



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:06 PM GMT

PDB ID : 4UW2  
Title : Crystal structure of Csm1 in T. onnurineus  
Authors : Jung, T.Y.; An, Y.; Park, K.H.; Lee, M.H.; Oh, B.H.; Woo, E.J.  
Deposited on : 2014-08-08  
Resolution : 2.63 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

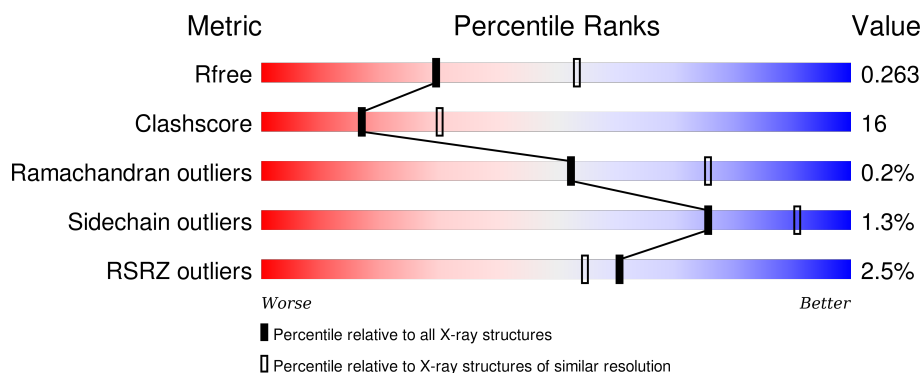
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	779	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	779	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>8%</div> </div> </div>
1	C	779	<div> <div>2%</div> <div> <div></div> <div>17%</div> <div>8%</div> <div>74%</div> </div> </div>
1	D	779	<div> <div>%</div> <div> <div></div> <div>8%</div> <div>•</div> <div>88%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14308 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 CSM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	Se	0	0	0
			5586	3596	959	1016	1	14			
1	B	713	Total	C	N	O	S	Se	0	0	0
			5719	3679	987	1038	2	13			
1	C	201	Total	C	N	O	S	Se	0	0	0
			1640	1063	287	286	4				
1	D	92	Total	C	N	O	S	Se	0	0	0
			753	487	135	130	1				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	EXPRESSION TAG	UNP B6YWB8
A	0	MSE	-	EXPRESSION TAG	UNP B6YWB8
B	-1	ALA	-	EXPRESSION TAG	UNP B6YWB8
B	0	MSE	-	EXPRESSION TAG	UNP B6YWB8
C	-1	ALA	-	EXPRESSION TAG	UNP B6YWB8
C	0	MSE	-	EXPRESSION TAG	UNP B6YWB8
D	-1	ALA	-	EXPRESSION TAG	UNP B6YWB8
D	0	MSE	-	EXPRESSION TAG	UNP B6YWB8

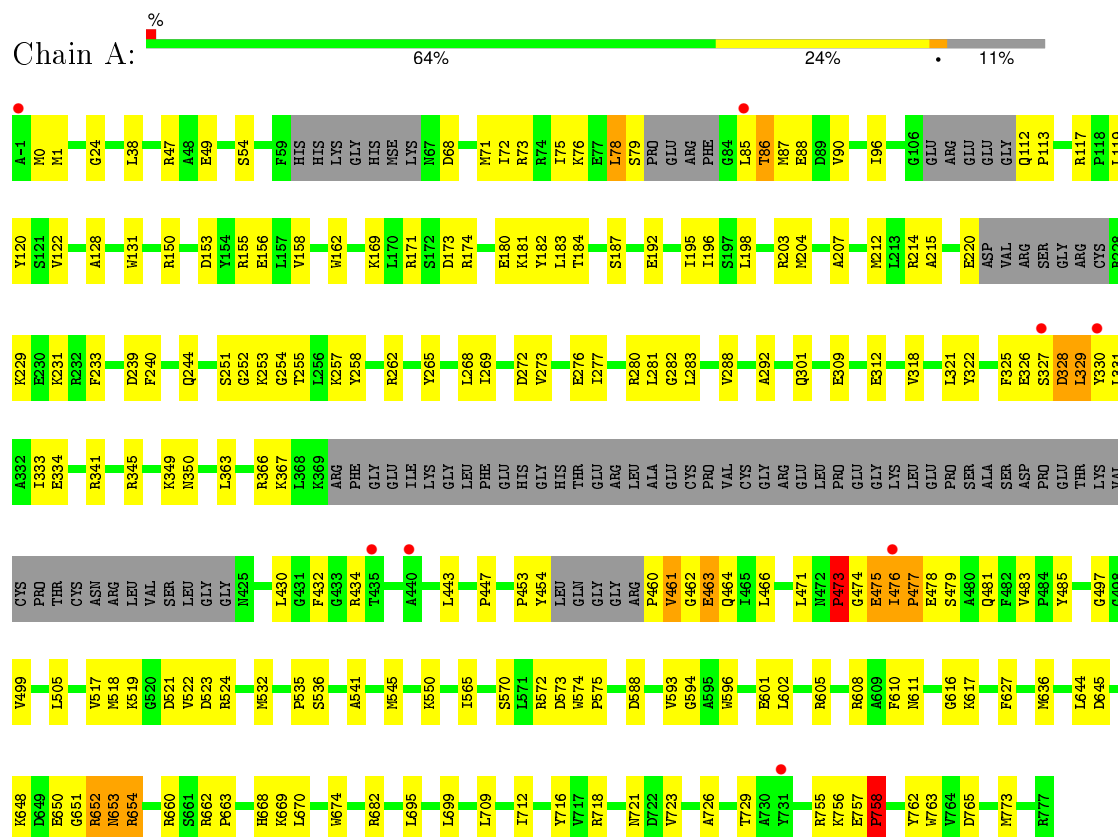
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	236	Total	O	0	0
			236	236		
2	B	263	Total	O	0	0
			263	263		
2	C	73	Total	O	0	0
			73	73		
2	D	38	Total	O	0	0
			38	38		

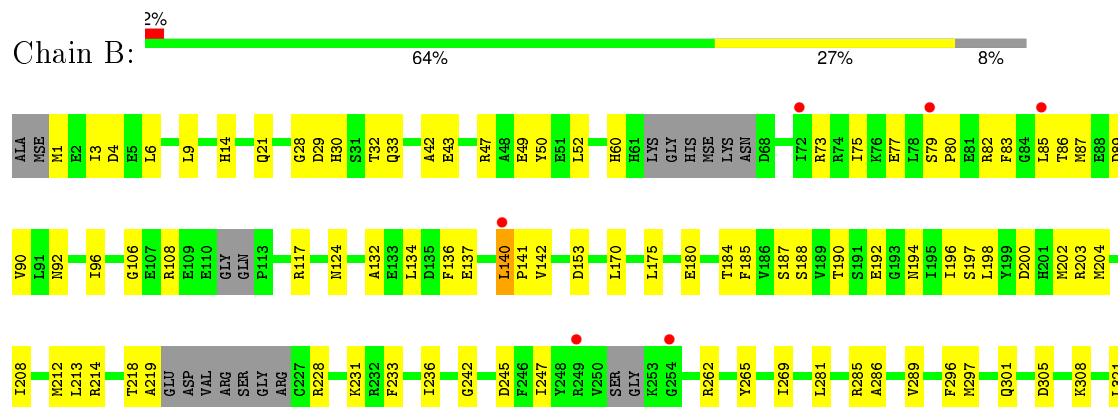
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

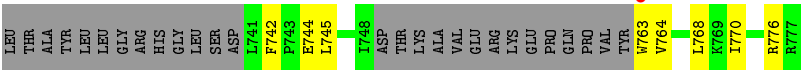
#### • Molecule 1: CSM1



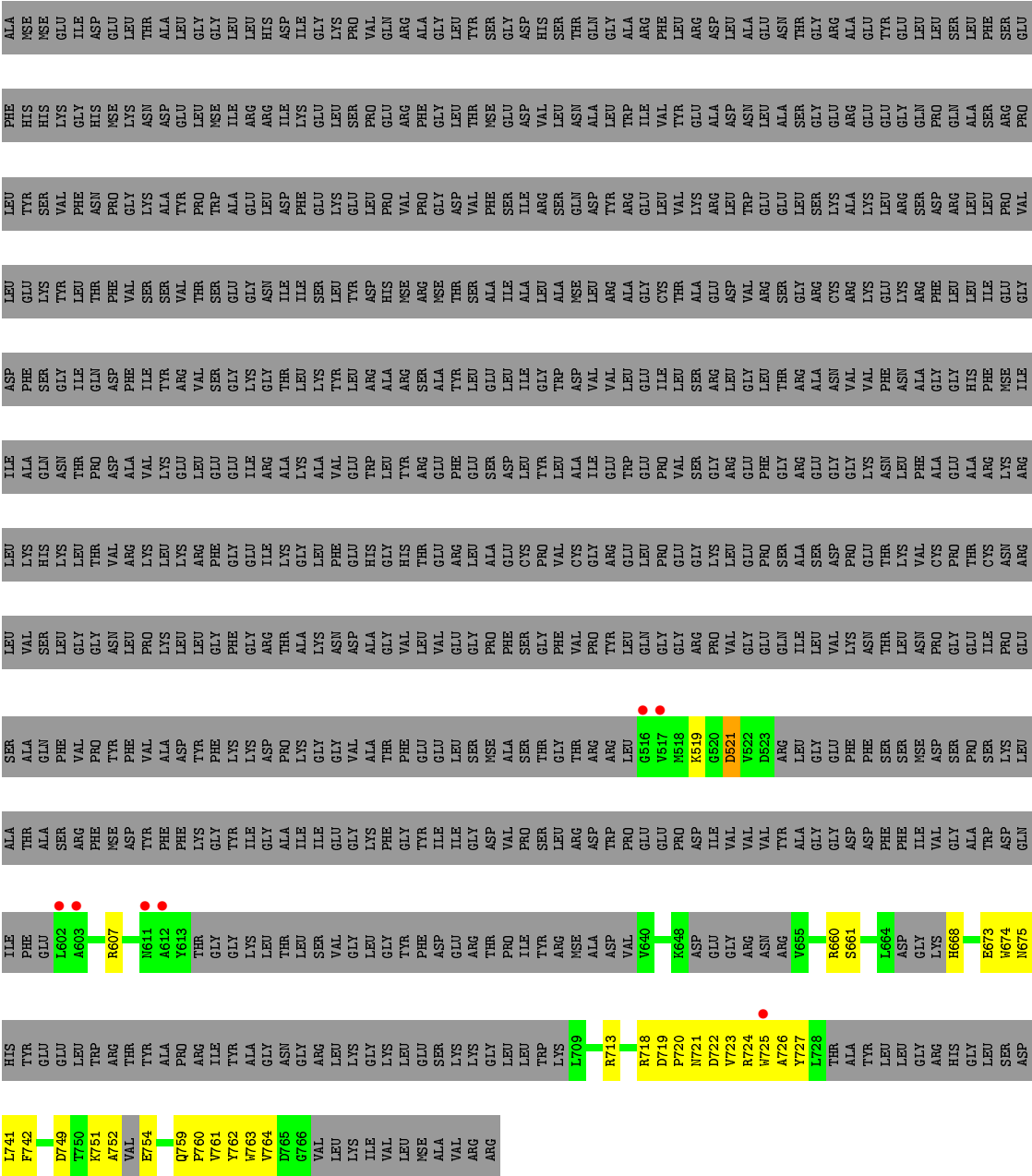
#### • Molecule 1: CSM1







● Molecule 1: CSM1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.89 Å   158.29 Å   299.27 Å 90.00°   89.97°   90.00°	Depositor
