



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:14 am BST

PDB ID : 5X9Z  
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain  
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.  
Deposited on : 2017-03-10  
Resolution : 7.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

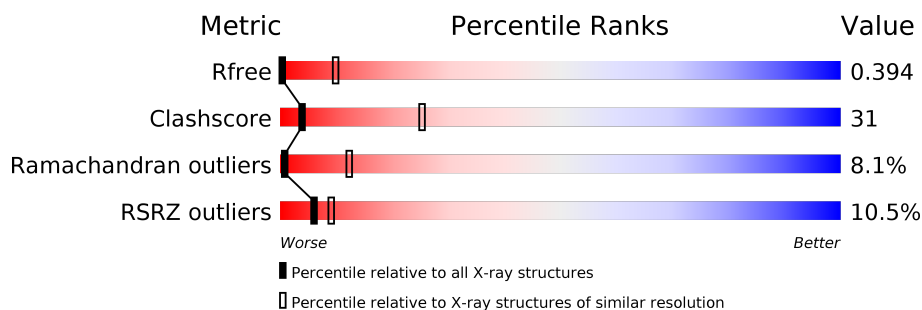
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.31 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))
$R_{free}$	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	2217	<div> <div>8%</div> <div>50%</div> <div>24%</div> <div>•</div> <div>23%</div> </div>
1	B	2217	<div> <div>8%</div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16948 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.

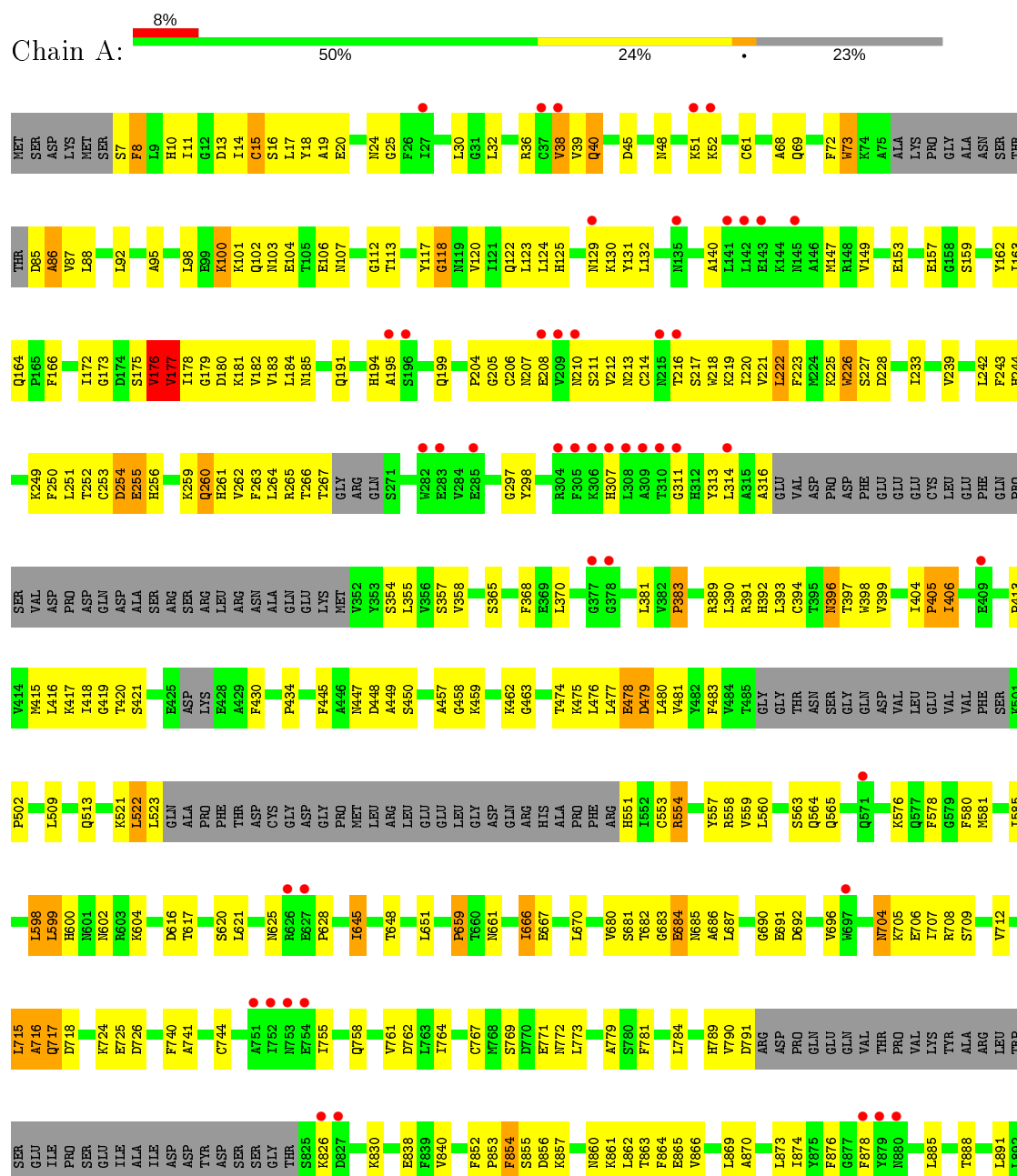
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	1710	Total	C	N	O	0	0	0
			8479	5059	1710	1710			
1	B	1708	Total	C	N	O	0	0	0
			8469	5053	1708	1708			

### 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 the various outlier classes 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: Inositol 1,4,5-trisphosphate receptor type 1









Q2206	I2207	V2208	F2209	P2210	V2211	P2212	C2215	E2216	F2217
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.50Å 221.73Å 318.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 7.31 49.15 – 7.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-7.31) 88.5 (49.15-7.31)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.317 , 0.394 0.316 , 0.394	Depositor DCC
$R_{free}$ test set	536 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	209.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 335.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.219 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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	0.48	1/8465 (0.0%)	0.72	6/11786 (0.1%)
1	B	0.49	1/8455 (0.0%)	0.72	1/11772 (0.0%)
All	All	0.48	2/16920 (0.0%)	0.72	7/23558 (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	25
1	B	0	22
All	All	0	47

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ILE	C-O	7.16	1.36	1.23
1	A	1048	THR	C-N	5.11	1.44	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	ARG	N-CA-C	-7.07	91.92	111.00
1	A	177	VAL	N-CA-C	6.68	129.03	111.00
1	B	743	MET	C-N-CA	5.66	135.84	121.70
1	A	176	VAL	C-N-CA	5.44	135.31	121.70
1	A	554	ARG	CA-C-O	-5.28	109.02	120.10
1	A	553	CYS	C-N-CA	-5.22	108.65	121.70
1	A	998	LYS	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	ASP	Peptide
1	A	1055	HIS	Peptide
1	A	118	GLY	Peptide
1	A	1202	GLN	Peptide
1	A	1375	ILE	Peptide
1	A	1380	LEU	Peptide
1	A	1383	VAL	Peptide
1	A	1461	CYS	Peptide
1	A	15	CYS	Peptide
1	A	1639	ASN	Peptide
1	A	176	VAL	Peptide
1	A	1815	SER	Peptide
1	A	2009	ILE	Peptide
1	A	2016	GLY	Peptide
1	A	2071	ASN	Peptide
1	A	2115	MET	Peptide
1	A	2142	GLU	Peptide
1	A	2184	ALA	Peptide
1	A	2192	THR	Peptide
1	A	254	ASP	Peptide
1	A	260	GLN	Peptide
1	A	406	ILE	Peptide
1	A	73	TRP	Peptide
1	A	8	PHE	Peptide
1	A	989	ARG	Peptide
1	B	1269	GLU	Peptide
1	B	1287	ILE	Peptide
1	B	1310	LYS	Peptide
1	B	1461	CYS	Peptide
1	B	1639	ASN	Peptide
1	B	176	VAL	Peptide
1	B	179	GLY	Peptide
1	B	1816	SER	Peptide
1	B	1883	ASN	Peptide
1	B	190	GLY	Peptide
1	B	191	GLN	Peptide
1	B	251	LEU	Peptide
1	B	252	THR	Peptide
1	B	299	TRP	Peptide
1	B	306	LYS	Peptide
1	B	424	LYS	Peptide
1	B	464	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	670	LEU	Peptide
1	B	7	SER	Peptide
1	B	744	CYS	Peptide
1	B	749	TYR	Peptide
1	B	759	LEU	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	8479	0	3697	386	0
1	B	8469	0	3697	360	0
All	All	16948	0	7394	745	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 31.

