B:2101:TRP:HA	1:B:2104:TYR:HB2	2.03	0.40
2:D:68:TYR:CE2	2:D:77:PRO:HD3	2.57	0.40
2:C:168:GLU:N	2:C:169:PRO:CD	2.84	0.40
1:B:2421:PHE:HD1	1:B:2430:ARG:HH22	1.68	0.40
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.47	0.40
2:C:200:THR:HB	2:C:209:GLN:HB2	2.02	0.40
2:C:239:SER:OG	2:C:240:ALA:N	2.54	0.40
1:B:2297:ASP:O	1:B:2299:LEU:N	2.54	0.40
1:B:1722:GLN:HA	1:B:1725:GLN:HE21	1.86	0.40
2:C:68:TYR:CE2	2:C:77:PRO:HD3	2.57	0.40
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.86	0.40
2:C:12:PRO:O	2:C:54:ARG:NH2	2.54	0.40
1:B:1618:ILE:H	1:B:1618:ILE:HG13	1.71	0.40
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.21	0.40
1:B:1980:SER:O	1:B:1988:HIS:HB2	2.22	0.40
2:D:85:ASN:H	2:D:85:ASN:ND2	2.19	0.40
1:B:1905:ARG:HD3	1:B:1905:ARG:HA	1.80	0.40
1:A:1401:GLU:CG	1:A:2389:VAL:HG22	2.51	0.40
1:B:2332:TYR:O	1:B:2507:LYS:NZ	2.38	0.40
1:A:2332:TYR:CE1	1:A:2507:LYS:HE2	2.56	0.40
2:C:101:TYR:HA	2:C:110:ARG:O	2.20	0.40
2:D:313:LYS:HA	2:D:313:LYS:HD3	1.86	0.40
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1046/1174 (89%)	904 (86%)	111 (11%)	31 (3%)	5	40
1	B	1052/1174 (90%)	913 (87%)	108 (10%)	31 (3%)	6	40
2	C	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	2	20
2	D	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	2	20
All	All	2728/3000 (91%)	2349 (86%)	279 (10%)	100 (4%)	4	35

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1680	ASP
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
1	B	2364	VAL
2	D	74	ASN
2	D	97	GLY
2	D	203	ILE
2	D	269	SER
1	A	1454	HIS
1	A	1525	GLN
1	A	1630	VAL
1	A	1650	MET
1	A	1680	ASP
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
1	A	2364	VAL
2	C	35	THR

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Mol	Chain	Res	Type
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	203	ILE
2	C	269	SER
1	B	1444	GLU
1	B	1454	HIS
1	B	1682	SER
1	B	1709	ARG
1	B	1735	GLU
1	B	1786	TRP
1	B	1914	GLY
1	B	1937	GLN
1	B	2000	GLU
2	D	35	THR
2	D	73	ASN
2	D	75	PRO
2	D	118	ASN
2	D	160	ASP
2	D	167	PRO
2	D	204	GLY
1	A	1444	GLU
1	A	1445	ILE
1	A	1682	SER
1	A	1709	ARG
1	A	1735	GLU
1	A	1786	TRP
1	A	1914	GLY
1	A	1937	GLN
1	A	2000	GLU
2	C	75	PRO
2	C	118	ASN
2	C	160	ASP
2	C	167	PRO
2	C	204	GLY
1	B	1445	ILE
1	B	1896	ARG
1	B	1933	ASP
1	B	2001	HIS
1	B	2093	ASN
1	B	2135	ASP
2	D	169	PRO

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Mol	Chain	Res	Type
2	D	264	ASN
1	A	1896	ARG
1	A	1933	ASP
1	A	2093	ASN
2	C	129	ALA
2	C	169	PRO
2	C	264	ASN
1	B	2357	ASP
1	B	2387	MET
2	D	129	ALA
1	A	2001	HIS
1	A	2135	ASP
1	A	2357	ASP
2	C	263	GLY
1	B	1583	TYR
1	B	1681	PRO
1	B	2515	HIS
2	D	140	GLN
2	D	263	GLY
1	A	1681	PRO
1	A	1784	ARG
1	A	2191	ASP
1	A	2515	HIS
2	C	262	SER
1	B	1474	PRO
1	B	2191	ASP
1	A	1474	PRO
1	A	2168	ARG
1	A	2387	MET
1	B	2168	ARG
2	D	201	GLY
2	C	76	ASN
2	C	201	GLY
2	C	310	GLY
2	D	76	ASN
2	D	310	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	927/1024 (90%)	837 (90%)	90 (10%)	10	41
1	B	931/1024 (91%)	830 (89%)	101 (11%)	8	36
2	C	269/276 (98%)	233 (87%)	36 (13%)	5	25
2	D	269/276 (98%)	233 (87%)	36 (13%)	5	25
All	All	2396/2600 (92%)	2133 (89%)	263 (11%)	8	35