Resolution (Å)	30.66 – 2.63 30.66 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.66-2.63) 98.2 (30.66-2.63)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.64 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.203   ,   0.261 0.209   ,   0.263	Depositor DCC
$R_{free}$ test set	1986 reflections (2.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33   ,   27.8	EDS
Estimated twinning fraction	0.500 for H,-K,-L 0.460 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for H,-K,-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 78224 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	14308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.31	4/5695 (0.1%)	0.54	12/7657 (0.2%)
1	B	0.23	1/5834 (0.0%)	0.46	5/7849 (0.1%)
1	C	0.27	0/1674	0.46	1/2245 (0.0%)
1	D	0.22	0/765	0.41	1/1025 (0.1%)
All	All	0.27	5/13968 (0.0%)	0.49	19/18776 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	PRO	N-CD	12.45	1.65	1.47
1	A	477	PRO	N-CD	5.56	1.55	1.47
1	B	141	PRO	N-CD	5.39	1.55	1.47
1	A	113	PRO	N-CD	5.31	1.55	1.47
1	A	758	PRO	N-CD	5.14	1.55	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	ARG	CB-CA-C	-17.39	75.63	110.40
1	B	652	ARG	N-CA-C	15.61	153.15	111.00
1	A	652	ARG	N-CA-C	14.01	148.83	111.00
1	B	652	ARG	CB-CA-C	-10.53	89.34	110.40
1	B	653	ASN	N-CA-C	-8.46	88.15	111.00
1	A	653	ASN	CB-CA-C	8.33	127.06	110.40
1	A	473	PRO	CA-N-CD	-7.45	101.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	PRO	N-CA-C	7.16	130.71	112.10
1	A	654	ARG	N-CA-CB	-7.07	97.88	110.60
1	A	654	ARG	N-CA-C	6.48	128.50	111.00
1	C	574	TRP	C-N-CD	6.04	141.09	128.40
1	A	653	ASN	N-CA-C	-6.01	94.76	111.00
1	A	473	PRO	N-CA-CB	-5.98	96.02	102.60
1	B	461	VAL	CB-CA-C	-5.88	100.22	111.40
1	A	757	GLU	C-N-CD	5.83	140.63	128.40
1	A	112	GLN	C-N-CD	5.59	140.14	128.40
1	B	140	LEU	C-N-CD	5.45	139.83	128.40
1	D	742	PHE	N-CA-C	5.35	125.45	111.00
1	A	497	GLY	N-CA-C	5.33	126.44	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	474	GLY	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	5586	0	5595	174	0
1	B	5719	0	5710	182	0
1	C	1640	0	1619	59	0
1	D	753	0	733	37	0
2	A	236	0	0	21	0
2	B	263	0	0	17	0
2	C	73	0	0	8	0
2	D	38	0	0	5	0
All	All	14308	0	13657	447	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 16.