All (745) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:MET:O	1:A:1212:ALA:HB3	1.49	1.10
1:A:405:PRO:HA	1:A:416:LEU:HA	1.39	1.04
1:A:162:TYR:O	1:A:184:LEU:C	1.97	1.02
1:B:1682:MET:O	1:B:1686:ARG:N	1.93	1.01
1:A:1472:SER:O	1:A:1476:LYS:CB	2.10	1.00
1:A:1371:LEU:O	1:A:1375:ILE:N	1.94	1.00
1:A:1605:ASP:O	1:A:1609:ALA:HB2	1.62	1.00
1:A:866:VAL:O	1:A:870:ALA:HB2	1.62	1.00
1:B:8:PHE:HA	1:B:177:VAL:HA	1.42	0.99
1:A:1208:MET:O	1:A:1212:ALA:CB	2.10	0.98
1:A:2020:LEU:O	1:A:2024:ILE:N	1.96	0.98
1:A:162:TYR:O	1:A:184:LEU:CA	2.11	0.98
1:A:314:LEU:HA	1:A:357:SER:HA	1.47	0.95
1:A:1125:ILE:O	1:A:1129:SER:CB	2.14	0.94
1:A:1798:LEU:HA	1:A:1802:GLY:HA3	1.50	0.94
1:A:581:MET:O	1:A:585:ILE:N	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:O	1:B:251:LEU:N	2.00	0.94
1:A:243:PHE:HA	1:A:250:PHE:HA	1.50	0.94
1:A:521:LYS:O	1:A:523:LEU:N	2.01	0.93
1:A:1118:ASP:O	1:A:1122:LEU:N	2.01	0.93
1:B:2040:THR:O	1:B:2044:GLN:CB	2.17	0.93
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.17	0.92
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.47	0.92
1:B:1417:GLU:O	1:B:1421:ALA:N	2.02	0.91
1:A:1210:ALA:O	1:A:1214:VAL:CB	2.19	0.91
1:A:708:ARG:O	1:A:712:VAL:N	2.03	0.91
1:B:314:LEU:HA	1:B:357:SER:HA	1.52	0.91
1:A:117:TYR:O	1:A:173:GLY:N	2.02	0.91
1:A:458:GLY:O	1:A:462:LYS:CB	2.18	0.91
1:A:981:ILE:O	1:A:985:ARG:CB	2.19	0.90
1:A:2125:LYS:O	1:A:2129:MET:CB	2.20	0.90
1:B:1095:GLN:O	1:B:1099:GLN:N	2.05	0.90
1:B:467:GLN:O	1:B:470:ARG:N	2.04	0.90
1:B:7:SER:O	1:B:178:ILE:N	2.04	0.89
1:B:1214:VAL:O	1:B:1218:LEU:N	2.06	0.89
1:A:1378:VAL:O	1:A:1382:ALA:HB2	1.73	0.88
1:B:315:ALA:HA	1:B:366:SER:HA	1.55	0.88
1:A:2083:LEU:O	1:A:2087:LEU:CB	2.22	0.88
1:A:856:ASP:O	1:A:860:ASN:CB	2.22	0.88
1:B:117:TYR:C	1:B:173:GLY:H	1.77	0.88
1:A:1864:LYS:O	1:A:1868:GLN:N	2.07	0.87
1:A:2189:ALA:O	1:A:2193:ALA:N	2.06	0.87
1:A:1380:LEU:O	1:A:1384:CYS:CB	2.23	0.86
1:B:981:ILE:O	1:B:985:ARG:CB	2.23	0.86
1:A:2124:ILE:O	1:A:2128:TYR:CB	2.24	0.86
1:A:19:ALA:N	1:A:25:GLY:O	2.09	0.85
1:B:696:VAL:O	1:B:700:TRP:N	2.10	0.85
1:B:2183:GLU:O	1:B:2187:PHE:CB	2.24	0.85
1:B:686:ALA:O	1:B:689:ALA:HB3	1.77	0.84
1:A:8:PHE:H	1:A:177:VAL:C	1.80	0.84
1:B:19:ALA:HA	1:B:218:TRP:HA	1.58	0.84
1:A:2036:LEU:O	1:A:2040:THR:CB	2.25	0.84
1:A:162:TYR:O	1:A:184:LEU:HA	1.74	0.84
1:B:244:HIS:O	1:B:248:GLU:N	2.10	0.83
1:B:140:ALA:N	1:B:146:ALA:O	2.11	0.83
1:B:1212:ALA:O	1:B:1216:GLU:CB	2.26	0.83
1:B:130:LYS:HA	1:B:153:GLU:HA	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.26	0.83
1:B:1594:ARG:O	1:B:1598:ASN:CB	2.27	0.83
1:B:391:ARG:HA	1:B:398:TRP:HA	1.59	0.83
1:A:125:HIS:O	1:A:129:ASN:N	2.11	0.83
1:A:1861:ASP:O	1:A:1865:VAL:CB	2.26	0.83
1:B:103:ASN:O	1:B:107:ASN:CB	2.26	0.83
1:B:865:GLU:O	1:B:869:LEU:CB	2.27	0.82
1:A:1605:ASP:O	1:A:1609:ALA:CB	2.27	0.82
1:A:354:SER:HA	1:A:419:GLY:HA3	1.61	0.82
1:B:1096:ALA:O	1:B:1100:VAL:N	2.13	0.82
1:A:2189:ALA:O	1:A:2192:THR:N	2.13	0.82
1:A:1849:ASP:O	1:A:1853:GLU:N	2.12	0.81
1:A:621:LEU:O	1:A:625:ASN:N	2.10	0.81
1:A:298:TYR:HA	1:A:381:LEU:HA	1.61	0.81
1:A:480:LEU:O	1:A:483:PHE:N	2.14	0.81
1:B:392:HIS:N	1:B:397:THR:O	2.12	0.81
1:A:975:ILE:O	1:A:979:GLN:CB	2.28	0.81
1:A:1417:GLU:O	1:A:1421:ALA:N	2.10	0.81
1:A:162:TYR:CB	1:A:185:ASN:O	2.29	0.81
1:A:2188:TYR:O	1:A:2192:THR:CB	2.29	0.81
1:B:392:HIS:O	1:B:396:ASN:N	2.13	0.81
1:B:764:ILE:O	1:B:768:MET:CB	2.29	0.81
1:A:1224:LYS:HA	1:A:1270:ALA:HB3	1.63	0.80
1:B:666:ILE:CB	1:B:670:LEU:H	1.93	0.80
1:B:697:TRP:O	1:B:701:ARG:N	2.10	0.80
1:A:866:VAL:O	1:A:870:ALA:CB	2.30	0.80
1:B:767:CYS:O	1:B:771:GLU:CB	2.30	0.80
1:A:251:LEU:HA	1:A:264:LEU:HA	1.64	0.80
1:A:8:PHE:N	1:A:177:VAL:O	2.14	0.79
1:B:670:LEU:HA	1:B:673:SER:H	1.47	0.79
1:B:605:LEU:O	1:B:608:LYS:N	2.16	0.79
1:B:163:ILE:HA	1:B:184:LEU:HA	1.63	0.78
1:B:398:TRP:H	1:B:422:PRO:HA	1.47	0.78
1:A:118:GLY:N	1:A:163:ILE:O	2.13	0.78
1:A:1381:LEU:O	1:A:1385:THR:CB	2.32	0.78
1:A:761:VAL:O	1:A:764:ILE:N	2.17	0.78
1:A:1992:ASN:O	1:A:1994:THR:N	2.15	0.78
1:A:1252:GLN:O	1:A:1256:HIS:CB	2.31	0.78
1:B:61:CYS:CB	1:B:122:GLN:O	2.32	0.78
1:B:162:TYR:CB	1:B:185:ASN:O	2.31	0.78
1:A:252:THR:O	1:A:263:PHE:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1862:ARG:O	1:A:1866:ALA:CB	2.33	0.77
1:B:1813:ASN:O	1:B:1815:SER:N	2.17	0.77
1:A:1792:ALA:O	1:A:1796:CYS:CB	2.31	0.77
1:B:1632:PRO:O	1:B:1635:LEU:N	2.17	0.77
1:A:1862:ARG:O	1:A:1866:ALA:HB3	1.85	0.77
1:A:853:PRO:O	1:A:855:SER:N	2.17	0.77
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.33	0.76
1:B:15:CYS:HA	1:B:222:LEU:HA	1.67	0.76
1:B:313:TYR:CB	1:B:358:VAL:O	2.34	0.76
1:A:666:ILE:CB	1:A:670:LEU:H	1.98	0.76
1:A:16:SER:O	1:A:221:VAL:N	2.19	0.76
1:A:2035:THR:O	1:A:2039:LEU:CB	2.34	0.76
1:B:162:TYR:O	1:B:184:LEU:C	2.24	0.76
1:A:194:HIS:H	1:A:211:SER:HA	1.51	0.76
1:A:2116:ARG:O	1:A:2120:LEU:N	2.18	0.75
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.34	0.75
1:A:392:HIS:O	1:A:396:ASN:N	2.20	0.75
1:B:1795:GLN:O	1:B:1799:ASP:N	2.20	0.75
1:A:1795:GLN:O	1:A:1799:ASP:N	2.19	0.74
1:B:161:PHE:HA	1:B:186:PRO:HA	1.68	0.74
1:B:891:LEU:O	1:B:895:LEU:CB	2.35	0.74
1:A:767:CYS:O	1:A:771:GLU:CB	2.35	0.74
1:A:32:LEU:H	1:A:448:ASP:CB	2.01	0.74
1:B:252:THR:O	1:B:262:VAL:HA	1.88	0.74
1:A:254:ASP:O	1:A:261:HIS:CB	2.36	0.74
1:B:185:ASN:HA	1:B:192:PRO:HA	1.68	0.74
1:B:15:CYS:HA	1:B:223:PHE:H	1.53	0.73
1:B:252:THR:O	1:B:262:VAL:CA	2.36	0.73
1:A:1848:GLU:O	1:A:1850:LYS:N	2.18	0.73
1:B:305:PHE:O	1:B:314:LEU:N	2.20	0.73
1:A:2088:LYS:O	1:A:2092:SER:N	2.22	0.72
1:A:365:SER:HA	1:A:394:CYS:CB	2.19	0.72
1:A:2147:SER:O	1:A:2151:VAL:CB	2.38	0.72
1:B:162:TYR:O	1:B:184:LEU:HA	1.89	0.72
1:A:212:VAL:O	1:A:214:CYS:N	2.21	0.72
1:A:255:GLU:HA	1:A:260:GLN:HA	1.72	0.72
1:B:509:LEU:O	1:B:513:GLN:N	2.19	0.72
1:B:982:LEU:O	1:B:986:LEU:N	2.23	0.72
1:B:102:GLN:O	1:B:106:GLU:CB	2.37	0.72
1:B:1818:ARG:O	1:B:1821:HIS:N	2.22	0.72
1:B:1052:LEU:O	1:B:1057:GLY:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLN:HA	1:B:207:ASN:HA	1.71	0.71
1:B:252:THR:HA	1:B:280:ALA:HA	1.72	0.71
1:B:315:ALA:HB3	1:B:356:VAL:O	1.89	0.71
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.38	0.71
1:A:474:THR:O	1:A:477:LEU:N	2.24	0.71
1:A:15:CYS:HA	1:A:222:LEU:HA	1.72	0.71
1:B:773:LEU:O	1:B:775:TYR:N	2.20	0.71
1:A:741:ALA:HB2	1:A:876:PHE:HA	1.73	0.71
1:A:253:CYS:C	1:A:261:HIS:O	2.29	0.71
1:A:2021:GLY:O	1:A:2025:ASN:N	2.24	0.71
1:A:973:LYS:O	1:A:977:ILE:CB	2.39	0.71
1:A:181:LYS:HA	1:A:218:TRP:O	1.90	0.70
1:B:2152:GLY:O	1:B:2156:TYR:CB	2.39	0.70
1:A:1371:LEU:O	1:A:1374:HIS:N	2.24	0.70
1:A:20:GLU:N	1:A:217:SER:O	2.22	0.70
1:A:1297:HIS:HA	1:A:1301:THR:HA	1.73	0.70
1:A:102:GLN:O	1:A:106:GLU:CB	2.40	0.70
1:A:1040:ILE:O	1:A:1043:GLY:N	2.25	0.70
1:A:8:PHE:N	1:A:176:VAL:O	2.26	0.69
1:B:104:GLU:O	1:B:108:ARG:CB	2.40	0.69
1:B:1636:PHE:O	1:B:1638:GLU:N	2.23	0.69
1:A:2189:ALA:C	1:A:2193:ALA:H	1.96	0.69
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.41	0.69
1:A:253:CYS:O	1:A:261:HIS:O	2.10	0.69
1:A:1378:VAL:O	1:A:1382:ALA:CB	2.40	0.69
1:A:1118:ASP:O	1:A:1121:GLN:N	2.25	0.69
1:A:2115:MET:O	1:A:2119:GLU:N	2.22	0.69
1:A:307:HIS:O	1:A:311:GLY:N	2.26	0.69
1:B:55:ASP:HA	1:B:127:LYS:CB	2.23	0.68
1:B:14:ILE:O	1:B:223:PHE:N	2.26	0.68
1:A:1294:HIS:O	1:A:1298:CYS:N	2.21	0.68
1:B:162:TYR:O	1:B:184:LEU:CA	2.41	0.68
1:B:853:PRO:O	1:B:855:SER:N	2.25	0.68
1:A:874:ILE:O	1:A:878:PHE:N	2.26	0.68
1:A:243:PHE:HA	1:A:250:PHE:CA	2.23	0.68
1:B:1593:SER:O	1:B:1597:ARG:N	2.18	0.68
1:A:2117:PRO:O	1:A:2121:VAL:CB	2.41	0.68
1:B:315:ALA:HB2	1:B:358:VAL:CB	2.23	0.68
1:A:162:TYR:O	1:A:184:LEU:O	2.10	0.67
1:B:1991:ASN:CB	1:B:1998:LEU:HA	2.25	0.67
1:B:11:ILE:H	1:B:113:THR:C	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2050:ASN:O	1:B:2054:ILE:CB	2.42	0.67
1:B:628:PRO:O	1:B:632:ASP:N	2.22	0.67
1:A:390:LEU:O	1:A:398:TRP:HA	1.93	0.67
1:B:398:TRP:O	1:B:421:SER:O	2.13	0.67
1:B:476:LEU:O	1:B:479:ASP:N	2.28	0.67
1:A:14:ILE:O	1:A:223:PHE:N	2.23	0.67
1:B:8:PHE:HA	1:B:177:VAL:CA	2.22	0.67
1:A:244:HIS:N	1:A:249:LYS:O	2.28	0.67
1:A:255:GLU:HA	1:A:259:LYS:O	1.95	0.67
1:A:769:SER:HA	1:A:779:ALA:HA	1.77	0.67
1:A:1476:LYS:HA	1:A:1884:LYS:HA	1.75	0.66
1:A:998:LYS:O	1:A:1007:GLN:HA	1.95	0.66
1:A:391:ARG:HA	1:A:398:TRP:HA	1.77	0.66
1:B:421:SER:O	1:B:423:LEU:N	2.28	0.66
1:B:135:ASN:CB	1:B:148:ARG:O	2.42	0.66
1:B:279:LYS:HA	1:B:309:ALA:H	1.60	0.66
1:A:255:GLU:CA	1:A:259:LYS:O	2.42	0.66
1:B:1986:PHE:O	1:B:1990:GLN:N	2.29	0.66
1:B:152:ASP:O	1:B:155:GLY:N	2.28	0.66
1:B:223:PHE:HA	1:B:293:ARG:HA	1.76	0.66
1:B:398:TRP:N	1:B:422:PRO:HA	2.10	0.66
1:B:680:VAL:O	1:B:682:THR:N	2.28	0.66
1:A:1062:ARG:O	1:A:1066:HIS:N	2.23	0.66
1:A:7:SER:HA	1:A:177:VAL:N	2.11	0.65
1:A:19:ALA:O	1:A:25:GLY:N	2.29	0.65
1:B:1597:ARG:O	1:B:1601:GLU:CB	2.44	0.65
1:A:1108:ASP:O	1:A:1112:TYR:N	2.26	0.65
1:B:1225:ALA:H	1:B:1270:ALA:HB3	1.60	0.65
1:A:118:GLY:H	1:A:163:ILE:C	2.00	0.65
1:B:252:THR:CB	1:B:280:ALA:HA	2.27	0.65
1:A:478:GLU:O	1:A:480:LEU:N	2.29	0.65
1:A:179:GLY:HA2	1:A:220:ILE:O	1.96	0.65
1:A:355:LEU:H	1:A:419:GLY:HA2	1.61	0.64
1:B:1850:LYS:O	1:B:1854:LYS:N	2.30	0.64
1:B:621:LEU:O	1:B:625:ASN:N	2.30	0.64
1:A:2076:LEU:HA	1:A:2080:ARG:CB	2.27	0.64
1:A:61:CYS:CB	1:A:122:GLN:O	2.45	0.64
1:A:32:LEU:CB	1:A:445:PHE:HA	2.28	0.64
1:B:70:LYS:O	1:B:74:LYS:CB	2.46	0.64
1:A:2123:VAL:O	1:A:2127:ALA:HB3	1.98	0.63
1:A:100:LYS:O	1:A:103:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:CA	1:B:280:ALA:HA	2.27	0.63
1:B:2091:ALA:O	1:B:2095:LEU:CB	2.46	0.63
1:A:16:SER:N	1:A:221:VAL:O	2.31	0.63
1:B:1489:PHE:HA	1:B:1493:PRO:C	2.18	0.63
1:A:313:TYR:O	1:A:358:VAL:CB	2.46	0.63
1:A:124:LEU:HA	1:A:131:TYR:HA	1.80	0.63
1:A:253:CYS:CB	1:A:262:VAL:HA	2.28	0.62
1:B:134:VAL:O	1:B:136:LYS:N	2.32	0.62
1:B:125:HIS:N	1:B:130:LYS:O	2.25	0.62
1:B:1986:PHE:O	1:B:1989:CYS:N	2.32	0.62
1:B:132:LEU:HA	1:B:150:THR:O	1.99	0.62
1:B:1966:GLN:O	1:B:1970:ARG:CB	2.48	0.62
1:B:138:LEU:O	1:B:148:ARG:N	2.22	0.62
1:A:2168:GLU:O	1:A:2172:MET:CB	2.48	0.62
1:B:1820:PHE:C	1:B:1822:GLU:H	2.04	0.62
1:A:1033:ILE:HA	1:A:1036:GLN:CB	2.30	0.61
1:A:404:ILE:O	1:A:417:LYS:N	2.33	0.61
1:B:1269:GLU:HA	1:B:1319:GLU:CB	2.30	0.61
1:B:789:HIS:O	1:B:791:ASP:N	2.33	0.61
1:A:7:SER:C	1:A:176:VAL:O	2.39	0.61
1:B:1457:ILE:O	1:B:1459:ARG:N	2.33	0.61
1:A:39:VAL:N	1:A:207:ASN:O	2.32	0.61
1:A:888:THR:O	1:A:891:LEU:N	2.33	0.61
1:B:666:ILE:H	1:B:667:GLU:HA	1.66	0.61
1:B:118:GLY:H	1:B:163:ILE:C	2.04	0.61
1:B:1849:ASP:O	1:B:1852:SER:N	2.34	0.61
1:B:279:LYS:N	1:B:309:ALA:HB2	2.15	0.61
1:A:69:GLN:O	1:A:73:TRP:CB	2.49	0.61
