



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4AV3  
Title : Crystal structure of Thermotoga Maritima sodium pumping membrane integral pyrophosphatase with metal ions in active site  
Authors : Kajander, T.; Kogan, K.; Kellosalo, J.; Pokharel, K.; Goldman, A.  
Deposited on : 2012-05-23  
Resolution : 2.60 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

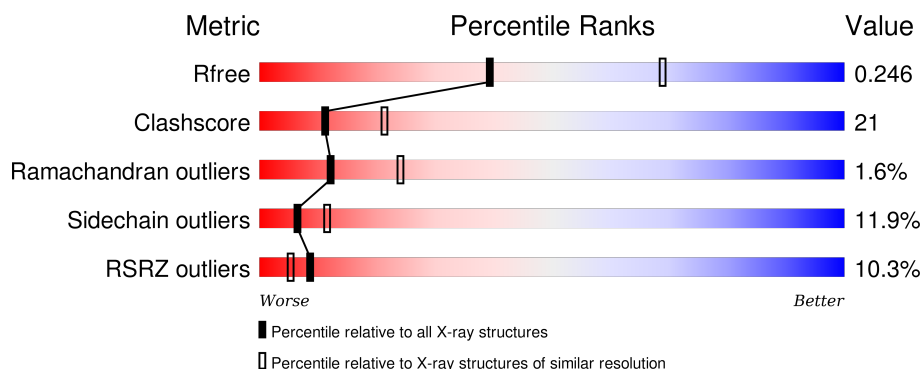
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	735	<div> <div>10%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	735	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9988 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 K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	0	0
			4926	3230	769	900	27			
1	B	707	Total	C	N	O	S	0	0	0
			5039	3294	789	929	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q9S5X0
A	-7	ARG	-	EXPRESSION TAG	UNP Q9S5X0
A	-6	GLY	-	EXPRESSION TAG	UNP Q9S5X0
A	-5	SER	-	EXPRESSION TAG	UNP Q9S5X0
A	-4	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	-3	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	-2	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	-1	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	0	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	1	HIS	-	EXPRESSION TAG	UNP Q9S5X0
A	353	LEU	VAL	ENGINEERED MUTATION	UNP Q9S5X0
A	395	GLY	SER	ENGINEERED MUTATION	UNP Q9S5X0
B	-8	MET	-	EXPRESSION TAG	UNP Q9S5X0
B	-7	ARG	-	EXPRESSION TAG	UNP Q9S5X0
B	-6	GLY	-	EXPRESSION TAG	UNP Q9S5X0
B	-5	SER	-	EXPRESSION TAG	UNP Q9S5X0
B	-4	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	-3	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	-2	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	-1	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	0	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	1	HIS	-	EXPRESSION TAG	UNP Q9S5X0
B	353	LEU	VAL	ENGINEERED MUTATION	UNP Q9S5X0
B	395	GLY	SER	ENGINEERED MUTATION	UNP Q9S5X0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

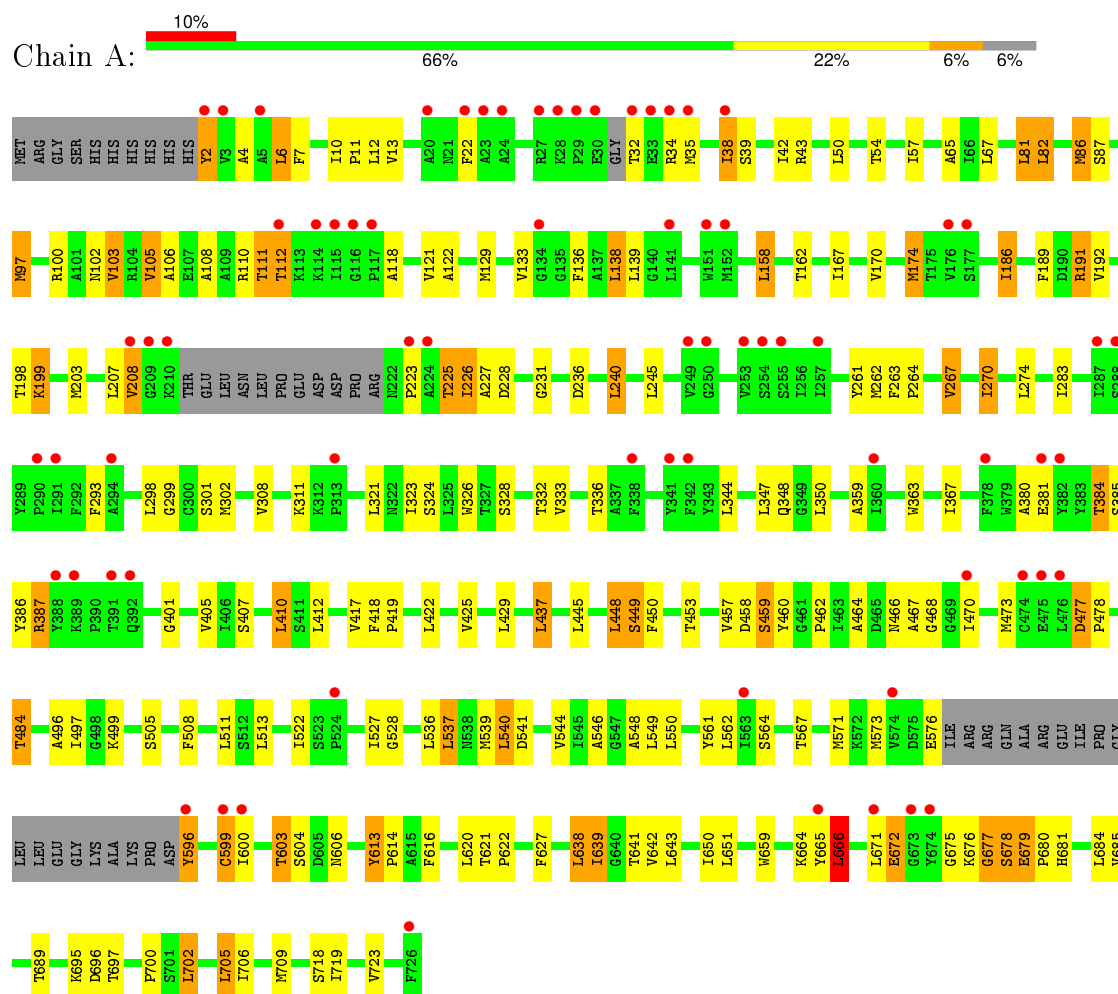
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	8	Total	O	0	0
			8	8		

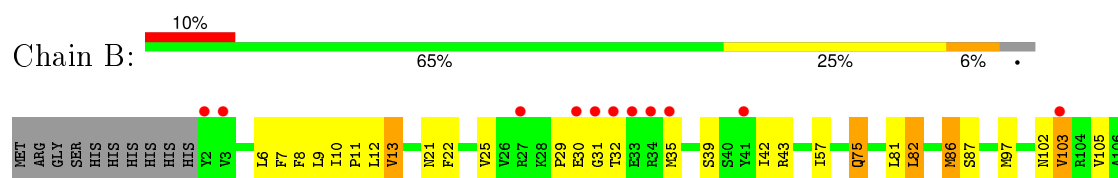
### 3 Residue-property plots

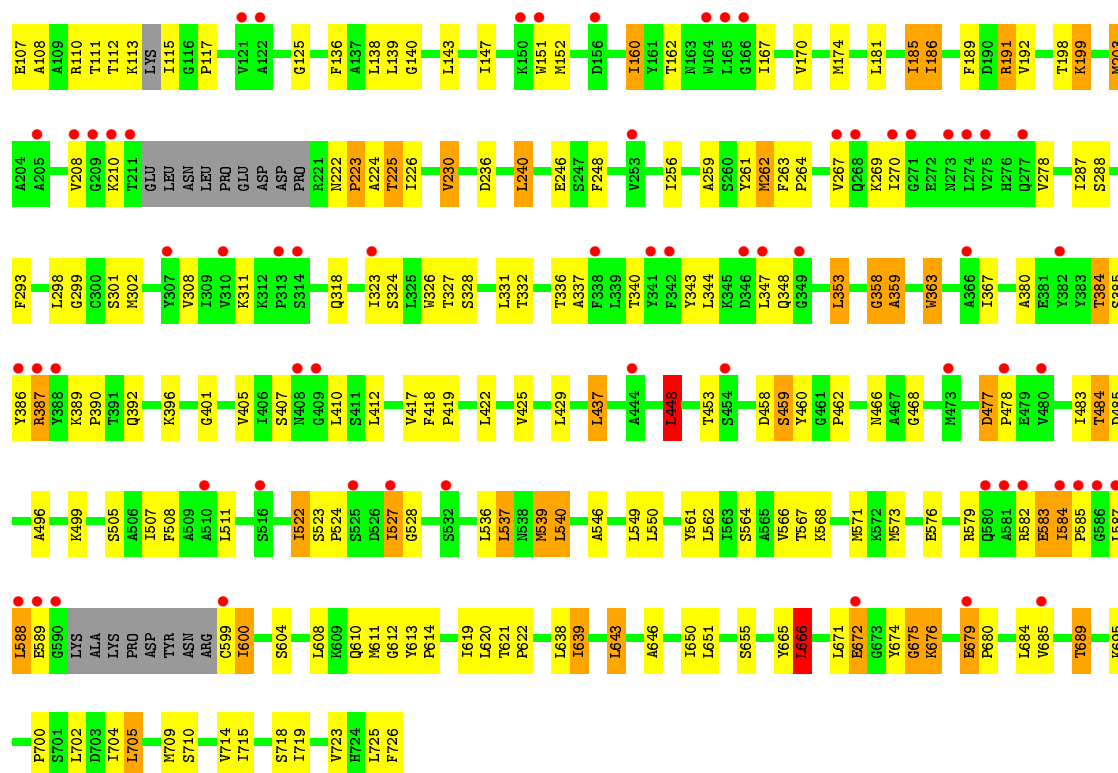
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.52Å 107.78Å 102.52Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 29.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.60) 97.9 (29.09-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.205 , 0.245 0.209 , 0.246	Depositor DCC
$R_{free}$ test set	2622 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 91.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 51920 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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 [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.71	1/5031 (0.0%)	0.83	7/6867 (0.1%)
1	B	0.71	2/5142 (0.0%)	0.81	4/7011 (0.1%)