All (447) 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:653:ASN:O	1:A:674:TRP:CD1	1.80	1.34
1:C:654:ARG:NH1	1:C:671:SER:HB3	1.45	1.29
1:B:52:LEU:CD2	1:B:85:LEU:HD11	1.70	1.22
1:B:52:LEU:HD22	1:B:85:LEU:CD1	1.74	1.18
1:A:653:ASN:O	1:A:674:TRP:NE1	1.76	1.16
1:A:272:ASP:OD2	1:A:447:PRO:HD2	1.44	1.15
1:A:322:TYR:HA	1:A:326:GLU:HB2	1.28	1.15
1:B:52:LEU:CD2	1:B:85:LEU:CD1	2.28	1.12
1:A:322:TYR:O	1:A:326:GLU:HB3	1.51	1.10
1:B:52:LEU:HD22	1:B:85:LEU:HD11	1.16	1.10
1:D:521:ASP:OD1	2:D:2004:HOH:O	1.75	1.03
1:B:140:LEU:HD23	1:B:564:ILE:HD12	1.41	1.01
1:D:723:VAL:HG22	1:D:724:ARG:H	1.28	0.98
1:C:654:ARG:NH1	1:C:671:SER:CB	2.27	0.97
1:A:272:ASP:OD2	1:A:447:PRO:CD	2.13	0.96
1:A:322:TYR:HA	1:A:326:GLU:CB	1.95	0.95
1:C:654:ARG:HH11	1:C:671:SER:HB3	1.15	0.93
1:B:203:ARG:NH1	1:B:542:SER:OG	2.01	0.92
1:A:651:GLY:O	1:A:652:ARG:HB2	1.67	0.91
1:B:140:LEU:HD22	1:B:561:PHE:HB3	1.51	0.90
1:B:184:THR:HG23	1:B:543:ARG:HH12	1.38	0.89
1:B:661:SER:OG	1:B:713:ARG:NH1	2.05	0.88
1:A:85:LEU:HD13	1:A:90:VAL:HG22	1.57	0.86
1:B:89:ASP:OD1	1:B:90:VAL:N	2.11	0.83
1:B:52:LEU:HD21	1:B:85:LEU:CD1	2.07	0.83
1:B:140:LEU:CD2	1:B:564:ILE:HD12	2.08	0.83
1:B:523:ASP:OD2	1:B:652:ARG:O	1.97	0.82
1:C:654:ARG:CZ	1:C:671:SER:HB3	2.10	0.81
1:B:700:GLU:O	1:B:701:SER:OG	1.99	0.81
1:B:697:GLY:O	2:B:2234:HOH:O	1.99	0.80
1:B:434:ARG:NH1	1:B:464:GLN:OE1	2.14	0.80
1:C:607:ARG:HG2	1:C:674:TRP:CE2	2.17	0.80
1:B:140:LEU:HD23	1:B:564:ILE:CD1	2.11	0.80
1:B:140:LEU:HB3	1:B:564:ILE:CD1	2.12	0.80
1:B:117:ARG:NH1	1:B:192:GLU:OE1	2.14	0.80
1:B:52:LEU:CD2	1:B:85:LEU:HD13	2.12	0.79
1:C:654:ARG:HH11	1:C:671:SER:CB	1.89	0.79
1:A:601:GLU:OE2	1:A:605:ARG:NH2	2.14	0.79
1:D:719:ASP:OD2	1:D:722:ASP:HB2	1.85	0.77
1:A:322:TYR:HE1	1:A:330:TYR:HD2	1.32	0.76
1:D:660:ARG:NH2	1:D:762:TYR:O	2.20	0.75
1:A:660:ARG:NH1	1:A:670:LEU:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:VAL:HG13	1:A:726:ALA:HB3	1.68	0.74
1:B:435:THR:HB	1:B:462:GLY:HA2	1.71	0.73
1:B:579:ASP:OD2	2:B:2153:HOH:O	2.07	0.72
1:B:140:LEU:HD22	1:B:561:PHE:CB	2.20	0.72
1:B:703:LYS:HE2	1:B:707:TRP:HE1	1.54	0.71
1:B:42:ALA:HB2	1:B:50:TYR:HB2	1.71	0.71
1:D:741:LEU:N	2:D:2027:HOH:O	2.24	0.71
1:B:285:ARG:NH1	2:B:2111:HOH:O	2.10	0.71
1:B:52:LEU:HD21	1:B:85:LEU:CD2	2.21	0.70
1:A:723:VAL:CG1	1:A:726:ALA:HB3	2.20	0.70
1:A:0:MSE:HB2	1:A:1:MSE:HB2	1.73	0.70
1:A:272:ASP:OD2	1:A:447:PRO:CG	2.39	0.70
1:A:258:TYR:HB3	1:A:262:ARG:NH1	2.07	0.70
1:C:650:GLU:OE1	1:C:654:ARG:NH1	2.25	0.69
1:A:272:ASP:OD2	1:A:447:PRO:HG2	1.93	0.69
1:B:153:ASP:OD2	2:B:2056:HOH:O	2.09	0.69
1:D:723:VAL:HG22	1:D:724:ARG:N	2.03	0.69
1:A:122:VAL:HG23	1:A:195:ILE:HD12	1.74	0.68
1:A:653:ASN:O	1:A:674:TRP:HD1	1.67	0.68
1:B:6:LEU:HD22	1:B:85:LEU:HD21	1.76	0.68
1:B:558:GLU:OE1	1:B:560:LYS:NZ	2.23	0.67
1:A:322:TYR:HE1	1:A:330:TYR:CD2	2.13	0.67
1:B:49:GLU:OE1	1:B:49:GLU:N	2.28	0.67
1:A:617:LYS:NZ	2:A:2049:HOH:O	2.27	0.67
1:A:156:GLU:OE2	2:A:2063:HOH:O	2.14	0.66
1:B:621:SER:OG	1:B:652:ARG:O	2.12	0.66
1:B:228:ARG:HH22	1:B:233:PHE:HE2	1.43	0.66
1:D:725:TRP:CZ2	1:D:761:VAL:HG11	2.31	0.66
1:B:654:ARG:NH2	1:B:671:SER:O	2.29	0.65
1:B:642:GLU:OE2	2:B:2211:HOH:O	2.14	0.65
1:B:4:ASP:HB3	1:B:214:ARG:HH22	1.62	0.65
1:C:654:ARG:HD3	1:C:671:SER:HB3	1.79	0.64
1:A:322:TYR:CA	1:A:326:GLU:CB	2.75	0.64
1:B:79:SER:HB2	1:B:82:ARG:HB3	1.80	0.64
1:C:512:THR:HA	1:C:776:ARG:HD2	1.78	0.64
1:A:85:LEU:CD1	1:A:90:VAL:HG22	2.28	0.64
1:C:648:LYS:HE3	1:C:652:ARG:NH1	2.12	0.64
1:B:425:ASN:HA	1:B:429:LEU:HD22	1.77	0.64
1:B:650:GLU:O	1:B:669:LYS:NZ	2.31	0.64
1:A:755:ARG:NH1	2:A:2222:HOH:O	2.31	0.64