1:B:125:HIS:O	1:B:129:ASN:N	2.33	0.61
1:A:1848:GLU:C	1:A:1850:LYS:H	2.03	0.60
1:A:666:ILE:N	1:A:667:GLU:HA	2.16	0.60
1:A:683:GLY:O	1:A:685:ASN:N	2.34	0.60
1:B:1459:ARG:C	1:B:1461:CYS:H	2.04	0.60
1:B:449:ALA:O	1:B:452:VAL:N	2.34	0.60
1:B:1051:ASP:O	1:B:1055:HIS:N	2.32	0.60
1:B:2120:LEU:O	1:B:2123:VAL:N	2.34	0.60
1:A:885:LEU:O	1:A:888:THR:N	2.34	0.60
1:A:1030:PHE:O	1:A:1034:GLU:CB	2.50	0.60
1:B:1609:ALA:O	1:B:1613:ARG:CB	2.50	0.60
1:B:2061:GLY:O	1:B:2064:ILE:N	2.31	0.60
1:A:1480:GLU:CB	1:A:1882:GLY:H	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:LYS:O	1:B:1132:TRP:CB	2.50	0.60
1:B:2188:TYR:O	1:B:2192:THR:CB	2.49	0.60
1:B:692:ASP:O	1:B:696:VAL:N	2.35	0.60
1:A:130:LYS:HA	1:A:153:GLU:HA	1.83	0.59
1:B:117:TYR:O	1:B:173:GLY:N	2.35	0.59
1:A:103:ASN:O	1:A:107:ASN:CB	2.50	0.59
1:A:1291:VAL:O	1:A:1295:PHE:N	2.35	0.59
1:B:398:TRP:H	1:B:422:PRO:CA	2.13	0.59
1:A:893:ALA:O	1:A:897:CYS:CB	2.51	0.59
1:B:1231:GLN:HA	1:B:1275:HIS:CB	2.33	0.59
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.51	0.59
1:B:2157:ILE:O	1:B:2161:GLN:CB	2.51	0.59
1:A:755:ILE:O	1:A:758:GLN:N	2.35	0.59
1:B:313:TYR:O	1:B:357:SER:C	2.41	0.59
1:B:691:GLU:O	1:B:695:GLU:N	2.35	0.59
1:B:117:TYR:O	1:B:119:ASN:N	2.37	0.58
1:B:962:LYS:O	1:B:966:MET:CB	2.51	0.58
1:A:680:VAL:O	1:A:682:THR:N	2.34	0.58
1:A:2020:LEU:O	1:A:2021:GLY:C	2.42	0.58
1:A:1251:ASN:O	1:A:1255:LEU:CB	2.51	0.58
1:A:1417:GLU:O	1:A:1420:ILE:N	2.36	0.58
1:A:1453:PHE:O	1:A:1457:ILE:CB	2.52	0.58
1:B:978:LEU:O	1:B:982:LEU:CB	2.52	0.58
1:A:1208:MET:O	1:A:1212:ALA:HB2	2.02	0.58
1:A:164:GLN:CB	1:A:183:VAL:O	2.52	0.57
1:A:242:LEU:O	1:A:250:PHE:HA	2.04	0.57
1:B:252:THR:O	1:B:262:VAL:C	2.42	0.57
1:B:1489:PHE:HA	1:B:1493:PRO:HA	1.86	0.57
1:B:1839:GLN:O	1:B:1842:PHE:CB	2.52	0.57
1:A:256:HIS:H	1:A:261:HIS:H	1.51	0.57
1:B:45:ASP:O	1:B:49:PRO:HA	2.05	0.57
1:A:978:LEU:O	1:A:982:LEU:CB	2.53	0.56
1:A:125:HIS:N	1:A:130:LYS:O	2.38	0.56
1:B:11:ILE:C	1:B:13:ASP:H	2.09	0.56
1:B:233:ILE:HA	1:B:384:ARG:N	2.19	0.56
1:B:399:VAL:HA	1:B:420:THR:HA	1.87	0.56
1:A:30:LEU:CB	1:A:36:ARG:H	2.18	0.56
1:B:313:TYR:O	1:B:357:SER:CA	2.53	0.56
1:A:1798:LEU:CA	1:A:1802:GLY:HA3	2.30	0.56
1:B:277:SER:O	1:B:280:ALA:HB3	2.06	0.56
1:B:1849:ASP:O	1:B:1850:LYS:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1976:CYS:O	1:B:1979:HIS:N	2.39	0.56
1:B:253:CYS:HA	1:B:262:VAL:HA	1.88	0.56
1:B:386:SER:O	1:B:432:ILE:N	2.29	0.56
1:B:1200:GLN:O	1:B:1203:ARG:N	2.39	0.56
1:B:1595:ASP:O	1:B:1599:ILE:CB	2.54	0.56
1:B:856:ASP:O	1:B:860:ASN:CB	2.53	0.56
1:A:563:SER:O	1:A:565:GLN:N	2.39	0.56
1:A:1048:THR:O	1:A:1050:LEU:N	2.36	0.56
1:A:1476:LYS:CA	1:A:1884:LYS:HA	2.36	0.56
1:A:256:HIS:H	1:A:261:HIS:N	2.03	0.56
1:A:254:ASP:O	1:A:256:HIS:N	2.39	0.56
1:A:233:ILE:HA	1:A:383:PRO:HA	1.86	0.56
1:B:2181:GLY:HA2	1:B:2184:ALA:HB3	1.88	0.56
1:A:1682:MET:O	1:A:1686:ARG:N	2.39	0.55
1:A:40:GLN:HA	1:A:206:CYS:HA	1.87	0.55
1:A:252:THR:C	1:A:263:PHE:O	2.44	0.55
1:A:551:HIS:O	1:A:554:ARG:N	2.37	0.55
1:B:676:GLU:O	1:B:680:VAL:N	2.35	0.55
1:B:7:SER:O	1:B:178:ILE:C	2.44	0.55
1:A:998:LYS:C	1:A:1007:GLN:HA	2.26	0.55
1:A:617:THR:O	1:A:621:LEU:CB	2.55	0.55
1:A:682:THR:O	1:A:686:ALA:HB3	2.07	0.55
1:B:1638:GLU:O	1:B:1640:THR:N	2.39	0.55
1:A:263:PHE:CB	1:A:416:LEU:H	2.19	0.55
1:A:457:ALA:HA	1:A:522:LEU:HA	1.88	0.55
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.05	0.55
1:A:297:GLY:O	1:A:381:LEU:HA	2.06	0.55
1:A:1371:LEU:O	1:A:1372:MET:C	2.42	0.55
1:A:1952:ALA:O	1:A:1954:ASP:N	2.40	0.55
1:B:1286:GLU:O	1:B:1289:GLU:O	2.25	0.55
1:B:1682:MET:CB	1:B:1687:GLY:H	2.19	0.55
1:B:1797:HIS:O	1:B:1802:GLY:N	2.29	0.55
1:A:1864:LYS:O	1:A:1867:GLN:N	2.39	0.55
1:A:704:ASN:C	1:A:706:GLU:H	2.10	0.55
1:A:7:SER:CB	1:A:179:GLY:N	2.69	0.55
1:B:2062:ILE:O	1:B:2066:THR:CB	2.55	0.55
1:B:848:VAL:O	1:B:850:GLN:N	2.40	0.55
1:A:195:ALA:HB3	1:A:216:THR:CB	2.37	0.55
1:B:680:VAL:C	1:B:682:THR:H	2.11	0.55
1:A:40:GLN:CA	1:A:206:CYS:HA	2.37	0.54
1:A:1317:LYS:HA	1:A:1323:ILE:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:LYS:CB	1:A:1883:ASN:HA	2.38	0.54
1:B:117:TYR:C	1:B:119:ASN:H	2.11	0.54
1:B:139:PRO:HA	1:B:147:MET:HA	1.89	0.54
1:A:1862:ARG:O	1:A:1866:ALA:HB2	2.07	0.54
1:B:1129:SER:CB	1:B:1180:LEU:HA	2.38	0.54
1:B:127:LYS:C	1:B:129:ASN:N	2.57	0.54
1:B:91:LYS:O	1:B:95:ALA:HB2	2.07	0.54
1:A:11:ILE:H	1:A:113:THR:C	2.09	0.54
1:B:1093:VAL:HA	1:B:1176:VAL:N	2.22	0.54
1:B:863:THR:O	1:B:867:VAL:CB	2.55	0.54
1:A:253:CYS:HA	1:A:263:PHE:H	1.73	0.54
1:A:475:LYS:O	1:A:479:ASP:CB	2.56	0.54
1:B:2185:LEU:HA	1:B:2188:TYR:CB	2.38	0.54
1:B:1405:ILE:O	1:B:1408:VAL:N	2.41	0.54
1:A:11:ILE:H	1:A:113:THR:N	2.06	0.54
1:B:1235:ARG:O	1:B:1238:HIS:N	2.41	0.54
1:B:1445:HIS:C	1:B:1447:TRP:H	2.11	0.54
1:B:780:SER:O	1:B:783:ARG:N	2.40	0.54
1:A:199:GLN:HA	1:A:207:ASN:HA	1.89	0.54
1:B:1682:MET:O	1:B:1685:ASP:N	2.41	0.54
1:A:1682:MET:C	1:A:1685:ASP:H	2.12	0.53
1:A:2020:LEU:O	1:A:2023:TYR:N	2.40	0.53
1:A:45:ASP:N	1:A:48:ASN:O	2.36	0.53
1:B:1052:LEU:HA	1:B:1056:GLY:H	1.72	0.53
1:A:123:LEU:O	1:A:132:LEU:N	2.36	0.53
1:B:570:ASN:O	1:B:573:TYR:N	2.42	0.53
1:A:1798:LEU:HA	1:A:1802:GLY:CA	2.30	0.53
1:B:299:TRP:H	1:B:380:SER:C	2.10	0.53
1:A:1682:MET:HA	1:A:1685:ASP:CB	2.39	0.53
1:B:1026:GLY:HA2	1:B:1594:ARG:CB	2.38	0.53
1:B:1796:CYS:HA	1:B:1799:ASP:CB	2.39	0.53
1:B:729:ILE:O	1:B:732:TYR:N	2.41	0.53
1:A:38:VAL:HA	1:A:208:GLU:HA	1.91	0.53
1:B:62:PRO:O	1:B:64:ASN:N	2.42	0.53
1:A:865:GLU:O	1:A:869:LEU:CB	2.57	0.53
1:A:1209:GLY:O	1:A:1213:VAL:CB	2.57	0.52
1:A:2010:CYS:O	1:A:2012:SER:N	2.43	0.52
1:B:1211:HIS:O	1:B:1214:VAL:N	2.42	0.52
1:B:1341:VAL:O	1:B:1345:TYR:N	2.42	0.52
1:B:1277:PHE:O	1:B:1280:ASN:N	2.43	0.52
1:B:200:LEU:O	1:B:203:ASN:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HA	1:A:219:LYS:O	2.10	0.52
1:B:10:HIS:H	1:B:13:ASP:CB	2.22	0.52
1:B:163:ILE:O	1:B:164:GLN:O	2.27	0.52
1:B:236:GLY:HA3	1:B:286:VAL:H	1.74	0.52
1:A:85:ASP:HA	1:A:86:ALA:C	2.30	0.52
1:B:127:LYS:C	1:B:129:ASN:H	2.11	0.52
1:B:315:ALA:HA	1:B:366:SER:CA	2.35	0.52
1:B:315:ALA:H	1:B:357:SER:HA	1.75	0.52
1:B:577:GLN:O	1:B:581:MET:N	2.32	0.52
1:A:1111:ASN:O	1:A:1115:ILE:N	2.43	0.52
1:B:242:LEU:C	1:B:251:LEU:H	2.06	0.52
1:A:1297:HIS:O	1:A:1301:THR:N	2.43	0.52
1:B:1608:SER:O	1:B:1612:ASP:CB	2.57	0.52
1:B:2186:GLU:O	1:B:2189:ALA:N	2.41	0.52
1:A:19:ALA:HA	1:A:217:SER:O	2.09	0.52
1:A:2184:ALA:HA	1:A:2187:PHE:CB	2.40	0.52
1:A:684:GLU:O	1:A:687:LEU:CB	2.58	0.52
1:A:977:ILE:O	1:A:981:ILE:CB	2.58	0.52
1:A:1986:PHE:O	1:A:1990:GLN:N	2.43	0.52
1:A:2114:ASN:O	1:A:2116:ARG:N	2.43	0.52
1:A:265:ARG:O	1:A:267:THR:N	2.44	0.51
1:A:459:LYS:O	1:A:463:GLY:N	2.31	0.51
1:A:7:SER:HA	1:A:177:VAL:CA	2.40	0.51
1:B:136:LYS:HA	1:B:147:MET:CB	2.40	0.51
1:A:854:PHE:O	1:A:857:LYS:N	2.41	0.51
1:A:896:ASP:C	1:A:898:VAL:H	2.13	0.51
1:B:117:TYR:HA	1:B:163:ILE:O	2.10	0.51
1:B:654:LYS:O	1:B:658:ASN:N	2.39	0.51
1:B:984:VAL:O	1:B:989:ARG:N	2.43	0.51
1:B:421:SER:O	1:B:422:PRO:C	2.49	0.51
1:A:1341:VAL:O	1:A:1344:PHE:N	2.43	0.51
1:A:316:ALA:HA	1:A:354:SER:O	2.10	0.51
1:B:1488:THR:O	1:B:1492:SER:N	2.42	0.51
1:B:1850:LYS:O	1:B:1854:LYS:CB	2.59	0.51
1:B:242:LEU:O	1:B:250:PHE:HA	2.10	0.51
1:A:1179:ILE:O	1:A:1183:LEU:CB	2.58	0.51
1:B:2063:ASP:HA	1:B:2113:TYR:CB	2.41	0.51
1:B:7:SER:N	1:B:177:VAL:CB	2.73	0.51
1:B:867:VAL:O	1:B:870:ALA:N	2.43	0.51
1:A:19:ALA:O	1:A:24:ASN:HA	2.11	0.51
1:A:399:VAL:HA	1:A:421:SER:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2129:MET:O	1:B:2131:GLY:N	2.43	0.51
1:A:692:ASP:O	1:A:696:VAL:N	2.43	0.51
1:B:11:ILE:C	1:B:13:ASP:N	2.63	0.51
1:A:1636:PHE:O	1:A:1638:GLU:N	2.44	0.51
1:B:1387:GLY:O	1:B:1389:ASN:N	2.44	0.51
1:B:165:PRO:HA	1:B:182:VAL:HA	1.92	0.51
1:B:885:LEU:C	1:B:888:THR:H	2.14	0.51
1:A:1085:ARG:O	1:A:1087:PHE:N	2.44	0.50
1:A:100:LYS:O	1:A:101:LYS:C	2.48	0.50
1:B:397:THR:HA	1:B:422:PRO:HA	1.93	0.50
1:B:652:ILE:O	1:B:655:ALA:HB3	2.12	0.50
1:A:2003:LEU:O	1:A:2007:ASP:CB	2.60	0.50
1:B:1489:PHE:HA	1:B:1493:PRO:CA	2.42	0.50
1:B:1867:GLN:O	1:B:1871:LYS:N	2.27	0.50
1:B:665:LEU:O	1:B:671:VAL:N	2.45	0.50
1:B:1095:GLN:O	1:B:1096:ALA:C	2.50	0.50
1:A:2018:GLY:C	1:A:2020:LEU:N	2.62	0.50
1:A:221:VAL:O	1:A:222:LEU:O	2.29	0.50
1:B:1289:GLU:C	1:B:1291:VAL:N	2.64	0.50
1:A:476:LEU:O	1:A:479:ASP:N	2.44	0.50
1:A:1238:HIS:O	1:A:1240:PHE:N	2.45	0.49
1:B:1636:PHE:C	1:B:1638:GLU:H	2.13	0.49
1:B:1820:PHE:O	1:B:1822:GLU:N	2.45	0.49
1:A:2114:ASN:C	1:A:2116:ARG:N	2.66	0.49
1:A:554:ARG:HA	1:A:557:TYR:CB	2.42	0.49
1:B:2036:LEU:O	1:B:2040:THR:CB	2.60	0.49
1:B:243:PHE:HA	1:B:249:LYS:O	2.11	0.49
1:B:281:LEU:O	1:B:308:LEU:CB	2.60	0.49
1:B:387:TYR:HA	1:B:431:ALA:HA	1.94	0.49
1:A:2173:LEU:O	1:A:2177:GLY:N	2.45	0.49
1:A:391:ARG:HA	1:A:398:TRP:N	2.27	0.49
1:B:1115:ILE:C	1:B:1117:GLN:H	2.16	0.49
1:B:1225:ALA:HB1	1:B:1226:GLU:HA	1.94	0.49
1:A:15:CYS:HA	1:A:223:PHE:N	2.27	0.49
1:A:255:GLU:C	1:A:259:LYS:O	2.51	0.49
1:A:1863:MET:O	1:A:1867:GLN:N	2.38	0.49
1:A:2119:GLU:O	1:A:2123:VAL:CB	2.60	0.49
1:B:2007:ASP:O	1:B:2011:GLY:N	2.46	0.49
1:B:666:ILE:H	1:B:667:GLU:CA	2.26	0.49
1:B:2044:GLN:C	1:B:2046:PRO:N	2.65	0.49
1:B:279:LYS:H	1:B:309:ALA:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLY:HA2	1:B:226:TRP:CB	2.43	0.49
1:A:391:ARG:HA	1:A:398:TRP:CA	2.42	0.49
1:B:1682:MET:C	1:B:1686:ARG:H	2.16	0.49
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.43	0.49
1:A:2019:LEU:O	1:A:2021:GLY:N	2.46	0.49
1:B:1127:GLU:O	1:B:1130:GLU:N	2.41	0.49
1:B:763:LEU:O	1:B:767:CYS:CB	2.60	0.49
1:B:860:ASN:O	1:B:861:LYS:C	2.51	0.49
1:A:2189:ALA:O	1:A:2191:HIS:N	2.45	0.48
1:A:1872:ALA:O	1:A:1876:VAL:CB	2.61	0.48
1:A:13:ASP:HA	1:A:226:TRP:N	2.28	0.48
1:A:826:LYS:O	1:A:830:LYS:CB	2.61	0.48
1:B:1843:PHE:O	1:B:1846:LEU:N	2.45	0.48
1:B:16:SER:N	1:B:221:VAL:O	2.30	0.48
1:A:39:VAL:C	1:A:207:ASN:H	2.16	0.48
1:A:2043:CYS:C	1:A:2097:ALA:HB1	2.34	0.48
1:A:2043:CYS:O	1:A:2097:ALA:HB1	2.14	0.48
1:A:724:LYS:O	1:A:726:ASP:N	2.47	0.48
1:B:298:TYR:HA	1:B:381:LEU:CA	2.43	0.48
1:B:298:TYR:HA	1:B:381:LEU:HA	1.95	0.48
1:B:986:LEU:C	1:B:988:TYR:H	2.16	0.48
1:A:2150:ASN:O	1:A:2153:HIS:N	2.46	0.48
1:A:355:LEU:H	1:A:419:GLY:CA	2.27	0.48
1:A:558:ARG:C	1:A:560:LEU:N	2.67	0.48
1:A:1631:ARG:CB	1:A:1648:SER:H	2.26	0.48
1:A:8:PHE:N	1:A:177:VAL:C	2.59	0.48
1:B:1634:LEU:O	1:B:1638:GLU:O	2.31	0.48
1:B:180:ASP:C	1:B:219:LYS:HA	2.34	0.48
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.44	0.48
1:A:781:PHE:O	1:A:784:LEU:N	2.46	0.48
1:B:1199:LYS:C	1:B:1201:GLN:N	2.67	0.48
1:B:233:ILE:CB	1:B:383:PRO:HA	2.44	0.48