All	All	0.71	3/10173 (0.0%)	0.82	11/13878 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	326	TRP	CD2-CE2	6.53	1.49	1.41
1	A	326	TRP	CD2-CE2	5.71	1.48	1.41
1	B	363	TRP	CD2-CE2	5.47	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	MET	CG-SD-CE	-8.70	86.28	100.20
1	A	174	MET	CG-SD-CE	-7.14	88.77	100.20
1	B	666	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	191	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	666	LEU	CA-CB-CG	6.02	129.16	115.30
1	A	677	GLY	N-CA-C	-5.71	98.84	113.10
1	B	448	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	191	ARG	NE-CZ-NH2	-5.35	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	449	SER	N-CA-C	-5.16	97.07	111.00
1	A	702	LEU	CB-CG-CD1	5.08	119.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	528	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	4926	0	4792	195	0
1	B	5039	0	4932	222	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	11	0	0	0	0
4	B	8	0	0	2	0
All	All	9988	0	9724	408	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 21.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:O	1:B:112:THR:HG22	1.21	1.31
1:A:105:VAL:HG21	1:A:467:ALA:CB	1.83	1.08
1:A:105:VAL:CG2	1:A:467:ALA:HB1	1.84	1.07
1:A:105:VAL:HG21	1:A:467:ALA:HB1	1.11	1.07
1:A:336:THR:HG22	1:A:363:TRP:HD1	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HG2	1:A:225:THR:HG22	1.33	1.05
1:B:336:THR:HG22	1:B:363:TRP:HD1	1.19	1.04
1:B:108:ALA:O	1:B:112:THR:CG2	2.07	1.02
1:B:584:ILE:HD13	1:B:588:LEU:HD13	1.37	1.01
1:A:336:THR:HG22	1:A:363:TRP:CD1	1.97	0.99
1:B:363:TRP:CZ2	1:B:367:ILE:HD11	1.99	0.98
1:B:336:THR:HG22	1:B:363:TRP:CD1	1.99	0.97
1:B:524:PRO:O	1:B:527:ILE:HD12	1.67	0.94
1:B:363:TRP:CE2	1:B:367:ILE:HD11	2.03	0.93
1:B:160:ILE:H	1:B:160:ILE:HD12	1.34	0.92
1:A:22:PHE:HA	1:A:97:MET:HE1	1.51	0.92
1:A:638:LEU:O	1:A:642:VAL:HG23	1.70	0.91
1:B:719:ILE:HG22	1:B:723:VAL:HG11	1.50	0.90
1:B:468:GLY:HA2	1:B:484:THR:HG23	1.53	0.90
1:B:719:ILE:O	1:B:723:VAL:HG12	1.73	0.89
1:A:719:ILE:HG22	1:A:723:VAL:HG11	1.54	0.89
1:B:223:PRO:HD2	1:B:225:THR:CG2	2.04	0.88
1:A:719:ILE:HG22	1:A:723:VAL:CG1	2.03	0.88
1:A:22:PHE:HA	1:A:97:MET:CE	2.05	0.87
1:A:105:VAL:CG2	1:A:106:ALA:N	2.39	0.85
1:A:540:LEU:HD22	1:B:437:LEU:HD21	1.58	0.85
1:B:223:PRO:HD2	1:B:225:THR:HG22	1.58	0.83
1:B:262:MET:HE3	1:B:353:LEU:HD21	1.60	0.83
1:A:118:ALA:O	1:A:121:VAL:HG22	1.78	0.83
1:A:468:GLY:HA2	1:A:484:THR:HG23	1.61	0.82
1:A:386:TYR:O	1:A:387:ARG:CB	2.28	0.81
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.17	0.80
1:B:386:TYR:O	1:B:387:ARG:CB	2.30	0.79
1:A:105:VAL:HG22	1:A:106:ALA:N	1.98	0.79
1:B:719:ILE:HG22	1:B:723:VAL:CG1	2.13	0.78
1:A:539:MET:HE2	1:B:539:MET:HG3	1.66	0.78
1:A:34:ARG:O	1:A:38:ILE:HG22	1.83	0.78
1:B:86:MET:HE1	1:B:139:LEU:HD23	1.66	0.77
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.20	0.77
1:A:270:ILE:HG23	1:A:270:ILE:O	1.85	0.77
1:B:7:PHE:HA	1:B:10:ILE:HD13	1.67	0.76
1:A:223:PRO:HG2	1:A:225:THR:CG2	2.13	0.76