1:A:464:GLN:HG3	1:A:481:GLN:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TYR:C	1:A:326:GLU:HB3	2.17	0.63
1:A:329:LEU:HG	1:A:330:TYR:N	2.13	0.63
1:B:140:LEU:CB	1:B:564:ILE:CD1	2.76	0.63
1:A:231:LYS:O	1:A:231:LYS:HG2	1.98	0.63
1:C:576:GLU:O	1:C:578:PRO:HD3	1.99	0.63
1:C:546:ASP:N	2:C:2016:HOH:O	2.31	0.63
1:D:725:TRP:NE1	1:D:761:VAL:HG11	2.14	0.63
1:C:650:GLU:HB3	1:C:669:LYS:HG2	1.80	0.63
1:B:608:ARG:NH1	1:B:678:GLU:OE1	2.31	0.63
1:B:86:THR:O	1:B:90:VAL:HG12	1.98	0.63
1:B:6:LEU:HD22	1:B:85:LEU:CD2	2.29	0.63
1:C:607:ARG:HG2	1:C:674:TRP:CD2	2.34	0.62
1:B:140:LEU:HD22	1:B:561:PHE:CG	2.34	0.62
1:B:755:ARG:NH2	1:B:757:GLU:OE2	2.31	0.62
1:D:725:TRP:HZ2	1:D:761:VAL:CG1	2.13	0.62
1:A:660:ARG:HD2	1:A:765:ASP:OD2	1.99	0.62
1:D:725:TRP:HE1	1:D:761:VAL:HG11	1.65	0.62
1:A:654:ARG:NH2	2:A:2190:HOH:O	2.25	0.62
1:A:478:GLU:HG2	1:A:478:GLU:O	2.00	0.62
1:B:140:LEU:CD2	1:B:561:PHE:HB3	2.25	0.62
1:C:763:TRP:N	2:C:2067:HOH:O	2.32	0.62
1:A:682:ARG:NH2	2:A:2202:HOH:O	2.33	0.62
1:A:87:MSE:HG2	1:A:87:MSE:O	1.99	0.62
1:C:699:LEU:HD11	1:C:706:LEU:HD11	1.83	0.61
1:B:200:ASP:OD2	1:B:540:THR:HA	1.99	0.61
1:A:322:TYR:CD1	1:A:326:GLU:OE1	2.53	0.61
1:A:85:LEU:HD13	1:A:90:VAL:CG2	2.29	0.61
1:A:350:ASN:ND2	1:A:532:MSE:O	2.30	0.61
1:A:292:ALA:HB1	1:A:550:LYS:HE2	1.83	0.61
1:B:428:LYS:HE2	1:B:456:GLN:HB3	1.83	0.60
1:B:180:GLU:O	1:B:184:THR:OG1	2.19	0.60
1:A:180:GLU:O	1:A:184:THR:OG1	2.18	0.60
1:B:140:LEU:CB	1:B:564:ILE:HD12	2.32	0.60
1:A:117:ARG:NH1	1:A:192:GLU:HG3	2.17	0.60
1:A:476:ILE:HG22	1:A:477:PRO:HD2	1.82	0.60
1:C:645:ASP:HA	1:C:648:LYS:HG3	1.84	0.60
1:A:521:ASP:OD2	1:A:648:LYS:NZ	2.23	0.59
1:A:180:GLU:OE2	2:A:2067:HOH:O	2.17	0.59
1:C:574:TRP:CE3	1:C:574:TRP:HA	2.37	0.59
1:B:132:ALA:HB2	1:B:185:PHE:HB2	1.83	0.59
1:B:136:PHE:O	1:B:137:GLU:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HZ3	1:A:499:VAL:HB	1.66	0.59
1:A:645:ASP:OD1	2:A:2182:HOH:O	2.17	0.59
1:B:426:LEU:HD11	1:B:499:VAL:HG23	1.84	0.58
1:A:345:ARG:NH2	2:A:2116:HOH:O	2.36	0.58
1:A:648:LYS:O	1:A:652:ARG:NH1	2.36	0.58
1:B:435:THR:OG1	1:B:439:ASP:OD2	2.21	0.58
1:B:187:SER:OG	1:B:194:ASN:ND2	2.37	0.58
1:A:212:MSE:HE2	1:A:233:PHE:HZ	1.66	0.58
1:D:725:TRP:CZ2	1:D:761:VAL:CG1	2.87	0.58
1:C:694:ARG:NH1	2:C:2061:HOH:O	2.11	0.58
1:B:661:SER:HG	1:B:713:ARG:NH1	2.01	0.58
1:D:725:TRP:CE2	1:D:761:VAL:HG11	2.39	0.57
2:A:2119:HOH:O	1:B:722:ASP:OD2	2.17	0.57
1:A:214:ARG:NH1	1:A:281:LEU:O	2.38	0.57
1:A:273:VAL:O	1:A:277:ILE:HG13	2.05	0.57
1:D:762:TYR:HD2	1:D:763:TRP:CE2	2.23	0.57
1:B:662:ARG:NH2	2:B:2219:HOH:O	2.34	0.57
1:A:648:LYS:HB3	1:A:652:ARG:NH1	2.19	0.57
1:A:463:GLU:O	1:A:481:GLN:N	2.38	0.57
1:C:698:LYS:O	1:C:698:LYS:HG2	2.04	0.57
1:C:592:ILE:O	2:C:2014:HOH:O	2.18	0.56
1:B:134:LEU:HD11	1:B:136:PHE:CE1	2.40	0.56
1:A:24:GLY:HA3	1:A:155:ARG:HH11	1.68	0.56
1:A:182:TYR:O	2:A:2069:HOH:O	2.18	0.56
1:A:517:VAL:HG22	1:A:593:VAL:HG12	1.87	0.56
1:A:239:ASP:OD1	1:A:240:PHE:N	2.38	0.56
1:B:77:GLU:O	1:B:80:PRO:HD3	2.06	0.56
1:A:215:ALA:HB2	1:A:301:GLN:HB2	1.87	0.56
1:B:706:LEU:HB2	1:B:772:LEU:HD21	1.86	0.56
1:B:52:LEU:HD21	1:B:85:LEU:HD13	1.83	0.56
1:A:329:LEU:HG	1:A:330:TYR:H	1.72	0.55
1:C:654:ARG:HD3	1:C:671:SER:CB	2.36	0.55
1:A:755:ARG:O	1:A:756:LYS:HB3	2.06	0.54
1:B:184:THR:HG23	1:B:543:ARG:NH1	2.17	0.54
1:A:611:ASN:O	1:A:616:GLY:N	2.40	0.54
1:A:709:LEU:HD22	1:A:729:THR:HG23	1.88	0.54
1:A:463:GLU:HG3	1:A:464:GLN:NE2	2.22	0.54
1:A:258:TYR:HB3	1:A:262:ARG:HH12	1.73	0.54
1:A:244:GLN:NE2	2:A:2087:HOH:O	2.40	0.53
1:A:318:VAL:O	2:A:2112:HOH:O	2.18	0.53