1:A:1049:PRO:O	1:A:1053:ASP:N	2.43	0.47
1:A:1332:ALA:O	1:A:1335:VAL:N	2.42	0.47
1:A:225:LYS:H	1:A:228:ASP:CB	2.25	0.47
1:B:2015:GLY:O	1:B:2067:ALA:HB1	2.14	0.47
1:A:15:CYS:HA	1:A:222:LEU:CA	2.42	0.47
1:A:239:VAL:O	1:A:434:PRO:HA	2.14	0.47
1:B:1061:LEU:O	1:B:1064:LEU:CB	2.63	0.47
1:B:111:LEU:C	1:B:113:THR:H	2.18	0.47
1:A:204:PRO:O	1:A:205:GLY:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2068:LEU:O	1:A:2072:ASP:HA	2.14	0.47
1:A:1789:MET:N	1:B:1789:MET:N	2.62	0.47
1:A:1341:VAL:O	1:A:1345:TYR:N	2.44	0.47
1:B:365:SER:HA	1:B:394:CYS:CB	2.44	0.47
1:B:680:VAL:C	1:B:682:THR:N	2.67	0.47
1:B:617:THR:O	1:B:621:LEU:CB	2.63	0.47
1:A:10:HIS:CB	1:A:112:GLY:HA2	2.45	0.47
1:B:315:ALA:CB	1:B:358:VAL:H	2.27	0.47
1:A:1980:ASN:HA	1:A:2038:SER:HA	1.97	0.47
1:B:2184:ALA:O	1:B:2188:TYR:CB	2.62	0.47
1:B:15:CYS:CA	1:B:223:PHE:H	2.25	0.47
1:B:696:VAL:O	1:B:697:TRP:C	2.53	0.47
1:A:149:VAL:CB	1:A:210:ASN:HA	2.45	0.46
1:A:576:LYS:O	1:A:578:PHE:N	2.48	0.46
1:B:125:HIS:O	1:B:127:LYS:N	2.48	0.46
1:A:869:LEU:O	1:A:873:LEU:CB	2.64	0.46
1:B:305:PHE:O	1:B:313:TYR:HA	2.16	0.46
1:A:98:LEU:O	1:A:101:LYS:N	2.48	0.46
1:B:1053:ASP:O	1:B:1057:GLY:HA3	2.16	0.46
1:B:1880:ASP:C	1:B:1882:GLY:H	2.18	0.46
1:B:299:TRP:H	1:B:380:SER:CB	2.28	0.46
1:B:620:SER:O	1:B:624:LYS:N	2.43	0.46
1:B:1632:PRO:O	1:B:1634:LEU:N	2.49	0.46
1:A:13:ASP:HA	1:A:225:LYS:C	2.36	0.46
1:A:1973:GLN:O	1:A:1976:CYS:N	2.48	0.46
1:A:180:ASP:O	1:A:219:LYS:HA	2.15	0.46
1:B:1632:PRO:O	1:B:1636:PHE:N	2.41	0.46
1:B:2197:ILE:HA	1:B:2212:PRO:CA	2.46	0.46
1:A:68:ALA:O	1:A:72:PHE:CB	2.63	0.46
1:B:1199:LYS:O	1:B:1202:GLN:N	2.47	0.46
1:B:476:LEU:O	1:B:477:LEU:C	2.53	0.46
1:A:1001:PHE:O	1:A:1003:GLU:N	2.44	0.46
1:A:1271:VAL:O	1:A:1275:HIS:N	2.46	0.46
1:A:979:GLN:O	1:A:982:LEU:N	2.49	0.46
1:B:117:TYR:CB	1:B:172:ILE:HA	2.46	0.46
1:B:773:LEU:C	1:B:775:TYR:H	2.13	0.46
1:A:1245:CYS:CB	1:A:1285:SER:O	2.64	0.45
1:B:131:TYR:O	1:B:152:ASP:O	2.34	0.45
1:A:393:LEU:C	1:A:396:ASN:H	2.20	0.45
1:A:659:PRO:O	1:A:661:ASN:N	2.48	0.45
1:B:2147:SER:O	1:B:2151:VAL:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:LEU:O	1:B:864:PHE:N	2.49	0.45
1:A:1966:GLN:O	1:A:1970:ARG:CB	2.63	0.45
1:B:1214:VAL:O	1:B:1215:LEU:C	2.55	0.45
1:B:1843:PHE:O	1:B:1847:THR:N	2.45	0.45
1:B:594:THR:O	1:B:597:ALA:HB3	2.15	0.45
1:B:444:ASP:O	1:B:447:ASN:N	2.49	0.45
1:A:616:ASP:O	1:A:620:SER:CB	2.65	0.45
1:B:11:ILE:O	1:B:13:ASP:N	2.50	0.45
1:B:1986:PHE:O	1:B:1987:LEU:C	2.54	0.45
1:B:356:VAL:O	1:B:358:VAL:N	2.50	0.45
1:A:140:ALA:HB2	1:A:147:MET:C	2.37	0.45
1:B:15:CYS:HA	1:B:223:PHE:N	2.25	0.45
1:B:183:VAL:O	1:B:185:ASN:N	2.44	0.45
1:B:1847:THR:O	1:B:1850:LYS:N	2.50	0.45
1:A:1116:LYS:O	1:A:1117:GLN:C	2.55	0.45
1:A:870:ALA:HA	1:A:873:LEU:CB	2.47	0.45
1:A:253:CYS:HA	1:A:263:PHE:N	2.31	0.45
1:A:716:ALA:O	1:A:718:ASP:N	2.50	0.45
1:A:7:SER:CB	1:A:180:ASP:N	2.80	0.45
1:B:313:TYR:O	1:B:357:SER:HA	2.17	0.45
1:A:445:PHE:O	1:A:449:ALA:HB2	2.17	0.45
1:B:1218:LEU:C	1:B:1220:ILE:H	2.20	0.45
1:A:1197:SER:O	1:A:1200:GLN:N	2.50	0.44
1:A:480:LEU:C	1:A:483:PHE:H	2.20	0.44
1:B:1820:PHE:C	1:B:1822:GLU:N	2.69	0.44
1:B:2202:ARG:CB	1:B:2206:GLN:HA	2.47	0.44
1:B:279:LYS:CA	1:B:309:ALA:HB2	2.47	0.44
1:B:397:THR:CA	1:B:422:PRO:HA	2.47	0.44
1:B:648:THR:O	1:B:651:LEU:N	2.49	0.44
1:A:40:GLN:N	1:A:206:CYS:HA	2.31	0.44
1:B:121:ILE:O	1:B:160:TRP:HA	2.17	0.44
1:B:1682:MET:O	1:B:1685:ASP:C	2.54	0.44
1:B:118:GLY:N	1:B:163:ILE:C	2.69	0.44
1:B:116:GLN:HA	1:B:175:SER:HA	1.99	0.44
1:A:2044:GLN:HA	1:A:2097:ALA:HB1	1.99	0.44
1:A:370:LEU:HA	1:A:389:ARG:O	2.17	0.44
1:A:399:VAL:HA	1:A:420:THR:HA	2.00	0.44
1:A:838:GLU:O	1:A:840:VAL:N	2.50	0.44
1:B:1211:HIS:O	1:B:1213:VAL:N	2.50	0.44
1:B:89:LEU:O	1:B:93:HIS:CB	2.65	0.44
1:A:1682:MET:CA	1:A:1686:ARG:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LYS:O	1:B:524:GLN:N	2.51	0.44
1:A:1476:LYS:HA	1:A:1884:LYS:CA	2.47	0.44
1:A:399:VAL:HA	1:A:421:SER:N	2.31	0.44
1:A:558:ARG:C	1:A:560:LEU:H	2.21	0.44
1:B:1682:MET:C	1:B:1685:ASP:H	2.21	0.44
1:B:179:GLY:HA2	1:B:220:ILE:O	2.18	0.44
1:B:113:THR:O	1:B:114:VAL:C	2.56	0.44
1:B:117:TYR:C	1:B:119:ASN:N	2.70	0.44
1:A:2126:LYS:O	1:A:2130:GLN:CB	2.66	0.44
1:A:398:TRP:O	1:A:421:SER:CB	2.66	0.44
1:A:690:GLY:O	1:A:691:GLU:C	2.56	0.44
1:A:979:GLN:O	1:A:983:ASN:N	2.41	0.44
1:B:1178:GLU:O	1:B:1182:ARG:CB	2.66	0.44
1:B:2186:GLU:O	1:B:2189:ALA:HB3	2.17	0.44
1:A:1680:GLU:C	1:A:1682:MET:N	2.71	0.44
1:A:1795:GLN:HA	1:A:1798:LEU:CB	2.48	0.44
1:B:1252:GLN:O	1:B:1255:LEU:N	2.51	0.44
1:B:2029:VAL:O	1:B:2030:ALA:C	2.55	0.44
1:B:2186:GLU:C	1:B:2189:ALA:H	2.19	0.44
1:B:440:VAL:O	1:B:443:LEU:N	2.51	0.44
1:B:893:ALA:O	1:B:896:ASP:N	2.51	0.44
1:A:1295:PHE:C	1:A:1297:HIS:N	2.72	0.43
1:A:1848:GLU:C	1:A:1850:LYS:N	2.64	0.43
1:A:645:ILE:O	1:A:648:THR:N	2.51	0.43
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.67	0.43
1:B:118:GLY:C	1:B:163:ILE:H	2.21	0.43
1:B:755:ILE:O	1:B:758:GLN:N	2.50	0.43
1:A:978:LEU:HA	1:A:981:ILE:CB	2.49	0.43
1:B:1289:GLU:O	1:B:1291:VAL:N	2.51	0.43
1:A:20:GLU:HA	1:A:24:ASN:HA	2.00	0.43
1:A:551:HIS:C	1:A:554:ARG:H	2.22	0.43
1:A:715:LEU:O	1:A:716:ALA:C	2.57	0.43
1:A:7:SER:HA	1:A:177:VAL:C	2.38	0.43
1:B:1682:MET:CA	1:B:1686:ARG:H	2.32	0.43
1:B:1682:MET:CB	1:B:1687:GLY:N	2.82	0.43
1:B:572:GLU:O	1:B:574:ILE:N	2.52	0.43
1:B:719:ALA:C	1:B:722:GLY:H	2.22	0.43
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.66	0.43
1:A:1883:ASN:HA	1:A:1884:LYS:HA	1.75	0.43
1:A:7:SER:CB	1:A:179:GLY:H	2.31	0.43
1:B:402:THR:CB	1:B:418:ILE:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:C	1:A:172:ILE:HA	2.39	0.43
1:A:13:ASP:HA	1:A:226:TRP:HA	2.00	0.43
1:A:659:PRO:C	1:A:661:ASN:H	2.21	0.43
1:A:761:VAL:O	1:A:762:ASP:C	2.56	0.43
1:B:670:LEU:HA	1:B:673:SER:CB	2.48	0.43
1:A:8:PHE:H	1:A:177:VAL:CA	2.31	0.43
1:B:1849:ASP:O	1:B:1850:LYS:O	2.36	0.43
1:B:860:ASN:O	1:B:863:THR:N	2.51	0.43
1:A:1417:GLU:O	1:A:1418:VAL:C	2.57	0.43
1:A:1477:TYR:HA	1:A:1881:LEU:O	2.19	0.43
1:A:862:LEU:O	1:A:863:THR:C	2.55	0.43
1:A:85:ASP:HA	1:A:86:ALA:O	2.18	0.43
1:A:480:LEU:O	1:A:481:VAL:C	2.57	0.42
1:A:715:LEU:O	1:A:717:GLN:N	2.51	0.42
1:B:118:GLY:H	1:B:164:GLN:N	2.17	0.42
1:B:1818:ARG:C	1:B:1820:PHE:N	2.72	0.42
1:B:181:LYS:HA	1:B:218:TRP:O	2.19	0.42
1:B:2061:GLY:C	1:B:2064:ILE:H	2.19	0.42
1:A:101:LYS:O	1:A:104:GLU:N	2.49	0.42
1:A:11:ILE:O	1:A:112:GLY:N	2.52	0.42
1:A:1375:ILE:HA	1:A:1378:VAL:CB	2.49	0.42
1:A:391:ARG:HA	1:A:397:THR:C	2.39	0.42
1:B:1457:ILE:C	1:B:1459:ARG:N	2.72	0.42
1:B:1649:GLY:O	1:B:1650:GLY:C	2.55	0.42
1:B:133:THR:O	1:B:149:VAL:HA	2.19	0.42
1:B:278:SER:O	1:B:279:LYS:C	2.58	0.42
1:A:2189:ALA:O	1:A:2190:LYS:C	2.58	0.42
1:A:598:LEU:O	1:A:599:LEU:C	2.57	0.42
1:B:773:LEU:C	1:B:775:TYR:N	2.72	0.42
1:B:1080:LEU:O	1:B:1084:PHE:N	2.35	0.42
1:B:134:VAL:HA	1:B:149:VAL:CB	2.49	0.42
1:B:315:ALA:CA	1:B:366:SER:HA	2.39	0.42
1:A:1369:SER:C	1:A:1371:LEU:N	2.73	0.42
1:A:354:SER:CA	1:A:419:GLY:HA3	2.40	0.42
1:A:982:LEU:O	1:A:986:LEU:N	2.36	0.42
1:B:622:VAL:O	1:B:626:ARG:HA	2.20	0.42
1:B:781:PHE:O	1:B:784:LEU:N	2.51	0.42
1:A:680:VAL:C	1:A:682:THR:H	2.21	0.42
1:B:1813:ASN:O	1:B:1814:ALA:C	2.58	0.42
1:B:1880:ASP:O	1:B:1882:GLY:N	2.44	0.42
1:A:1270:ALA:O	1:A:1272:THR:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2183:GLU:HA	1:A:2186:GLU:CB	2.50	0.42
1:A:19:ALA:HA	1:A:218:TRP:HA	2.02	0.42
1:A:252:THR:N	1:A:263:PHE:O	2.52	0.42
1:A:355:LEU:N	1:A:418:ILE:O	2.53	0.42
1:A:789:HIS:O	1:A:791:ASP:N	2.52	0.42
1:A:92:LEU:O	1:A:95:ALA:HB3	2.19	0.42
1:A:666:ILE:N	1:A:667:GLU:CA	2.80	0.42
1:B:690:GLY:O	1:B:691:GLU:C	2.58	0.42
1:A:1793:GLU:HA	1:A:1796:CYS:CB	2.50	0.41
1:A:648:THR:O	1:A:651:LEU:N	2.53	0.41
1:B:250:PHE:O	1:B:264:LEU:HA	2.20	0.41
1:A:191:GLN:CB	1:A:212:VAL:HA	2.50	0.41
1:A:16:SER:C	1:A:221:VAL:H	2.22	0.41
1:B:263:PHE:CB	1:B:416:LEU:O	2.68	0.41
1:A:1381:LEU:HA	1:A:1384:CYS:CB	2.50	0.41
1:A:2123:VAL:O	1:A:2127:ALA:CB	2.64	0.41
1:A:18:TYR:O	1:A:218:TRP:HA	2.21	0.41
1:B:1093:VAL:O	1:B:1096:ALA:HB3	2.20	0.41
1:B:1199:LYS:O	1:B:1200:GLN:C	2.58	0.41
1:B:62:PRO:O	1:B:63:MET:C	2.58	0.41
1:B:1236:LEU:O	1:B:1237:ALA:C	2.58	0.41
1:B:1633:GLU:HA	1:B:1636:PHE:CB	2.50	0.41
1:B:1840:HIS:O	1:B:1841:SER:C	2.58	0.41
1:B:305:PHE:C	1:B:314:LEU:H	2.15	0.41
1:B:91:LYS:O	1:B:95:ALA:CB	2.66	0.41
1:A:1118:ASP:O	1:A:1119:LEU:C	2.59	0.41
1:B:1080:LEU:O	1:B:1083:LEU:CB	2.68	0.41
1:B:756:SER:O	1:B:760:ASP:HA	2.20	0.41
1:A:166:PHE:N	1:A:182:VAL:HA	2.35	0.41
1:A:1836:THR:HA	1:A:1839:GLN:CB	2.50	0.41
1:A:724:LYS:C	1:A:726:ASP:H	2.22	0.41
1:B:1062:ARG:O	1:B:1063:VAL:C	2.59	0.41
1:B:253:CYS:O	1:B:279:LYS:CB	2.68	0.41
1:B:862:LEU:O	1:B:863:THR:C	2.59	0.41
1:A:772:ASN:O	1:A:773:LEU:C	2.57	0.41
1:B:2197:ILE:HA	1:B:2212:PRO:CB	2.51	0.41
1:B:251:LEU:HA	1:B:264:LEU:HA	2.03	0.41
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.50	0.41
1:A:1207:ASN:C	1:A:1209:GLY:N	2.73	0.41
1:A:1211:HIS:O	1:A:1215:LEU:CB	2.68	0.41
1:A:861:LYS:O	1:A:864:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:O	1:A:88:LEU:N	2.54	0.41
1:B:1106:SER:O	1:B:1107:GLN:CB	2.69	0.41
1:A:509:LEU:O	1:A:513:GLN:N	2.54	0.41
1:A:708:ARG:O	1:A:709:SER:C	2.59	0.41
1:B:675:PHE:O	1:B:679:GLY:HA3	2.21	0.41
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.34	0.41
1:B:706:GLU:O	1:B:708:ARG:N	2.44	0.41
1:A:1953:LYS:O	1:A:1954:ASP:C	2.59	0.40
1:A:368:PHE:HA	1:A:392:HIS:HA	2.04	0.40
1:B:1657:LYS:O	1:B:1660:LYS:N	2.44	0.40
1:B:1678:LEU:HA	1:B:1827:ALA:HA	2.02	0.40
1:A:243:PHE:O	1:A:430:PHE:CB	2.69	0.40
1:B:1214:VAL:O	1:B:1217:LEU:N	2.55	0.40
1:B:1824:ILE:O	1:B:1827:ALA:HB3	2.20	0.40
1:B:1966:GLN:C	1:B:1970:ARG:H	2.25	0.40
1:B:24:ASN:O	1:B:41:PRO:HA	2.22	0.40
1:B:740:PHE:O	1:B:742:ARG:N	2.55	0.40
1:A:1954:ASP:O	1:A:1955:ASP:C	2.60	0.40
1:A:255:GLU:HA	1:A:261:HIS:H	1.86	0.40
1:A:251:LEU:CA	1:A:264:LEU:HA	2.42	0.40
1:A:406:ILE:N	1:A:415:MET:O	2.55	0.40
1:A:580:PHE:O	1:A:581:MET:C	2.59	0.40
1:A:896:ASP:C	1:A:898:VAL:N	2.74	0.40
1:B:1459:ARG:C	1:B:1461:CYS:N	2.72	0.40
1:B:1682:MET:CB	1:B:1686:ARG:H	2.34	0.40
1:A:100:LYS:O	1:A:103:ASN:CB	2.70	0.40
1:A:1134:TYR:O	1:A:1230:MET:N	2.52	0.40
1:A:1680:GLU:C	1:A:1682:MET:H	2.24	0.40
1:B:2211:VAL:O	1:B:2212:PRO:C	2.59	0.40
1:A:157:GLU:C	1:A:159:SER:N	2.75	0.40
1:A:17:LEU:CB	1:A:220:ILE:HA	2.52	0.40
1:B:986:LEU:C	1:B:988:TYR:N	2.75	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	1682/2217 (76%)	1265 (75%)	296 (18%)	121 (7%)	1	14
1	B	1680/2217 (76%)	1193 (71%)	337 (20%)	150 (9%)	1	11
All	All	3362/4434 (76%)	2458 (73%)	633 (19%)	271 (8%)	1	12