1:B:672:GLU:CA	1:B:672:GLU:OE1	2.35	0.75
1:B:672:GLU:HA	1:B:672:GLU:OE1	1.86	0.75
1:B:468:GLY:HA2	1:B:484:THR:CG2	2.16	0.75
1:B:185:ILE:HD12	1:B:185:ILE:C	2.07	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HE3	1:A:323:ILE:HD12	1.69	0.74
1:B:386:TYR:O	1:B:387:ARG:HB3	1.86	0.73
1:A:158:LEU:HD23	1:A:263:PHE:CG	2.24	0.73
1:A:336:THR:CG2	1:A:363:TRP:HD1	1.98	0.73
1:A:225:THR:O	1:A:228:ASP:N	2.22	0.73
1:B:336:THR:CG2	1:B:363:TRP:HD1	2.01	0.72
1:B:584:ILE:HG23	1:B:588:LEU:HB2	1.72	0.72
1:B:75:GLN:H	1:B:75:GLN:HE21	1.37	0.70
1:B:174:MET:HE1	1:B:715:ILE:HG23	1.73	0.70
1:B:240:LEU:HD13	1:B:458:ASP:HB3	1.71	0.70
1:B:270:ILE:HG22	4:B:2004:HOH:O	1.90	0.70
1:B:674:TYR:O	1:B:676:LYS:N	2.25	0.70
1:A:293:PHE:CE2	1:A:336:THR:HG23	2.27	0.70
1:A:223:PRO:CG	1:A:225:THR:HG22	2.18	0.69
1:A:540:LEU:HD22	1:B:437:LEU:CD2	2.21	0.69
1:B:599:CYS:SG	1:B:600:ILE:N	2.65	0.69
1:B:226:ILE:O	1:B:230:VAL:HG13	1.91	0.69
1:B:380:ALA:O	1:B:384:THR:HB	1.92	0.69
1:B:203:MET:CE	1:B:567:THR:HG22	2.23	0.69
1:B:358:GLY:O	1:B:359:ALA:HB3	1.94	0.68
1:B:170:VAL:HG23	1:B:261:TYR:CE1	2.29	0.68
1:A:207:LEU:O	1:A:208:VAL:HG13	1.94	0.68
1:B:86:MET:CE	1:B:139:LEU:HD23	2.23	0.67
1:A:105:VAL:HG22	1:A:106:ALA:H	1.58	0.67
1:B:42:ILE:HD12	1:B:43:ARG:N	2.09	0.67
1:B:725:LEU:C	1:B:725:LEU:HD13	2.16	0.67
1:B:725:LEU:HD12	1:B:726:PHE:CG	2.30	0.66
1:B:75:GLN:HG2	1:B:152:MET:HE1	1.78	0.66
1:A:536:LEU:HD12	1:A:537:LEU:N	2.11	0.66
1:B:328:SER:CB	1:B:453:THR:HG21	2.25	0.66
1:A:311:LYS:HE3	1:A:323:ILE:CD1	2.26	0.66
1:B:174:MET:HE1	1:B:715:ILE:HG12	1.77	0.66
1:B:138:LEU:HD13	1:B:248:PHE:CE2	2.29	0.66
1:B:340:THR:HG23	1:B:344:LEU:HD12	1.76	0.66
1:B:208:VAL:HG22	1:B:210:LYS:H	1.60	0.66
1:B:86:MET:HE3	1:B:139:LEU:HB3	1.77	0.65
1:B:138:LEU:HD13	1:B:248:PHE:HE2	1.60	0.65
1:A:723:VAL:O	1:A:723:VAL:HG22	1.96	0.65
1:A:321:LEU:HD13	1:A:457:VAL:HG13	1.79	0.65
1:B:293:PHE:CE2	1:B:336:THR:HG23	2.31	0.65
1:A:600:ILE:O	1:A:604:SER:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PHE:CE2	1:A:336:THR:CG2	2.80	0.64
1:B:363:TRP:CH2	1:B:367:ILE:HD11	2.32	0.64
1:A:328:SER:CB	1:A:453:THR:HG21	2.27	0.64
1:B:353:LEU:HD13	1:B:353:LEU:O	1.98	0.63
1:A:32:THR:HG22	1:A:34:ARG:H	1.63	0.63
1:B:293:PHE:CE2	1:B:336:THR:CG2	2.81	0.63
1:B:527:ILE:HD13	1:B:528:GLY:H	1.62	0.63
1:A:380:ALA:O	1:A:384:THR:HB	1.98	0.63
1:B:278:VAL:HG11	1:B:353:LEU:HD23	1.81	0.63
1:A:363:TRP:CZ2	1:A:367:ILE:CD1	2.81	0.63
1:B:725:LEU:HD12	1:B:726:PHE:CD2	2.33	0.63
1:A:384:THR:HG21	1:A:496:ALA:HB1	1.80	0.62
1:A:613:TYR:HB3	1:A:614:PRO:HD3	1.81	0.62
1:B:600:ILE:O	1:B:604:SER:HB2	1.98	0.62
1:B:468:GLY:CA	1:B:484:THR:HG23	2.26	0.62
1:A:468:GLY:HA2	1:A:484:THR:CG2	2.28	0.62
1:B:39:SER:HB2	1:B:103:VAL:HG13	1.80	0.62
1:A:86:MET:HE3	1:A:139:LEU:HD23	1.81	0.62
1:B:262:MET:CE	1:B:353:LEU:HD21	2.29	0.62
1:A:719:ILE:HG22	1:A:723:VAL:HG12	1.82	0.61
1:B:344:LEU:HA	1:B:347:LEU:HD21	1.81	0.61
1:A:270:ILE:CG2	1:A:270:ILE:O	2.48	0.61
1:B:192:VAL:HG11	1:B:614:PRO:HB2	1.81	0.61