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1457	GLU
1	B	1475	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1557	PHE
1	B	1590	MET
1	B	1592	SER
1	B	1593	CYS
1	B	1611	ARG
1	B	1630	VAL
1	B	1650	MET
1	B	1685	LEU
1	B	1709	ARG
1	B	1740	LYS
1	B	1767	SER
1	B	1768	THR
1	B	1780	THR
1	B	1870	THR
1	B	1872	ASP
1	B	1878	LEU
1	B	1891	SER
1	B	1895	SER
1	B	1896	ARG

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Mol	Chain	Res	Type
1	B	1898	ASN
1	B	1899	ASN
1	B	1908	THR
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL
1	B	1956	LEU
1	B	1959	GLN
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2035	SER
1	B	2036	ARG
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2080	GLU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS
1	B	2098	THR
1	B	2102	ASP
1	B	2123	LEU
1	B	2124	GLN
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2155	SER
1	B	2164	THR
1	B	2165	SER
1	B	2167	GLN
1	B	2168	ARG
1	B	2173	THR
1	B	2181	GLU
1	B	2189	HIS
1	B	2190	GLU
1	B	2195	ASP

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Mol	Chain	Res	Type
1	B	2228	ILE
1	B	2232	THR
1	B	2240	VAL
1	B	2244	ASP
1	B	2245	THR
1	B	2254	ARG
1	B	2259	ILE
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2301	LYS
1	B	2318	THR
1	B	2342	SER
1	B	2354	LEU
1	B	2363	GLU
1	B	2378	ARG
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2503	ARG
1	B	2515	HIS
1	B	2530	LYS
1	B	2533	THR
1	B	2538	LEU
1	B	2548	PHE
2	D	13	VAL
2	D	37	THR
2	D	44	GLN
2	D	82	ASP
2	D	84	VAL
2	D	85	ASN
2	D	91	VAL
2	D	98	ARG
2	D	128	ASN
2	D	135	CYS
2	D	140	GLN
2	D	159	THR
2	D	160	ASP

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Mol	Chain	Res	Type
2	D	162	ASN
2	D	164	GLN
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	175	SER
2	D	183	SER
2	D	199	LEU
2	D	214	THR
2	D	215	LYS
2	D	242	GLN
2	D	243	THR
2	D	248	ARG
2	D	261	LYS
2	D	262	SER
2	D	286	VAL
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1443	LEU
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1557	PHE
1	A	1590	MET
1	A	1593	CYS
1	A	1611	ARG
1	A	1630	VAL
1	A	1650	MET
1	A	1685	LEU
1	A	1709	ARG
1	A	1740	LYS
1	A	1768	THR

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Mol	Chain	Res	Type
1	A	1780	THR
1	A	1872	ASP
1	A	1878	LEU
1	A	1891	SER
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1908	THR
1	A	1916	TRP
1	A	1932	ILE
1	A	1956	LEU
1	A	1959	GLN
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2035	SER
1	A	2036	ARG
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2080	GLU
1	A	2090	LYS
1	A	2093	ASN
1	A	2095	LYS
1	A	2102	ASP
1	A	2123	LEU
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2155	SER
1	A	2164	THR
1	A	2165	SER
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2181	GLU
1	A	2189	HIS

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Mol	Chain	Res	Type
1	A	2190	GLU
1	A	2195	ASP
1	A	2228	ILE
1	A	2232	THR
1	A	2240	VAL
1	A	2244	ASP
1	A	2245	THR
1	A	2254	ARG
1	A	2259	ILE
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2301	LYS
1	A	2318	THR
1	A	2342	SER
1	A	2354	LEU
1	A	2363	GLU
1	A	2367	THR
1	A	2378	ARG
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2503	ARG
1	A	2530	LYS
1	A	2533	THR
1	A	2548	PHE
2	C	13	VAL
2	C	37	THR
2	C	44	GLN
2	C	82	ASP
2	C	84	VAL
2	C	85	ASN
2	C	91	VAL
2	C	98	ARG
2	C	123	ARG
2	C	128	ASN
2	C	135	CYS
2	C	140	GLN
2	C	159	THR

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Mol	Chain	Res	Type
2	C	160	ASP
2	C	162	ASN
2	C	164	GLN
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	175	SER
2	C	183	SER
2	C	214	THR
2	C	215	LYS
2	C	242	GLN
2	C	243	THR
2	C	248	ARG
2	C	261	LYS
2	C	262	SER
2	C	286	VAL
2	C	287	THR
2	C	289	SER
2	C	301	THR
2	C	312	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1398	HIS
1	B	1496	GLN
1	B	1509	GLN
1	B	1594	HIS
1	B	1687	HIS
1	B	1760	ASN
1	B	1782	HIS
1	B	1807	GLN
1	B	1898	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN