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ALA
1	A	87	VAL
1	A	213	ASN
1	A	222	LEU
1	A	226	TRP
1	A	255	GLU
1	A	266	THR
1	A	478	GLU
1	A	479	ASP
1	A	502	PRO
1	A	522	LEU
1	A	598	LEU
1	A	628	PRO
1	A	659	PRO
1	A	666	ILE
1	A	681	SER
1	A	744	CYS
1	A	899	HIS
1	A	990	ILE
1	A	1239	GLU
1	A	1264	ASN
1	A	1370	PRO
1	A	1400	LEU
1	A	1637	PRO
1	A	1849	ASP
1	A	1864	LYS
1	A	1885	LYS
1	A	1966	GLN
1	A	1993	LYS
1	A	2013	THR
1	A	2046	PRO

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Mol	Chain	Res	Type
1	A	2071	ASN
1	A	2104	ASP
1	A	2143	ASP
1	A	2178	GLN
1	A	2210	PRO
1	B	38	VAL
1	B	113	THR
1	B	164	GLN
1	B	165	PRO
1	B	223	PHE
1	B	293	ARG
1	B	300	ASN
1	B	357	SER
1	B	405	PRO
1	B	513	GLN
1	B	628	PRO
1	B	659	PRO
1	B	666	ILE
1	B	681	SER
1	B	696	VAL
1	B	741	ALA
1	B	744	CYS
1	B	760	ASP
1	B	773	LEU
1	B	774	PRO
1	B	854	PHE
1	B	990	ILE
1	B	999	ARG
1	B	1008	SER
1	B	1095	GLN
1	B	1096	ALA
1	B	1107	GLN
1	B	1214	VAL
1	B	1220	ILE
1	B	1285	SER
1	B	1292	VAL
1	B	1300	GLU
1	B	1311	PHE
1	B	1400	LEU
1	B	1458	CYS
1	B	1462	ASN
1	B	1463	ASN