1:B:75:GLN:CG	1:B:152:MET:HE1	2.30	0.61
1:A:677:GLY:O	1:A:678:SER:OG	2.16	0.61
1:A:86:MET:CE	1:A:139:LEU:HD23	2.31	0.61
1:A:264:PRO:O	1:A:267:VAL:HG13	2.01	0.60
1:B:160:ILE:H	1:B:160:ILE:CD1	2.06	0.60
1:B:536:LEU:HD12	1:B:537:LEU:N	2.16	0.60
1:A:105:VAL:HA	1:A:121:VAL:HG21	1.82	0.60
1:B:22:PHE:HA	1:B:97:MET:CE	2.32	0.59
1:A:121:VAL:HG23	1:A:122:ALA:N	2.16	0.59
1:A:616:PHE:CD2	1:A:620:LEU:CD1	2.85	0.59
1:B:167:ILE:HD13	1:B:719:ILE:HG12	1.85	0.59
1:A:2:TYR:CZ	1:A:4:ALA:HB2	2.38	0.58
1:A:105:VAL:O	1:A:108:ALA:HB3	2.02	0.58
1:B:666:LEU:HB2	1:B:671:LEU:HD12	1.85	0.58
1:A:39:SER:HB2	1:A:103:VAL:HG13	1.84	0.58
1:A:199:LYS:HD3	1:A:696:ASP:HB2	1.85	0.58
1:A:308:VAL:HG21	1:A:324:SER:HB3	1.85	0.58
1:A:105:VAL:HG23	1:A:106:ALA:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ALA:O	1:A:467:ALA:HB3	2.03	0.58
1:B:685:VAL:O	1:B:689:THR:HG23	2.04	0.58
1:B:705:LEU:HD21	1:B:709:MET:CE	2.33	0.57
1:B:112:THR:O	1:B:113:LYS:CB	2.52	0.57
1:A:38:ILE:HD13	1:A:470:ILE:HA	1.85	0.57
1:B:224:ALA:HB1	1:B:573:MET:HE1	1.87	0.57
1:B:31:GLY:HA3	1:B:35:MET:HE2	1.87	0.57
1:A:12:LEU:CD1	1:A:139:LEU:HD13	2.35	0.57
1:A:381:GLU:OE1	1:A:497:ILE:HD11	2.05	0.57
1:A:616:PHE:CD2	1:A:620:LEU:HD12	2.39	0.56
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.86	0.56
1:B:385:SER:C	1:B:386:TYR:O	2.40	0.56
1:B:384:THR:HG21	1:B:496:ALA:HB1	1.87	0.56
1:A:199:LYS:HD3	1:A:696:ASP:CB	2.35	0.56
1:A:596:TYR:CD1	1:A:596:TYR:N	2.73	0.56
1:A:599:CYS:O	1:A:603:THR:HG22	2.06	0.56
1:A:192:VAL:HG13	1:A:562:LEU:HD21	1.87	0.56
1:B:562:LEU:O	1:B:566:VAL:HG23	2.06	0.56
1:A:651:LEU:HD23	1:A:651:LEU:C	2.26	0.56
1:A:42:ILE:HD12	1:A:43:ARG:N	2.21	0.56
1:B:651:LEU:C	1:B:651:LEU:HD23	2.27	0.55
1:B:448:LEU:HD21	1:B:505:SER:HB3	1.88	0.55
1:A:105:VAL:CG2	1:A:467:ALA:CB	2.61	0.55
1:A:385:SER:C	1:A:386:TYR:O	2.43	0.55
1:A:459:SER:O	1:A:462:PRO:HD2	2.07	0.55
1:A:468:GLY:CA	1:A:484:THR:HG23	2.35	0.55
1:A:573:MET:O	1:A:576:GLU:N	2.39	0.55
1:B:223:PRO:HG2	1:B:224:ALA:H	1.72	0.54
1:B:358:GLY:O	1:B:359:ALA:CB	2.53	0.54
1:A:719:ILE:CG2	1:A:723:VAL:HG11	2.31	0.54
1:B:459:SER:O	1:B:462:PRO:HD2	2.07	0.54
1:A:719:ILE:O	1:A:723:VAL:HG12	2.07	0.54
1:A:32:THR:HB	1:A:35:MET:HG3	1.88	0.54
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.89	0.54
1:B:675:GLY:O	1:B:676:LYS:CB	2.55	0.54
1:B:21:ASN:O	1:B:25:VAL:HG23	2.08	0.54
1:B:167:ILE:CG2	1:B:718:SER:HB3	2.38	0.54
1:A:344:LEU:HD22	1:A:347:LEU:CD1	2.37	0.53
1:A:437:LEU:HD21	1:B:540:LEU:HD22	1.90	0.53
1:A:118:ALA:O	1:A:121:VAL:CG2	2.52	0.53
1:A:344:LEU:CD2	1:A:347:LEU:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD11	1:B:511:LEU:HD11	1.90	0.53
1:A:671:LEU:O	1:A:672:GLU:CB	2.56	0.53
1:A:167:ILE:CG2	1:A:718:SER:HB3	2.39	0.53
1:B:584:ILE:O	1:B:587:LEU:N	2.40	0.53
1:B:672:GLU:OE1	1:B:672:GLU:N	2.41	0.53
1:A:336:THR:CG2	1:A:363:TRP:CD1	2.82	0.53
1:B:527:ILE:HD13	1:B:528:GLY:N	2.24	0.53
1:B:613:TYR:HB3	1:B:614:PRO:HD3	1.91	0.53
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.91	0.53