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Mol	Chain	Res	Type
1	B	2154	GLN
1	B	2161	GLN
1	B	2167	GLN
1	B	2189	HIS
1	B	2233	ASN
1	B	2262	ASN
1	B	2277	HIS
1	B	2385	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
1	B	2502	ASN
2	D	22	HIS
2	D	30	HIS
2	D	39	GLN
2	D	40	HIS
2	D	41	GLN
2	D	63	GLN
2	D	74	ASN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN
2	D	128	ASN
2	D	132	ASN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	311	HIS
2	D	312	GLN
1	A	1398	HIS
1	A	1496	GLN
1	A	1594	HIS
1	A	1627	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1744	HIS
1	A	1760	ASN
1	A	1898	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN

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Mol	Chain	Res	Type
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2161	GLN
1	A	2167	GLN
1	A	2189	HIS
1	A	2262	ASN
1	A	2292	ASN
1	A	2385	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2428	ASN
1	A	2502	ASN
2	C	30	HIS
2	C	39	GLN
2	C	40	HIS
2	C	41	GLN
2	C	63	GLN
2	C	74	ASN
2	C	85	ASN
2	C	94	HIS
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
2	C	312	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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	P2X	A	2601	-	23,26,26	1.08	2 (8%)	23,39,39	3.25	11 (47%)
3	P2X	B	2601	-	23,26,26	1.10	2 (8%)	23,39,39	3.40	10 (43%)