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Mol	Chain	Res	Type
1	B	1492	SER
1	B	1637	PRO
1	B	1814	ALA
1	B	1966	GLN
1	B	1967	PRO
1	B	1984	GLN
1	B	2046	PRO
1	B	2075	PRO
1	B	2117	PRO
1	B	2129	MET
1	B	2210	PRO
1	A	52	LYS
1	A	175	SER
1	A	177	VAL
1	A	564	GLN
1	A	600	HIS
1	A	684	GLU
1	A	716	ALA
1	A	717	GLN
1	A	725	GLU
1	A	740	PHE
1	A	854	PHE
1	A	1027	ALA
1	A	1095	GLN
1	A	1267	ILE
1	A	1288	ASN
1	A	1346	ASN
1	A	1347	ASP
1	A	1349	ALA
1	A	1372	MET
1	A	1435	VAL
1	A	1458	CYS
1	A	1461	CYS
1	A	1464	THR
1	A	1865	VAL
1	A	1881	LEU
1	A	1984	GLN
1	A	2011	GLY
1	A	2021	GLY
1	A	2115	MET
1	A	2146	ALA
1	A	2148	PRO

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Mol	Chain	Res	Type
1	B	12	GLY
1	B	63	MET
1	B	75	ALA
1	B	118	GLY
1	B	135	ASN
1	B	221	VAL
1	B	307	HIS
1	B	313	TYR
1	B	380	SER
1	B	381	LEU
1	B	414	VAL
1	B	422	PRO
1	B	423	LEU
1	B	450	SER
1	B	484	VAL
1	B	573	TYR
1	B	603	ARG
1	B	640	SER
1	B	665	LEU
1	B	767	CYS
1	B	790	VAL
1	B	849	CYS
1	B	893	ALA
1	B	1460	ALA
1	B	1461	CYS
1	B	1639	ASN
1	B	1797	HIS
1	B	1801	GLU
1	B	1817	ASP
1	B	1850	LYS
1	B	2146	ALA
1	A	100	LYS
1	A	227	SER
1	A	396	ASN
1	A	405	PRO
1	A	413	PRO
1	A	450	SER
1	A	604	LYS
1	A	1061	LEU
1	A	1086	HIS
1	A	1462	ASN
1	A	1630	HIS