1:B:160:ILE:N	1:B:160:ILE:HD12	2.13	0.53
1:B:185:ILE:HD12	1:B:185:ILE:O	2.09	0.53
1:B:621:THR:HB	1:B:622:PRO:HD3	1.90	0.53
1:A:203:MET:SD	1:A:567:THR:HG22	2.49	0.53
1:B:308:VAL:HG21	1:B:324:SER:HB3	1.90	0.53
1:A:548:ALA:HB1	1:B:643:LEU:HD21	1.91	0.52
1:B:112:THR:HG21	1:B:117:PRO:HG2	1.89	0.52
1:B:22:PHE:HA	1:B:97:MET:HE1	1.90	0.52
1:B:522:ILE:HD13	1:B:523:SER:N	2.24	0.52
1:A:86:MET:HE2	1:A:136:PHE:HA	1.91	0.52
1:A:448:LEU:HD21	1:A:505:SER:HB3	1.92	0.52
1:B:224:ALA:HB1	1:B:573:MET:CE	2.39	0.52
1:A:39:SER:OG	1:A:103:VAL:HG22	2.10	0.52
1:B:723:VAL:O	1:B:723:VAL:HG22	2.10	0.52
1:A:677:GLY:O	1:A:678:SER:CB	2.58	0.52
1:A:384:THR:HG21	1:A:496:ALA:CB	2.40	0.52
1:A:448:LEU:C	1:A:449:SER:O	2.47	0.51
1:B:174:MET:CE	1:B:715:ILE:HG23	2.40	0.51
1:B:138:LEU:CD1	1:B:248:PHE:CE2	2.92	0.51
1:A:223:PRO:C	1:A:225:THR:H	2.12	0.51
1:A:344:LEU:HD23	1:A:347:LEU:HD11	1.91	0.51
1:A:676:LYS:HA	1:A:681:HIS:CE1	2.45	0.51
1:A:158:LEU:HD23	1:A:263:PHE:CD2	2.46	0.51
1:B:9:LEU:HD23	1:B:9:LEU:N	2.26	0.51
1:A:621:THR:HB	1:A:622:PRO:HD3	1.93	0.51
1:B:725:LEU:HD12	1:B:726:PHE:CD1	2.45	0.50
1:B:39:SER:HB2	1:B:103:VAL:CG1	2.41	0.50
1:B:344:LEU:HA	1:B:347:LEU:CD2	2.41	0.50
1:B:7:PHE:HA	1:B:10:ILE:CD1	2.39	0.50
1:B:499:LYS:CE	1:B:695:LYS:O	2.59	0.50
1:B:181:LEU:O	1:B:185:ILE:HG23	2.12	0.50
1:A:42:ILE:HD11	1:A:102:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LYS:HE3	1:B:323:ILE:HD12	1.94	0.50
1:B:619:ILE:HG22	1:B:620:LEU:HD12	1.92	0.50
1:B:719:ILE:CG2	1:B:723:VAL:HG11	2.34	0.49
1:B:725:LEU:C	1:B:725:LEU:CD1	2.81	0.49
1:A:347:LEU:O	1:A:348:GLN:HB2	2.12	0.49
1:B:86:MET:HG3	1:B:136:PHE:HB3	1.94	0.49
1:A:616:PHE:CD2	1:A:620:LEU:HD13	2.46	0.49
1:A:685:VAL:O	1:A:689:THR:HG23	2.11	0.49
1:B:293:PHE:CE2	1:B:336:THR:HG21	2.46	0.49
1:B:236:ASP:HB2	1:B:462:PRO:HG3	1.94	0.49
1:A:57:ILE:HG13	1:A:189:PHE:CD2	2.48	0.49
1:B:412:LEU:HD23	1:B:412:LEU:C	2.33	0.49
1:A:596:TYR:HD1	1:A:596:TYR:N	2.09	0.49
1:B:327:THR:HG22	1:B:331:LEU:HD12	1.94	0.49
1:B:7:PHE:CA	1:B:10:ILE:HD13	2.41	0.49
1:A:616:PHE:CE2	1:A:620:LEU:HD13	2.48	0.49
1:A:38:ILE:HD12	1:A:473:MET:HG3	1.95	0.48
1:A:225:THR:O	1:A:226:ILE:C	2.51	0.48
1:B:666:LEU:HD12	1:B:666:LEU:C	2.33	0.48
1:A:207:LEU:O	1:A:208:VAL:CG1	2.60	0.48
1:B:39:SER:OG	1:B:103:VAL:HG22	2.13	0.48
1:A:174:MET:HE2	1:A:174:MET:O	2.14	0.48
1:A:10:ILE:N	1:A:11:PRO:CD	2.76	0.48
1:B:199:LYS:HA	1:B:199:LYS:HE3	1.95	0.48
1:A:641:THR:HG22	1:A:706:ILE:HG22	1.95	0.48
1:A:65:ALA:HB2	1:A:81:LEU:HD13	1.95	0.48
1:B:417:VAL:HG22	1:B:650:ILE:HB	1.94	0.48
1:B:363:TRP:CD2	1:B:367:ILE:HD11	2.47	0.48
1:B:222:ASN:OD1	1:B:222:ASN:O	2.30	0.48
1:A:86:MET:CE	1:A:139:LEU:HB3	2.44	0.48
1:A:541:ASP:HB3	1:A:544:VAL:HG23	1.95	0.48
1:A:32:THR:HB	1:A:35:MET:CG	2.44	0.48
1:A:39:SER:O	1:A:42:ILE:HG13	2.14	0.48
1:B:710:SER:O	1:B:714:VAL:HG23	2.14	0.48
1:B:6:LEU:O	1:B:10:ILE:HD12	2.14	0.47
1:A:86:MET:HG3	1:A:136:PHE:HB3	1.95	0.47
1:B:10:ILE:N	1:B:11:PRO:CD	2.76	0.47