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	P2X	A	2601	-	-	0/2/8/8	0/4/4/4
3	P2X	B	2601	-	-	0/2/8/8	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	P2X	C21-C23	2.36	1.41	1.36
3	B	2601	P2X	C21-C23	2.59	1.42	1.36
3	A	2601	P2X	N3-N2	2.62	1.40	1.37
3	B	2601	P2X	N3-N2	2.72	1.40	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	P2X	N4-C19-N6	-10.93	120.52	128.89
3	A	2601	P2X	N4-C19-N6	-9.84	121.36	128.89
3	B	2601	P2X	C16-C12-C9	-6.48	119.47	129.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	P2X	C16-C12-C9	-5.81	120.48	129.24
3	B	2601	P2X	C14-C8-N2	-3.29	107.22	111.46
3	A	2601	P2X	C23-C21-C18	-2.93	117.70	120.88
3	B	2601	P2X	C23-C21-C18	-2.64	118.02	120.88
3	A	2601	P2X	C12-C16-C17	-2.60	103.31	106.55
3	A	2601	P2X	C16-C17-C20	-2.45	127.83	136.55
3	B	2601	P2X	C16-C17-C20	-2.36	128.18	136.55
3	A	2601	P2X	C22-C20-C17	-2.24	117.74	120.48
3	A	2601	P2X	C21-C18-N5	2.02	136.72	130.72
3	B	2601	P2X	C21-C18-N5	2.03	136.75	130.72
3	B	2601	P2X	C12-N5-C18	2.36	109.33	104.47
3	A	2601	P2X	C21-C23-C22	2.55	123.31	120.18
3	B	2601	P2X	C21-C23-C22	2.70	123.49	120.18
3	A	2601	P2X	C12-N5-C18	2.77	110.18	104.47
3	B	2601	P2X	C16-C17-C18	3.41	109.25	106.27
3	A	2601	P2X	C16-C17-C18	4.36	110.08	106.27
3	B	2601	P2X	C9-N3-N2	6.01	109.65	105.34
3	A	2601	P2X	C9-N3-N2	6.11	109.73	105.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	P2X	3	0
3	B	2601	P2X	4	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	1054/1174 (89%)	0.33	80 (7%) 17 16	26, 62, 152, 178	0
1	B	1058/1174 (90%)	0.15	44 (4%) 40 34	23, 53, 128, 168	0
2	C	317/326 (97%)	0.23	13 (4%) 41 35	29, 61, 115, 156	0
2	D	317/326 (97%)	-0.03	3 (0%) 85 79	23, 40, 91, 142	0
All	All	2746/3000 (91%)	0.21	140 (5%) 32 27	23, 56, 140, 178	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2434	THR	6.2
1	A	2434	THR	6.0
1	B	1469	THR	5.7
1	A	2435	ASN	5.3
1	A	2044	VAL	5.0
1	A	1619	TRP	5.0
1	A	1582	SER	4.9
1	A	1580	GLY	4.9
2	C	205	ASP	4.9
1	B	1581	GLU	4.8
1	A	2048	PHE	4.5
1	A	1600	GLU	4.5
1	A	2436	THR	4.5
1	B	2435	ASN	4.4
1	A	2038	TYR	4.3
1	B	1504	VAL	4.3
1	A	2049	GLU	4.2
1	A	1469	THR	4.2
1	B	1587	TYR	4.1
1	B	1499	GLU	4.1
1	A	1599	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	1540	THR	4.0
1	A	1581	GLU	4.0
1	A	1558	SER	3.9
1	B	1580	GLY	3.9
1	A	1587	TYR	3.8
1	B	1577	ALA	3.8
1	B	2044	VAL	3.8
2	C	119	LEU	3.7
1	A	1468	ASP	3.7
1	B	1446	GLN	3.7
1	A	1554	GLN	3.6
1	A	2045	LYS	3.6
1	B	1582	SER	3.5
1	A	2055	HIS	3.5
2	C	202	GLY	3.5
1	B	1505	ASN	3.5
1	B	2436	THR	3.4
1	A	1386	ARG	3.4
1	A	2101	TRP	3.4
1	B	1386	ARG	3.3
2	C	90	SER	3.3
1	A	1546	TYR	3.3
2	C	201	GLY	3.3
1	A	2090	LYS	3.2
1	A	1584	SER	3.2
1	A	1388	ALA	3.2
2	C	8	VAL	3.2
1	A	1603	ILE	3.2
1	B	1573	ALA	3.2
1	B	1869	VAL	3.2
1	A	1606	LYS	3.2
2	D	202	GLY	3.2
1	A	2042	ARG	3.2
1	A	2433	ASP	3.1
1	B	1872	ASP	3.1
1	A	1387	ALA	3.1
2	C	10	SER	3.1
1	B	1578	MET	3.0
1	B	1385	GLU	3.0
1	A	1628	ARG	3.0
1	B	2040	GLY	3.0
1	B	2043	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2433	ASP	3.0
1	A	1504	VAL	3.0
1	A	1730	HIS	3.0
1	B	2045	LYS	2.9
1	A	1867	LYS	2.9
1	A	2104	TYR	2.9
2	D	205	ASP	2.9
1	A	1579	ALA	2.9
1	B	2039	PHE	2.9
2	C	204	GLY	2.8
1	A	2097	LEU	2.8
1	B	1579	ALA	2.7
1	A	2432	MET	2.7
1	A	1556	LEU	2.7
1	A	1470	ASN	2.7
1	B	1508	THR	2.7
1	A	1578	MET	2.7
1	A	1559	LEU	2.7
1	B	1572	ASP	2.6
1	B	1470	ASN	2.6
1	A	1604	GLN	2.6
1	A	1566	LYS	2.6
1	B	1468	ASP	2.6
1	A	1502	THR	2.6
1	B	1472	ASP	2.5
1	A	1627	GLN	2.5
2	C	207	VAL	2.5
1	B	1449	TRP	2.5
1	B	1868	LYS	2.5
1	A	1555	ASP	2.5
1	B	1731	ALA	2.5
1	A	2096	ASP	2.5
1	A	2428	ASN	2.5
1	A	2040	GLY	2.4
1	B	2038	TYR	2.4
1	B	1496	GLN	2.4
1	B	1871	GLU	2.4
1	A	2106	HIS	2.4
1	A	2118	LEU	2.4
2	C	9	GLY	2.4
1	A	1385	GLU	2.4
1	A	1611	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2043	ASN	2.4
2	C	269	SER	2.4
2	D	204	GLY	2.4
1	A	1573	ALA	2.3
1	A	1505	ASN	2.3
2	C	265	PRO	2.3
1	A	2034	ALA	2.3
1	A	1534	CYS	2.3
1	A	1869	VAL	2.3
1	A	2039	PHE	2.3
1	A	1812	ASP	2.3
1	A	1507	GLU	2.3
1	B	1507	GLU	2.2
1	A	2041	GLU	2.2
1	A	2033	GLU	2.2
1	A	1596	LEU	2.2
1	A	1549	VAL	2.2
1	A	1620	TRP	2.2
1	A	2051	LEU	2.2
1	A	1586	ALA	2.2
1	A	2078	LEU	2.2
1	B	1473	ASP	2.2
1	B	1812	ASP	2.2
1	A	1871	GLU	2.1
1	B	1467	MET	2.1
1	A	1614	ILE	2.1
1	B	1450	TYR	2.1
1	A	1814	LYS	2.1
1	A	2031	LEU	2.1
1	A	1509	GLN	2.1
1	A	1585	ARG	2.1
1	A	2050	VAL	2.1
1	B	1867	LYS	2.0
1	A	2037	LEU	2.0
2	C	118	ASN	2.0

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

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



### 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
3	P2X	B	2601	23/23	0.94	0.24	0.63	33,34,35,35	0
3	P2X	A	2601	23/23	0.95	0.21	-0.34	37,37,38,38	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.