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Mol	Chain	Res	Type
1	A	1820	PHE
1	A	1953	LYS
1	A	2060	ASN
1	A	2165	HIS
1	B	66	TYR
1	B	114	VAL
1	B	126	LEU
1	B	264	LEU
1	B	379	ASP
1	B	434	PRO
1	B	514	ASN
1	B	521	LYS
1	B	682	THR
1	B	686	ALA
1	B	707	ILE
1	B	722	GLY
1	B	776	ASP
1	B	993	LEU
1	B	1002	ASP
1	B	1116	LYS
1	B	1200	GLN
1	B	1241	LEU
1	B	1268	LEU
1	B	1388	LYS
1	B	1391	TYR
1	B	1821	HIS
1	B	2060	ASN
1	B	2085	LEU
1	B	2130	GLN
1	B	2165	HIS
1	B	2205	GLU
1	A	40	GLN
1	A	51	LYS
1	A	447	ASN
1	A	599	LEU
1	A	704	ASN
1	A	1096	ALA
1	A	1221	PRO
1	A	1299	ILE
1	A	1887	ASP
1	A	2202	ARG
1	B	41	PRO

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Mol	Chain	Res	Type
1	B	279	LYS
1	B	684	GLU
1	B	694	GLU
1	B	699	PHE
1	B	778	ARG
1	B	887	LEU
1	B	968	MET
1	B	982	LEU
1	B	1198	ARG
1	B	1211	HIS
1	B	1290	ARG
1	B	1632	PRO
1	B	1881	LEU
1	B	2070	LEU
1	A	602	ASN
1	A	645	ILE
1	A	790	VAL
1	A	852	PHE
1	A	895	LEU
1	A	897	CYS
1	A	1275	HIS
1	A	1463	ASN
1	A	2020	LEU
1	A	2190	LYS
1	A	2215	CYS
1	B	230	LYS
1	B	285	GLU
1	B	424	LYS
1	B	439	GLU
1	B	473	VAL
1	B	522	LEU
1	B	703	SER
1	B	863	THR
1	B	1271	VAL
1	B	1996	TYR
1	B	2029	VAL
1	B	2147	SER
1	B	2207	ILE
1	B	2209	PHE
1	A	120	VAL
1	A	705	LYS
1	A	715	LEU

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Mol	Chain	Res	Type
1	A	1369	SER
1	A	1466	ASP
1	A	1991	ASN
1	A	2147	SER
1	B	418	ILE
1	B	680	VAL
1	B	1466	ASP
1	B	1651	PHE
1	A	38	VAL
1	A	178	ILE
1	A	383	PRO
1	B	191	GLN
1	B	367	ILE
1	B	1299	ILE
1	A	559	VAL
1	A	707	ILE
1	A	1874	VAL
1	A	2062	ILE
1	B	1291	VAL
1	B	1341	VAL
1	B	1370	PRO
1	A	1418	VAL
1	B	179	GLY
1	B	1631	ARG
1	A	894	ILE
1	A	1838	ILE
1	A	1967	PRO
1	B	212	VAL
1	B	2045	GLY
1	B	186	PRO

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1710/2217 (77%)	0.34	184 (10%) 5 9	0, 157, 428, 888	0
1	B	1708/2217 (77%)	0.29	175 (10%) 6 10	0, 136, 432, 776	0
All	All	3418/4434 (77%)	0.31	359 (10%) 6 9	0, 147, 430, 888	0