1:D:724:ARG:O	1:D:724:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ALA:HA	1:B:542:SER:HB3	1.90	0.53
1:B:86:THR:HG22	1:B:87:MSE:H	1.74	0.53
1:A:122:VAL:HG21	1:A:541:ALA:HB2	1.90	0.53
1:B:660:ARG:NH2	1:B:762:TYR:O	2.40	0.53
1:A:322:TYR:CE1	1:A:330:TYR:HD2	2.21	0.53
1:A:183:LEU:HB3	1:A:198:LEU:HD23	1.89	0.53
1:A:463:GLU:HG3	1:A:464:GLN:OE1	2.09	0.53
1:D:607:ARG:HE	1:D:674:TRP:HB3	1.74	0.53
1:A:72:ILE:HG13	1:A:73:ARG:HG2	1.91	0.53
1:B:29:ASP:N	1:B:32:THR:OG1	2.42	0.53
1:D:764:VAL:HG22	1:D:764:VAL:O	2.09	0.53
1:A:572:ARG:NE	1:A:573:ASP:O	2.42	0.52
1:B:542:SER:HA	1:B:545:MSE:HE3	1.90	0.52
1:B:550:LYS:NZ	2:B:2177:HOH:O	2.11	0.52
1:A:309:GLU:HA	1:A:312:GLU:HB3	1.92	0.52
1:A:463:GLU:HG3	1:A:464:GLN:CD	2.30	0.52
1:A:523:ASP:HB3	1:A:652:ARG:HD2	1.91	0.52
1:A:171:ARG:NE	1:A:173:ASP:OD1	2.43	0.52
1:A:325:PHE:O	1:A:328:ASP:HB2	2.10	0.52
1:A:325:PHE:HB3	1:A:328:ASP:HB2	1.91	0.52
1:B:86:THR:HB	1:B:89:ASP:CG	2.30	0.52
1:A:522:VAL:HG21	1:A:545:MSE:HE2	1.90	0.52
1:B:212:MSE:HE2	1:B:233:PHE:HZ	1.74	0.52
1:A:169:LYS:HB2	1:A:174:ARG:HG3	1.91	0.52
1:B:524:ARG:NH2	2:B:2170:HOH:O	2.42	0.52
1:B:204:MSE:HE1	1:B:289:VAL:HA	1.92	0.52
1:B:680:LEU:HD22	1:B:684:TYR:HE2	1.75	0.51
1:D:661:SER:OG	1:D:713:ARG:NH1	2.42	0.51
1:A:181:LYS:HG3	1:A:471:LEU:HD12	1.92	0.51
1:B:716:TYR:N	2:B:2240:HOH:O	2.39	0.51
1:C:576:GLU:C	1:C:578:PRO:HD3	2.30	0.51
1:B:108:ARG:NH2	1:B:188:SER:HB2	2.25	0.51
1:A:322:TYR:CA	1:A:326:GLU:HB3	2.41	0.51
1:A:476:ILE:HG22	1:A:477:PRO:CD	2.41	0.51
1:A:229:LYS:HG3	1:A:341:ARG:HB2	1.92	0.51
1:A:240:PHE:CD2	1:A:329:LEU:HD21	2.46	0.51
1:D:762:TYR:CD2	1:D:763:TRP:CE2	2.98	0.51
1:A:24:GLY:HA3	1:A:155:ARG:NH1	2.24	0.51
1:A:322:TYR:CE1	1:A:330:TYR:CD2	2.97	0.51
1:B:140:LEU:O	1:B:142:VAL:HG23	2.11	0.51
1:A:96:ILE:HG23	1:A:212:MSE:SE	2.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ALA:N	1:C:504:GLU:OE1	2.44	0.51
1:B:321:LEU:O	1:B:325:PHE:N	2.44	0.51
1:D:749:ASP:OD2	1:D:760:PRO:HG3	2.10	0.51
1:B:345:ARG:NH1	1:B:533:ASP:OD2	2.44	0.51
1:B:14:HIS:HB2	1:B:60:HIS:CE1	2.46	0.51
1:A:272:ASP:OD1	1:A:434:ARG:NH2	2.38	0.51
1:B:79:SER:N	1:B:80:PRO:HD3	2.26	0.51
1:B:203:ARG:HD3	1:B:539:ALA:HB1	1.92	0.51
1:B:86:THR:HG22	1:B:87:MSE:N	2.27	0.51
1:A:119:LEU:HD13	1:A:187:SER:HA	1.92	0.51
1:B:485:TYR:O	2:B:2143:HOH:O	2.19	0.51
1:A:758:PRO:HD2	2:A:2228:HOH:O	2.11	0.51
1:A:466:LEU:O	1:A:485:TYR:HE1	1.94	0.51
1:B:47:ARG:HB3	1:B:49:GLU:OE1	2.11	0.50
1:A:627:PHE:CD2	1:A:636:MSE:HB2	2.46	0.50
1:D:668:HIS:N	2:D:2018:HOH:O	2.44	0.50
1:D:722:ASP:OD1	1:D:723:VAL:N	2.44	0.50
1:B:21:GLN:OE1	1:B:30:HIS:N	2.44	0.50
1:C:632:PRO:HB2	1:C:634:TYR:HD2	1.76	0.50
1:B:728:LEU:O	1:B:732:LEU:N	2.44	0.50
1:B:52:LEU:HD22	1:B:85:LEU:HD13	1.72	0.50
1:B:4:ASP:CB	1:B:214:ARG:HH22	2.22	0.50
1:D:723:VAL:CG2	1:D:724:ARG:H	2.11	0.50
1:B:543:ARG:HB3	1:B:547:TYR:CZ	2.46	0.50
1:A:203:ARG:NH1	2:A:2076:HOH:O	2.35	0.50
1:C:518:MSE:HE1	1:C:602:LEU:HB3	1.93	0.50
1:C:518:MSE:N	2:C:2014:HOH:O	2.45	0.50
1:B:108:ARG:NH2	1:B:196:ILE:HB	2.27	0.50
1:C:652:ARG:HG3	1:C:653:ASN:H	1.76	0.49
1:A:570:SER:OG	1:A:572:ARG:O	2.29	0.49
1:C:703:LYS:NZ	1:C:707:TRP:HE1	2.10	0.49
1:A:479:SER:O	2:A:2129:HOH:O	2.19	0.49
1:A:321:LEU:CD2	1:A:325:PHE:CE2	2.95	0.49
1:B:648:LYS:NZ	2:B:2215:HOH:O	2.15	0.49
1:D:725:TRP:HZ2	1:D:761:VAL:HG12	1.78	0.49
1:A:650:GLU:HB3	1:A:669:LYS:HD3	1.95	0.49
1:A:473:PRO:O	1:A:475:GLU:HG3	2.12	0.49
1:A:203:ARG:NH2	1:A:288:VAL:O	2.45	0.49
1:D:751:LYS:O	1:D:752:ALA:HB3	2.12	0.49
1:B:231:LYS:NZ	2:B:2090:HOH:O	2.44	0.49
1:B:689:TYR:O	2:B:2230:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HB	1:B:89:ASP:OD1	2.12	0.49