1:A:328:SER:HB2	1:A:453:THR:HG21	1.96	0.47
1:B:401:GLY:O	1:B:405:VAL:HG23	2.14	0.47
1:A:536:LEU:HD12	1:A:536:LEU:C	2.35	0.47
1:A:723:VAL:CG2	1:A:723:VAL:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:THR:HG21	1:B:496:ALA:CB	2.45	0.47
1:A:42:ILE:HD12	1:A:42:ILE:C	2.35	0.47
1:B:328:SER:HB2	1:B:453:THR:HG21	1.97	0.47
1:B:613:TYR:HB3	1:B:614:PRO:CD	2.44	0.47
1:A:666:LEU:CD1	1:A:675:GLY:HA2	2.44	0.47
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.66	0.47
1:B:639:ILE:HD13	1:B:639:ILE:HA	1.62	0.47
1:A:198:THR:HG22	1:A:231:GLY:HA2	1.97	0.47
1:B:105:VAL:O	1:B:108:ALA:HB3	2.14	0.47
1:A:192:VAL:HG11	1:A:614:PRO:HB2	1.97	0.47
1:A:344:LEU:HD22	1:A:347:LEU:HD12	1.96	0.47
1:A:410:LEU:HD13	1:A:659:TRP:HH2	1.80	0.47
1:A:613:TYR:HB3	1:A:614:PRO:CD	2.44	0.47
1:A:225:THR:O	1:A:227:ALA:N	2.48	0.47
1:B:499:LYS:HE2	1:B:695:LYS:O	2.15	0.47
1:A:32:THR:HG22	1:A:34:ARG:N	2.30	0.46
1:A:236:ASP:HB2	1:A:462:PRO:HG3	1.97	0.46
1:B:386:TYR:HB2	1:B:665:TYR:CD1	2.50	0.46
1:A:263:PHE:HB3	1:A:264:PRO:HD3	1.98	0.46
1:A:675:GLY:C	1:A:677:GLY:H	2.19	0.46
1:B:240:LEU:HD13	1:B:458:ASP:CB	2.43	0.46
1:A:267:VAL:HG21	1:A:527:ILE:HG23	1.98	0.46
1:A:293:PHE:CE2	1:A:336:THR:HG21	2.49	0.46
1:B:666:LEU:CD1	1:B:675:GLY:HA2	2.46	0.46
1:B:192:VAL:HG11	1:B:614:PRO:CB	2.44	0.46
1:A:344:LEU:HB3	1:A:347:LEU:HD12	1.98	0.46
1:B:30:GLU:CA	1:B:107:GLU:OE1	2.64	0.46
1:B:191:ARG:CZ	1:B:700:PRO:HB3	2.46	0.46
1:B:337:ALA:HB2	1:B:363:TRP:NE1	2.30	0.46
1:B:25:VAL:HB	1:B:97:MET:HE1	1.98	0.46
1:A:198:THR:HG22	1:A:231:GLY:CA	2.46	0.46
1:A:561:TYR:C	1:A:561:TYR:CD1	2.88	0.46
1:B:86:MET:HE2	1:B:140:GLY:N	2.31	0.46
1:A:666:LEU:HD12	1:A:666:LEU:C	2.36	0.46
1:B:138:LEU:HD11	1:B:248:PHE:CZ	2.50	0.45
1:B:288:SER:OG	1:B:343:TYR:OH	2.16	0.45
1:B:57:ILE:HG13	1:B:189:PHE:CD2	2.51	0.45
1:A:121:VAL:CG2	1:A:122:ALA:N	2.79	0.45
1:B:167:ILE:HG23	1:B:718:SER:HB3	1.99	0.45
1:B:203:MET:HE3	1:B:567:THR:HG22	1.97	0.45
1:B:460:TYR:CD1	1:B:460:TYR:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:C	1:B:107:GLU:OE1	2.54	0.45
1:B:259:ALA:HA	1:B:262:MET:CE	2.46	0.45
1:B:246:GLU:OE1	1:B:704:ILE:HD12	2.16	0.45
1:A:445:LEU:O	1:A:449:SER:N	2.50	0.45
1:A:13:VAL:HG22	1:A:302:MET:SD	2.57	0.45
1:B:527:ILE:CD1	1:B:527:ILE:N	2.80	0.45
1:B:262:MET:SD	1:B:353:LEU:HD11	2.57	0.45
1:B:192:VAL:HG13	1:B:562:LEU:HD21	1.99	0.45
1:B:573:MET:O	1:B:576:GLU:N	2.50	0.45
1:A:267:VAL:HG21	1:A:527:ILE:CG2	2.46	0.45
1:A:6:LEU:HD12	1:A:7:PHE:HD1	1.82	0.45
1:A:111:THR:HG22	1:A:112:THR:N	2.30	0.45
1:A:511:LEU:HD11	1:B:549:LEU:HD11	1.97	0.45
1:A:191:ARG:CZ	1:A:700:PRO:HB3	2.47	0.45
1:A:87:SER:HB2	1:A:186:ILE:HG12	1.99	0.45
1:A:301:SER:HA	1:A:328:SER:OG	2.17	0.45
1:B:568:LYS:HD2	1:B:610:GLN:OE1	2.16	0.45
1:B:679:GLU:N	1:B:680:PRO:CD	2.80	0.45
1:A:299:GLY:HA2	1:A:302:MET:HE2	1.99	0.45
1:B:160:ILE:N	1:B:160:ILE:CD1	2.75	0.44
1:B:263:PHE:HB3	1:B:264:PRO:HD3	1.97	0.44
1:A:386:TYR:HB2	1:A:665:TYR:CD1	2.52	0.44
1:A:627:PHE:HE1	1:A:723:VAL:CG1	2.30	0.44