All (359) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2102	ARG	18.5
1	A	2103	HIS	16.7
1	A	2101	SER	13.2
1	A	2107	ASN	13.0
1	A	1395	LYS	11.4
1	A	1387	GLY	11.0
1	B	1442	THR	10.8
1	B	1439	GLU	10.8
1	A	2104	ASP	10.7
1	B	2216	GLU	10.5
1	B	1443	SER	10.5
1	B	1438	LYS	10.4
1	B	1437	MET	10.3
1	A	1396	CYS	10.1
1	A	1385	THR	9.7
1	B	1436	GLU	9.5
1	A	2105	SER	9.4
1	B	588	ASP	9.4
1	B	1326	CYS	9.0
1	A	1458	CYS	9.0
1	B	1329	MET	8.8
1	A	1388	LYS	8.6
1	A	2106	GLU	8.6
1	A	1454	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	1457	ILE	8.3
1	B	2018	GLY	7.9
1	B	1328	ASP	7.8
1	B	2019	LEU	7.7
1	A	2099	MET	7.6
1	B	639	VAL	7.5
1	A	2142	GLU	7.4
1	A	2140	ASN	7.3
1	A	2141	GLY	7.2
1	B	2163	ALA	7.0
1	A	1386	GLU	7.0
1	B	585	ILE	7.0
1	B	2215	CYS	6.9
1	B	463	GLY	6.9
1	B	2205	GLU	6.8
1	B	1370	PRO	6.7
1	B	2020	LEU	6.6
1	A	1389	ASN	6.6
1	B	584	GLN	6.6
1	B	1389	ASN	6.5
1	A	1384	CYS	6.5
1	A	1455	VAL	6.5
1	B	1413	ASP	6.4
1	A	215	ASN	6.3
1	A	1456	ASP	6.2
1	B	2164	ARG	6.2
1	B	638	CYS	6.2
1	A	2210	PRO	6.1
1	B	1327	GLN	6.1
1	A	1468	LYS	6.1
1	B	1416	PRO	6.1
1	B	1307	GLN	6.0
1	B	582	GLN	6.0
1	A	1026	GLY	6.0
1	B	1325	LYS	6.0
1	B	1369	SER	5.9
1	B	462	LYS	5.9
1	B	2206	GLN	5.8
1	B	1415	ILE	5.7
1	B	1385	THR	5.7
1	B	1440	ILE	5.7
1	A	2196	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	2143	ASP	5.6
1	B	1444	ASN	5.5
1	A	309	ALA	5.5
1	A	2100	GLU	5.5
1	A	2098	ILE	5.5
1	A	1027	ALA	5.4
1	B	1429	CYS	5.4
1	B	1388	LYS	5.4
1	B	1414	CYS	5.3
1	B	1387	GLY	5.3
1	B	1465	SER	5.3
1	A	2108	ALA	5.3
1	A	1177	LYS	5.2
1	A	305	PHE	5.2
1	B	583	LYS	5.2
1	B	586	GLY	5.2
1	A	2042	TYR	5.1
1	B	1834	GLY	5.1
1	B	2023	TYR	5.1
1	A	1984	GLN	5.1
1	A	1178	GLU	5.1
1	B	1330	VAL	5.1
1	A	1368	ASN	5.0
1	B	1427	ASN	5.0
1	A	2198	VAL	4.9
1	A	1367	GLU	4.9
1	B	1835	ASN	4.9
1	A	1451	GLU	4.9
1	B	1428	HIS	4.9
1	A	310	THR	4.8
1	B	1386	GLU	4.8
1	A	37	CYS	4.8
1	B	1348	ARG	4.8
1	A	2043	CYS	4.7
1	B	195	ALA	4.7
1	B	1430	TYR	4.7
1	B	459	LYS	4.6
1	B	587	TYR	4.6
1	B	1431	VAL	4.6
1	B	640	SER	4.6
1	B	194	HIS	4.5
1	A	2197	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	2209	PHE	4.4
1	B	2204	MET	4.4
1	A	1398	SER	4.4
1	B	589	VAL	4.4
1	A	209	VAL	4.4
1	A	1132	TRP	4.4
1	A	1394	ILE	4.4
1	A	2050	ASN	4.3
1	A	2110	ARG	4.3
1	A	987	ASP	4.3
1	A	1414	CYS	4.2
1	B	461	GLU	4.2
1	B	1333	GLU	4.2
1	B	1441	TYR	4.1
1	B	23	THR	4.1
1	B	2217	PHE	4.1
1	A	1983	LEU	4.0
1	A	2047	CYS	4.0
1	A	1642	ALA	4.0
1	B	1350	SER	4.0
1	A	1887	ASP	4.0
1	B	581	MET	4.0
1	A	1397	ASN	4.0
1	B	1349	ALA	4.0
1	B	2017	LEU	4.0
1	A	1288	ASN	4.0
1	B	1306	VAL	3.9
1	A	753	ASN	3.9
1	B	2207	ILE	3.9
1	B	1833	GLY	3.9
1	A	900	VAL	3.9
1	A	283	GLU	3.9
1	B	2165	HIS	3.8
1	A	2046	PRO	3.8
1	B	2160	HIS	3.8
1	A	879	TYR	3.8
1	A	1888	ASP	3.8
1	B	1305	ASN	3.7
1	B	405	PRO	3.7
1	B	403	ASN	3.7
1	B	1002	ASP	3.7
1	A	2051	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	2139	GLU	3.6
1	B	1466	ASP	3.6
1	A	195	ALA	3.6
1	A	2048	HIS	3.6
1	A	307	HIS	3.6
1	B	402	THR	3.6
1	B	1405	ILE	3.6
1	A	196	SER	3.6
1	A	1467	ARG	3.5
1	A	216	THR	3.5
1	A	1459	ARG	3.5
1	B	2074	ASN	3.5
1	A	306	LYS	3.5
1	B	1373	TYR	3.5
1	A	308	LEU	3.5
1	A	2199	ARG	3.5
1	B	404	ILE	3.4
1	B	2138	GLY	3.4
1	A	1492	SER	3.4
1	A	2045	GLY	3.4
1	B	25	GLY	3.4
1	A	880	ASN	3.4
1	A	2052	ASN	3.3
1	B	295	GLY	3.3
1	B	418	ILE	3.3
1	A	1434	GLU	3.3
1	A	1310	LYS	3.3
1	A	2029	VAL	3.2
1	A	1491	SER	3.2
1	A	754	GLU	3.2
1	A	2165	HIS	3.2
1	B	1371	LEU	3.2
1	A	2137	ASP	3.2
1	A	2109	GLU	3.2
1	B	1417	GLU	3.2
1	B	1310	LYS	3.2
1	A	1279	ASN	3.2
1	A	1438	LYS	3.2
1	A	1280	ASN	3.2
1	A	878	PHE	3.2
1	B	2166	ASN	3.2
1	A	285	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	3.2
1	A	2144	GLY	3.1
1	B	1324	LYS	3.1
1	A	314	LEU	3.1
1	A	1436	GLU	3.1
1	A	2027	LYS	3.1
1	A	2095	LEU	3.1
1	B	460	LEU	3.1
1	A	2097	ALA	3.1
1	B	2203	THR	3.1
1	A	210	ASN	3.1
1	B	66	TYR	3.0
1	B	2139	GLU	3.0
1	B	2162	LEU	3.0
1	A	1982	ASP	3.0
1	B	24	ASN	3.0
1	A	1392	THR	3.0
1	B	1372	MET	3.0
1	A	1441	TYR	3.0
1	B	464	THR	3.0
1	A	1493	PRO	3.0
1	A	1435	VAL	3.0
1	B	2079	LYS	3.0
1	A	1488	THR	3.0
1	A	409	GLU	2.9
1	B	2202	ARG	2.9
1	B	2161	GLN	2.9
1	B	1467	ARG	2.9
1	A	1433	THR	2.9
1	A	2138	GLY	2.9
1	A	1289	GLU	2.9
1	B	28	SER	2.9
1	A	129	ASN	2.9
1	A	2200	LEU	2.9
1	B	1435	VAL	2.9
1	B	1384	CYS	2.9
1	A	1089	GLN	2.8
1	A	135	ASN	2.8
1	A	626	ARG	2.8
1	B	1177	LYS	2.8
1	B	579	GLY	2.8
1	A	627	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2028	ASN	2.8
1	A	304	ARG	2.8
1	A	2161	GLN	2.8
1	B	704	ASN	2.8
1	A	1415	ILE	2.8
1	A	52	LYS	2.8
1	A	751	ALA	2.8
1	A	1439	GLU	2.7
1	B	578	PHE	2.7
1	B	1829	ALA	2.7
1	B	2193	ALA	2.7
1	A	1989	CYS	2.7
1	A	208	GLU	2.7
1	A	2041	GLU	2.7
1	A	38	VAL	2.7
1	B	267	THR	2.7
1	B	1404	ASP	2.6
1	B	85	ASP	2.6
1	B	1464	THR	2.6
1	B	2194	GLN	2.6
1	A	311	GLY	2.6
1	B	2201	ASP	2.6
1	A	1300	GLU	2.6
1	A	143	GLU	2.6
1	A	1179	ILE	2.6
1	A	1099	GLN	2.6
1	B	2159	ALA	2.6
1	B	2024	ILE	2.6
1	A	282	TRP	2.6
1	B	417	LYS	2.6
1	A	377	GLY	2.6
1	B	1681	MET	2.6
1	B	1003	GLU	2.5
1	A	1889	GLU	2.5
1	A	2211	VAL	2.5
1	A	1278	MET	2.5
1	A	1437	MET	2.5
1	A	1242	GLN	2.5
1	B	1304	ARG	2.5
1	A	2166	ASN	2.5
1	B	1303	GLY	2.5
1	A	1086	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2049	GLU	2.5
1	A	899	HIS	2.5
1	B	213	ASN	2.5
1	B	196	SER	2.4
1	B	458	GLY	2.4
1	B	1302	HIS	2.4
1	B	1432	ASP	2.4
1	B	969	ASP	2.4
1	B	1004	SER	2.4
1	A	1180	LEU	2.4
1	A	1360	SER	2.4
1	A	1489	PHE	2.4
1	A	1243	ASN	2.4
1	B	1390	VAL	2.4
1	B	580	PHE	2.4
1	B	660	THR	2.4
1	A	1886	LYS	2.4
1	B	1346	ASN	2.3
1	B	1679	ARG	2.3
1	A	1416	PRO	2.3
1	B	661	ASN	2.3
1	A	51	LYS	2.3
1	A	2112	LEU	2.3
1	B	2045	GLY	2.3
1	A	2044	GLN	2.3
1	B	294	GLY	2.3
1	B	1339	GLU	2.3
1	A	1133	VAL	2.3
1	A	1452	ASN	2.3
1	A	752	ILE	2.3
1	A	2096	LEU	2.3
1	B	1001	PHE	2.3
1	B	1300	GLU	2.3
1	A	1462	ASN	2.3
1	A	1641	ASP	2.3
1	A	2082	ASP	2.3
1	B	575	ALA	2.3
1	B	1830	LEU	2.3
1	B	1832	GLU	2.2
1	A	1329	MET	2.2
1	B	2146	ALA	2.2
1	B	1456	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1347	ASP	2.2
1	B	1605	ASP	2.2
1	A	826	LYS	2.2
1	B	1243	ASN	2.2
1	B	2046	PRO	2.2
1	B	1988	ARG	2.2
1	B	1053	ASP	2.2
1	A	145	ASN	2.2
1	B	419	GLY	2.2
1	A	27	ILE	2.2
1	A	1352	GLN	2.2
1	A	571	GLN	2.2
1	B	2002	THR	2.2
1	A	141	LEU	2.2
1	B	2080	ARG	2.2
1	B	52	LYS	2.1
1	B	2001	GLU	2.1
1	B	1434	GLU	2.1
1	B	401	SER	2.1
1	B	1412	GLU	2.1
1	B	960	PRO	2.1
1	A	1366	ASP	2.1
1	B	137	ARG	2.1
1	A	2026	GLU	2.1
1	B	27	ILE	2.1
1	A	1277	PHE	2.1
1	A	1333	GLU	2.1
1	A	1461	CYS	2.1
1	A	2030	ALA	2.1
1	A	2160	HIS	2.1
1	B	2021	GLY	2.1
1	B	2073	ILE	2.0
1	A	1985	ASN	2.0
1	B	210	ASN	2.0
1	A	697	TRP	2.0
1	A	2212	PRO	2.0
1	B	1029	ASP	2.0
1	B	1461	CYS	2.0
1	A	378	GLY	2.0
1	B	1402	LEU	2.0
1	A	827	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.