1:A:349:LYS:NZ	1:D:718:ARG:HG2	2.28	0.49
1:B:502:PHE:HE1	1:B:593:VAL:HG21	1.76	0.49
1:B:43:GLU:HG2	1:B:43:GLU:O	2.12	0.48
1:C:678:GLU:OE1	2:C:2024:HOH:O	2.19	0.48
1:B:231:LYS:H	1:B:339:SER:HA	1.78	0.48
1:B:704:GLY:HA2	1:B:707:TRP:HD1	1.77	0.48
1:B:461:VAL:O	1:B:461:VAL:CG1	2.59	0.48
1:A:322:TYR:N	2:A:2112:HOH:O	2.34	0.48
1:B:1:MSE:SE	1:B:49:GLU:HG2	2.63	0.48
1:B:47:ARG:HD2	1:B:170:LEU:HD23	1.95	0.48
1:B:461:VAL:HG13	1:B:461:VAL:O	2.14	0.48
1:A:325:PHE:HB3	1:A:328:ASP:CB	2.43	0.48
1:B:136:PHE:C	1:B:137:GLU:HG2	2.34	0.48
1:C:507:MSE:HA	1:C:513:ARG:HD3	1.96	0.48
1:C:503:GLU:HG3	1:C:630:ARG:NH1	2.29	0.48
1:C:744:GLU:H	1:C:744:GLU:HG2	1.40	0.48
1:A:443:LEU:HB2	1:A:453:PRO:HD3	1.96	0.47
1:A:268:LEU:O	2:A:2098:HOH:O	2.20	0.47
1:B:198:LEU:HG	1:B:202:MSE:HE3	1.95	0.47
1:A:204:MSE:SE	1:A:535:PRO:HB2	2.64	0.47
1:B:242:GLY:HA2	1:B:245:ASP:OD2	2.15	0.47
1:B:557:ILE:O	1:B:574:TRP:NE1	2.41	0.47
1:D:754:GLU:N	2:D:2033:HOH:O	2.47	0.47
1:B:184:THR:CG2	1:B:543:ARG:HH12	2.16	0.47
1:B:696:LYS:HB3	1:B:699:LEU:HD12	1.95	0.47
1:C:512:THR:HG22	1:C:514:ARG:HG2	1.95	0.47
1:C:662:ARG:HD3	1:C:670:LEU:HD11	1.96	0.47
1:B:607:ARG:NH1	1:B:678:GLU:OE2	2.48	0.47
1:B:296:PHE:N	2:B:2095:HOH:O	2.40	0.47
1:B:52:LEU:HD21	1:B:85:LEU:HD21	1.96	0.47
1:A:321:LEU:HD22	1:A:325:PHE:CD2	2.50	0.47
1:B:607:ARG:HG3	1:B:674:TRP:CD2	2.50	0.47
1:C:631:THR:HB	1:C:632:PRO:HD2	1.97	0.47
1:B:553:ILE:HA	1:B:556:ILE:HD12	1.96	0.47
1:A:131:TRP:CE2	1:A:153:ASP:HB3	2.50	0.47
1:A:334:GLU:OE2	1:A:366:ARG:NH1	2.48	0.47
1:C:549:PHE:HA	1:C:553:ILE:HG13	1.97	0.47
1:A:158:VAL:O	1:A:162:TRP:N	2.46	0.47
1:D:759:GLN:OE1	2:D:2028:HOH:O	2.20	0.47
1:B:188:SER:OG	1:B:198:LEU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:O	1:A:78:LEU:O	2.33	0.47
1:B:654:ARG:NH2	1:B:669:LYS:HD3	2.31	0.46
1:A:76:LYS:HD3	1:A:87:MSE:SE	2.65	0.46
1:A:565:ILE:O	1:A:608:ARG:NH1	2.45	0.46
1:B:469:ASN:N	2:B:2143:HOH:O	2.44	0.46
1:A:430:LEU:N	1:A:454:TYR:O	2.46	0.46
1:B:197:SER:HB3	1:B:200:ASP:OD2	2.15	0.46
1:B:108:ARG:CZ	1:B:188:SER:HB2	2.46	0.46
1:A:432:PHE:O	1:A:466:LEU:N	2.49	0.46
1:B:733:LEU:HB3	1:B:738:LEU:O	2.16	0.46
1:B:305:ASP:HA	1:B:308:LYS:HB3	1.97	0.46
1:A:150:ARG:NH2	2:A:2060:HOH:O	2.48	0.46
1:A:648:LYS:CA	1:A:652:ARG:NH1	2.78	0.46
1:B:548:PHE:HA	1:B:552:TYR:HD2	1.81	0.46
1:A:505:LEU:HD13	1:A:594:GLY:HA2	1.98	0.46
1:A:120:TYR:HA	1:A:128:ALA:HA	1.98	0.46
1:A:276:GLU:OE2	1:A:280:ARG:NE	2.49	0.46
1:A:0:MSE:HB3	1:A:0:MSE:HE2	1.90	0.46
1:B:323:ARG:HB2	1:B:324:GLU:OE1	2.15	0.46
1:C:706:LEU:HD23	1:C:768:LEU:HD11	1.97	0.45
1:A:281:LEU:HD23	1:A:283:LEU:HD11	1.97	0.45
1:A:758:PRO:HG2	1:A:763:TRP:HE1	1.81	0.45
1:B:663:PRO:HG3	1:B:717:VAL:HA	1.97	0.45
1:A:321:LEU:HD23	1:A:325:PHE:CE2	2.51	0.45
1:C:722:ASP:HB3	1:C:724:ARG:HG2	1.99	0.45
1:A:474:GLY:C	1:A:475:GLU:HG3	2.34	0.45
1:B:247:ILE:HA	1:B:262:ARG:HE	1.81	0.45
1:A:662:ARG:NH1	1:A:670:LEU:HG	2.32	0.45
1:B:704:GLY:O	1:B:708:LYS:HG2	2.16	0.45
1:D:761:VAL:O	1:D:761:VAL:HG22	2.16	0.45
1:A:269:ILE:O	1:A:273:VAL:HG23	2.17	0.45
1:A:85:LEU:CD1	1:A:90:VAL:CG2	2.93	0.45
1:B:669:LYS:O	1:B:762:TYR:OH	2.27	0.45
1:B:476:ILE:HG12	1:B:478:GLU:H	1.80	0.45
1:A:38:LEU:HD12	1:A:54:SER:HA	1.98	0.45
1:C:633:ILE:HG13	1:C:633:ILE:O	2.17	0.45
1:B:208:ILE:HG22	1:B:212:MSE:HE3	2.00	0.44
1:B:82:ARG:O	1:B:83:PHE:HB2	2.16	0.44
1:C:687:ARG:NH1	1:C:744:GLU:OE2	2.49	0.44
1:B:9:LEU:HD22	1:B:175:LEU:HD12	1.99	0.44
1:B:688:ILE:HA	1:B:699:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:CZ	1:B:269:ILE:HD11	2.53	0.44
1:A:651:GLY:O	1:A:652:ARG:CB	2.48	0.44