1:B:666:LEU:HD13	1:B:675:GLY:HA2	2.00	0.44
1:B:392:GLN:O	1:B:396:LYS:HG3	2.18	0.44
1:B:222:ASN:N	1:B:223:PRO:CD	2.81	0.44
1:B:262:MET:SD	1:B:353:LEU:CD1	3.06	0.44
1:A:170:VAL:HG23	1:A:261:TYR:CE1	2.53	0.44
1:A:22:PHE:HA	1:A:97:MET:HE2	1.97	0.44
1:B:8:PHE:C	1:B:9:LEU:HD23	2.38	0.44
1:B:42:ILE:HD11	1:B:102:ASN:HD21	1.82	0.43
1:B:87:SER:HB2	1:B:186:ILE:HG12	1.99	0.43
1:A:412:LEU:HD23	1:A:412:LEU:C	2.38	0.43
1:A:245:LEU:HD23	1:A:245:LEU:C	2.38	0.43
1:B:256:ILE:HG23	1:B:287:ILE:HG23	1.99	0.43
1:A:425:VAL:HG13	1:B:546:ALA:HB1	2.00	0.43
1:B:675:GLY:O	1:B:676:LYS:HB3	2.17	0.43
1:B:203:MET:HE1	1:B:567:THR:HG22	1.97	0.43
1:B:608:LEU:HD23	1:B:611:MET:CE	2.49	0.43
1:A:332:THR:O	1:A:336:THR:HB	2.19	0.43
1:B:725:LEU:HD12	1:B:726:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HG2	1:A:697:THR:OG1	2.19	0.43
1:B:579:ARG:O	1:B:583:GLU:HB2	2.18	0.43
1:A:616:PHE:C	1:A:616:PHE:CD1	2.92	0.43
1:B:13:VAL:HG22	1:B:302:MET:SD	2.59	0.43
1:B:301:SER:HA	1:B:328:SER:OG	2.18	0.43
1:B:299:GLY:HA2	1:B:302:MET:HE2	2.01	0.43
1:B:347:LEU:O	1:B:348:GLN:HB2	2.19	0.43
1:B:263:PHE:HB3	1:B:264:PRO:CD	2.49	0.43
1:B:484:THR:HG22	1:B:485:ASP:N	2.33	0.43
1:A:499:LYS:HE2	1:A:695:LYS:O	2.19	0.43
1:A:240:LEU:HD13	1:A:458:ASP:CG	2.39	0.43
1:B:12:LEU:CD1	1:B:139:LEU:HD13	2.49	0.42
1:A:679:GLU:N	1:A:680:PRO:CD	2.82	0.42
1:B:363:TRP:CH2	1:B:367:ILE:CD1	3.02	0.42
1:A:240:LEU:HD13	1:A:458:ASP:OD2	2.19	0.42
1:B:332:THR:O	1:B:336:THR:HB	2.18	0.42
1:B:42:ILE:CD1	1:B:102:ASN:HD21	2.32	0.42
1:B:208:VAL:O	1:B:208:VAL:HG13	2.19	0.42
1:B:198:THR:HG22	1:B:199:LYS:NZ	2.34	0.42
1:B:507:ILE:HD13	1:B:646:ALA:HB1	2.01	0.42
1:A:38:ILE:CD1	1:A:470:ILE:HA	2.50	0.42
1:B:7:PHE:O	1:B:10:ILE:HD13	2.20	0.42
1:B:270:ILE:CG2	4:B:2004:HOH:O	2.57	0.42
1:A:199:LYS:HA	1:A:199:LYS:HE3	2.02	0.42
1:B:499:LYS:NZ	1:B:695:LYS:O	2.52	0.42
1:B:389:LYS:N	1:B:390:PRO:CD	2.82	0.42
1:A:129:MET:O	1:A:133:VAL:HG23	2.19	0.42
1:B:42:ILE:C	1:B:42:ILE:HD12	2.40	0.42
1:B:561:TYR:CD1	1:B:561:TYR:C	2.93	0.42
1:B:262:MET:CE	1:B:353:LEU:HD11	2.50	0.42
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.81	0.42
1:A:223:PRO:C	1:A:225:THR:N	2.73	0.42
1:A:263:PHE:HB3	1:A:264:PRO:CD	2.50	0.42
1:A:158:LEU:HD21	1:A:283:ILE:HG21	2.01	0.42
1:A:65:ALA:HB2	1:A:81:LEU:CD1	2.50	0.42
1:A:100:ARG:O	1:A:103:VAL:HG23	2.19	0.42
1:A:344:LEU:CD2	1:A:347:LEU:HD12	2.50	0.42
1:A:87:SER:CB	1:A:186:ILE:HG12	2.50	0.42
1:B:582:ARG:HA	1:B:582:ARG:HD2	1.90	0.42
1:A:417:VAL:HG22	1:A:650:ILE:HB	2.02	0.42
1:B:115:ILE:HA	1:B:483:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HB2	1:A:103:VAL:CG1	2.48	0.41
1:A:401:GLY:O	1:A:405:VAL:HG23	2.20	0.41
1:A:705:LEU:HD21	1:A:709:MET:CE	2.50	0.41
1:B:39:SER:O	1:B:42:ILE:HG13	2.19	0.41
1:B:725:LEU:CD1	1:B:726:PHE:CD1	3.03	0.41
1:B:82:LEU:O	1:B:86:MET:HB2	2.20	0.41
1:A:6:LEU:HD13	1:A:6:LEU:C	2.41	0.41
1:B:507:ILE:CD1	1:B:646:ALA:HB1	2.51	0.41
1:A:167:ILE:HG23	1:A:718:SER:HB3	2.02	0.41
1:B:147:ILE:O	1:B:151:TRP:HB3	2.21	0.41