1:A:204:MSE:HE2	1:A:204:MSE:HB3	1.84	0.44
1:C:698:LYS:HE2	1:C:702:LYS:NZ	2.33	0.44
1:A:758:PRO:HG2	1:A:763:TRP:NE1	2.32	0.44
1:B:124:ASN:HB2	1:B:615:GLY:HA3	1.99	0.44
1:B:420:VAL:O	1:B:443:LEU:HD21	2.18	0.44
1:C:595:ALA:O	1:C:599:ILE:HG12	2.18	0.44
1:D:726:ALA:O	1:D:727:TYR:CD1	2.70	0.44
1:B:86:THR:CB	1:B:89:ASP:CG	2.86	0.44
1:A:596:TRP:CH2	1:A:773:MSE:HG3	2.53	0.44
1:A:574:TRP:HA	1:A:575:PRO:HD3	1.80	0.44
1:A:220:GLU:N	2:A:2083:HOH:O	2.50	0.44
1:A:648:LYS:HB3	1:A:652:ARG:HH12	1.83	0.43
1:B:106:GLY:H	1:B:534:SER:HB3	1.83	0.43
1:A:331:LEU:HD21	1:A:333:ILE:HD11	1.99	0.43
1:B:82:ARG:HG3	1:B:83:PHE:CD1	2.52	0.43
1:B:361:HIS:O	1:B:365:VAL:HG13	2.18	0.43
1:B:334:GLU:OE2	1:B:366:ARG:NH1	2.51	0.43
1:B:47:ARG:HD2	1:B:170:LEU:CB	2.48	0.43
1:A:231:LYS:HB3	1:A:231:LYS:HE2	1.59	0.43
1:B:247:ILE:O	1:B:262:ARG:NH2	2.39	0.43
1:B:47:ARG:HD2	1:B:170:LEU:HB3	1.99	0.43
1:B:281:LEU:O	1:B:301:GLN:NE2	2.39	0.43
1:B:507:MSE:HA	1:B:513:ARG:HG3	1.99	0.43
1:B:607:ARG:HA	1:B:620:LEU:HD12	2.00	0.43
1:B:218:THR:HA	1:B:219:ALA:HA	1.69	0.43
1:A:518:MSE:HE1	1:A:602:LEU:HD23	1.99	0.43
1:A:326:GLU:HA	1:A:327:SER:HA	1.69	0.43
1:B:47:ARG:HD2	1:B:170:LEU:CD2	2.48	0.43
1:D:720:PRO:HG2	1:D:721:ASN:ND2	2.33	0.43
1:C:643:ARG:HH12	1:C:656:PHE:HZ	1.56	0.43
1:C:652:ARG:NH1	2:C:2049:HOH:O	2.51	0.43
1:B:4:ASP:HA	1:B:213:LEU:HD21	2.00	0.43
1:A:709:LEU:HD23	1:A:712:ILE:HD12	2.01	0.43
1:C:673:GLU:HB3	1:C:676:HIS:CB	2.49	0.43
1:C:654:ARG:CD	1:C:671:SER:HB3	2.47	0.43
1:A:466:LEU:HA	1:A:483:VAL:O	2.18	0.43
1:B:336:GLU:HB3	1:B:359:LEU:HD23	2.00	0.43
1:B:73:ARG:HA	1:B:75:ILE:HG22	2.01	0.43
1:A:253:LYS:HA	1:A:254:GLY:HA3	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:VAL:HA	1:B:592:ILE:HG23	2.00	0.42
1:B:697:GLY:O	1:B:699:LEU:N	2.46	0.42
1:A:301:GLN:N	1:A:301:GLN:OE1	2.52	0.42
1:A:325:PHE:C	1:A:328:ASP:HB2	2.39	0.42
1:B:28:GLY:O	1:B:33:GLN:NE2	2.44	0.42
1:C:653:ASN:OD1	1:C:674:TRP:CD1	2.71	0.42
1:A:252:GLY:N	2:A:2090:HOH:O	2.52	0.42
1:D:673:GLU:HG2	1:D:675:ASN:H	1.85	0.42
1:B:571:LEU:HA	1:B:689:TYR:HE2	1.84	0.42
1:A:695:LEU:HD13	1:A:699:LEU:HD23	2.01	0.42
1:D:762:TYR:HD2	1:D:763:TRP:NE1	2.18	0.42
1:B:233:PHE:HB2	1:B:338:VAL:HG23	2.01	0.42
1:B:755:ARG:NH2	2:B:2256:HOH:O	2.52	0.42
1:A:473:PRO:CG	1:A:474:GLY:H	2.32	0.42
1:B:715:LEU:HB3	1:B:724:ARG:HE	1.84	0.42
1:A:716:TYR:CE2	1:A:762:TYR:HB2	2.54	0.42
1:B:326:GLU:O	1:B:327:SER:OG	2.33	0.42
1:A:519:LYS:NZ	1:A:644:LEU:HD23	2.35	0.42
1:B:518:MSE:HE1	1:B:602:LEU:HB3	2.01	0.42
1:B:117:ARG:HB2	1:B:190:THR:HG22	2.01	0.42
1:B:739:SER:OG	1:D:751:LYS:HD2	2.19	0.42
1:C:662:ARG:HG3	1:C:664:LEU:CD2	2.50	0.42
1:B:92:ASN:O	1:B:96:ILE:N	2.45	0.42
1:A:545:MSE:HE1	1:A:610:PHE:CE1	2.55	0.42
1:A:460:PRO:HB2	1:A:476:ILE:HD11	2.02	0.42
1:C:722:ASP:O	1:C:724:ARG:N	2.52	0.42
1:C:502:PHE:HB3	1:C:515:LEU:HD22	2.01	0.42
1:B:6:LEU:CD2	1:B:85:LEU:CD2	2.98	0.41
1:D:607:ARG:HD2	1:D:674:TRP:HE3	1.84	0.41
1:B:4:ASP:HB3	1:B:214:ARG:NH2	2.31	0.41
1:A:461:VAL:HA	1:A:462:GLY:HA2	1.64	0.41
1:A:321:LEU:N	2:A:2112:HOH:O	2.53	0.41
1:C:768:LEU:N	2:C:2068:HOH:O	2.52	0.41
1:A:341:ARG:HA	1:A:341:ARG:HD2	1.81	0.41
1:A:721:ASN:O	1:C:722:ASP:OD1	2.39	0.41
1:A:254:GLY:HA2	1:A:255:THR:HA	1.81	0.41
1:B:430:LEU:O	1:B:468:LYS:N	2.53	0.41
1:A:321:LEU:CD2	1:A:325:PHE:HE2	2.33	0.41
1:B:3:ILE:HD12	1:B:89:ASP:HB2	2.03	0.41
1:B:324:GLU:OE1	1:B:324:GLU:N	2.54	0.41
1:A:196:ILE:HG23	1:A:536:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:HA	1:B:453:PRO:HD3	1.92	0.41
1:A:268:LEU:O	1:A:272:ASP:HB2	2.21	0.41
1:B:715:LEU:HD13	1:B:724:ARG:HG3	2.02	0.41
1:B:449:SER:OG	1:B:450:GLY:N	2.54	0.41
1:B:52:LEU:HD21	1:B:85:LEU:HD22	2.00	0.41
1:A:321:LEU:HD23	1:A:325:PHE:HE2	1.85	0.41
1:B:523:ASP:CG	1:B:652:ARG:O	2.58	0.41
1:A:214:ARG:NH2	1:A:282:GLY:O	2.54	0.41
1:A:204:MSE:HA	1:A:207:ALA:HB3	2.03	0.41
1:C:643:ARG:NH1	1:C:656:PHE:CZ	2.69	0.41
1:C:571:LEU:HD11	1:C:770:ILE:HG22	2.03	0.41
1:B:356:ARG:HH22	1:B:530:SER:HA	1.86	0.41
1:C:610:PHE:O	1:C:613:TYR:HB3	2.20	0.41
1:C:742:PHE:HB2	1:C:745:LEU:HB3	2.03	0.41
1:D:519:LYS:HB3	1:D:519:LYS:HE3	1.60	0.41
1:B:203:ARG:O	1:B:286:ALA:HB1	2.21	0.41
1:B:688:ILE:C	1:B:696:LYS:HB2	2.41	0.41
1:D:713:ARG:HG3	1:D:761:VAL:O	2.21	0.41
1:A:588:ASP:OD1	1:A:588:ASP:N	2.53	0.41
1:B:236:ILE:O	1:B:297:MSE:HA	2.21	0.41
1:A:718:ARG:NH2	1:B:368:LEU:HD11	2.36	0.41
1:A:523:ASP:CB	1:A:652:ARG:HD2	2.51	0.40
1:A:466:LEU:HD12	1:A:466:LEU:N	2.37	0.40
1:B:75:ILE:O	2:B:2021:HOH:O	2.22	0.40
1:A:363:LEU:HB3	1:A:367:LYS:NZ	2.36	0.40
1:B:519:LYS:HG2	1:B:644:LEU:HD22	2.03	0.40
1:B:748:ILE:HG21	1:D:726:ALA:HB3	2.02	0.40
1:A:68:ASP:HA	1:A:71:MSE:HG2	2.03	0.40
1:A:524:ARG:CZ	1:A:652:ARG:HH21	2.34	0.40
1:A:663:PRO:HG2	1:A:668:HIS:CG	2.57	0.40
1:A:86:THR:C	1:A:88:GLU:N	2.74	0.40
1:A:329:LEU:CG	1:A:330:TYR:N	2.83	0.40
1:A:541:ALA:O	1:A:545:MSE:HB2	2.21	0.40
1:B:552:TYR:O	1:B:556:ILE:HG13	2.21	0.40
1:C:648:LYS:HE2	1:C:648:LYS:HB3	1.90	0.40
1:C:652:ARG:CG	1:C:653:ASN:H	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	682/779 (88%)	622 (91%)	57 (8%)	3 (0%)	39	63
1	B	699/779 (90%)	609 (87%)	90 (13%)	0	100	100
1	C	187/779 (24%)	165 (88%)	21 (11%)	1 (0%)	34	57
1	D	76/779 (10%)	64 (84%)	12 (16%)	0	100	100
All	All	1644/3116 (53%)	1460 (89%)	180 (11%)	4 (0%)	52	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	633	ILE
1	A	461	VAL
1	A	473	PRO
1	A	758	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	584/638 (92%)	571 (98%)	13 (2%)	60	83
1	B	596/638 (93%)	596 (100%)	0	100	100
1	C	166/638 (26%)	161 (97%)	5 (3%)	48	75
1	D	77/638 (12%)	76 (99%)	1 (1%)	76	91
All	All	1423/2552 (56%)	1404 (99%)	19 (1%)	76	91

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	49	GLU
1	A	78	LEU
1	A	79	SER
1	A	86	THR
1	A	251	SER
1	A	265	TYR
1	A	328	ASP
1	A	329	LEU
1	A	463	GLU
1	A	473	PRO
1	A	475	GLU
1	A	476	ILE
1	C	574	TRP
1	C	576	GLU
1	C	577	GLU
1	C	630	ARG
1	C	764	VAL
1	D	521	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	B	60	HIS
1	B	194	ASN
1	D	759	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 [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	682/779 (87%)	-0.16	8 (1%) 81 78	5, 26, 54, 82	0
1	B	700/779 (89%)	-0.17	12 (1%) 73 68	5, 24, 56, 92	0
1	C	197/779 (25%)	0.36	14 (7%) 19 13	22, 41, 71, 97	0
1	D	91/779 (11%)	0.39	7 (7%) 16 12	19, 39, 71, 98	0
All	All	1670/3116 (53%)	-0.08	41 (2%) 61 55	5, 28, 61, 98	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	516	GLY	7.6
1	C	763	TRP	5.5
1	B	440	ALA	5.4
1	C	563	TYR	4.7
1	B	85	LEU	3.7
1	C	645	ASP	3.4
1	C	709	LEU	3.4
1	A	476	ILE	3.4
1	D	612	ALA	3.3
1	A	440	ALA	3.3
1	A	85	LEU	3.2
1	C	725	TRP	3.1
1	C	657	VAL	3.1
1	D	603	ALA	3.0
1	B	254	GLY	3.0
1	B	249	ARG	2.9
1	B	327	SER	2.8
1	C	662	ARG	2.7
1	D	611	ASN	2.6
1	B	441	GLY	2.6
1	C	646	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	435	THR	2.5
1	C	643	ARG	2.5
1	A	327	SER	2.4
1	D	517	VAL	2.4
1	B	415	THR	2.4
1	C	581	VAL	2.3
1	D	602	LEU	2.3
1	C	672	TYR	2.3
1	C	722	ASP	2.2
1	C	726	ALA	2.2
1	B	79	SER	2.2
1	B	347	GLY	2.2
1	A	731	TYR	2.2
1	B	140	LEU	2.2
1	A	330	TYR	2.1
1	C	500	ALA	2.1
1	A	-1	ALA	2.1
1	B	72	ILE	2.1
1	D	725	TRP	2.1
1	B	328	ASP	2.1

## 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.