1:B:75:GLN:H	1:B:75:GLN:NE2	2.11	0.41
1:A:344:LEU:CD2	1:A:347:LEU:HD11	2.51	0.41
1:A:192:VAL:HG11	1:A:614:PRO:CB	2.50	0.41
1:B:97:MET:HE3	1:B:125:GLY:HA2	2.01	0.41
1:A:448:LEU:CD2	1:A:505:SER:HB3	2.51	0.41
1:B:87:SER:CB	1:B:186:ILE:HG12	2.51	0.41
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.92	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.94	0.41
1:A:639:ILE:HA	1:A:639:ILE:HD13	1.78	0.41
1:A:460:TYR:CD1	1:A:460:TYR:C	2.92	0.41
1:B:719:ILE:C	1:B:723:VAL:HG12	2.39	0.40
1:B:6:LEU:O	1:B:10:ILE:CD1	2.70	0.40
1:A:333:VAL:HG13	1:A:367:ILE:HD11	2.03	0.40
1:B:674:TYR:CD1	1:B:680:PRO:HG2	2.56	0.40
1:A:606:ASN:ND2	1:A:606:ASN:O	2.54	0.40
1:B:174:MET:HE1	1:B:715:ILE:CG2	2.46	0.40
1:B:328:SER:OG	1:B:453:THR:HG21	2.20	0.40
1:B:138:LEU:CD1	1:B:248:PHE:CZ	3.05	0.40
1:A:639:ILE:HG23	1:A:639:ILE:HD12	1.95	0.40
1:B:448:LEU:CD2	1:B:505:SER:HB3	2.51	0.40
1:A:344:LEU:HA	1:A:347:LEU:CD1	2.52	0.40
1:B:611:MET:O	1:B:612:GLY:C	2.60	0.40
1:B:336:THR:CG2	1:B:363:TRP:CD1	2.85	0.40
1:B:269:LYS:C	1:B:270:ILE:HD12	2.41	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	686/735 (93%)	632 (92%)	45 (7%)	9 (1%)	15	30
1	B	699/735 (95%)	653 (93%)	33 (5%)	13 (2%)	10	19
All	All	1385/1470 (94%)	1285 (93%)	78 (6%)	22 (2%)	12	24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	ALA
1	B	32	THR
1	B	359	ALA
1	B	675	GLY
1	B	676	LYS
1	A	208	VAL
1	A	226	ILE
1	A	387	ARG
1	A	450	PHE
1	A	672	GLU
1	A	678	SER
1	B	223	PRO
1	B	358	GLY
1	B	387	ARG
1	A	477	ASP
1	A	478	PRO
1	B	477	ASP
1	B	478	PRO
1	B	589	GLU
1	B	584	ILE
1	B	585	PRO
1	B	600	ILE

### 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	470/575 (82%)	411 (87%)	59 (13%)	5	10
1	B	486/575 (84%)	431 (89%)	55 (11%)	7	13
All	All	956/1150 (83%)	842 (88%)	114 (12%)	6	11

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	6	LEU
1	A	38	ILE
1	A	50	LEU
1	A	54	THR
1	A	67	LEU
1	A	81	LEU
1	A	82	LEU
1	A	86	MET
1	A	97	MET
1	A	103	VAL
1	A	105	VAL
1	A	110	ARG
1	A	111	THR
1	A	112	THR
1	A	138	LEU
1	A	158	LEU
1	A	162	THR
1	A	186	ILE
1	A	199	LYS
1	A	225	THR
1	A	240	LEU
1	A	262	MET
1	A	267	VAL
1	A	270	ILE
1	A	274	LEU
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	350	LEU
1	A	384	THR
1	A	407	SER
1	A	410	LEU
1	A	422	LEU
1	A	429	LEU
1	A	437	LEU
1	A	448	LEU
1	A	459	SER
1	A	466	ASN
1	A	477	ASP
1	A	484	THR
1	A	508	PHE
1	A	522	ILE
1	A	537	LEU
1	A	540	LEU
1	A	550	LEU
1	A	564	SER
1	A	571	MET
1	A	596	TYR
1	A	599	CYS
1	A	603	THR
1	A	613	TYR
1	A	638	LEU
1	A	639	ILE
1	A	643	LEU
1	A	664	LYS
1	A	666	LEU
1	A	679	GLU
1	A	684	LEU
1	A	702	LEU
1	A	705	LEU
1	B	13	VAL
1	B	75	GLN
1	B	81	LEU
1	B	82	LEU
1	B	86	MET
1	B	103	VAL
1	B	110	ARG
1	B	111	THR
1	B	143	LEU
1	B	160	ILE

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Mol	Chain	Res	Type
1	B	162	THR
1	B	185	ILE
1	B	186	ILE
1	B	199	LYS
1	B	203	MET
1	B	225	THR
1	B	230	VAL
1	B	240	LEU
1	B	262	MET
1	B	267	VAL
1	B	298	LEU
1	B	318	GLN
1	B	353	LEU
1	B	384	THR
1	B	407	SER
1	B	410	LEU
1	B	422	LEU
1	B	429	LEU
1	B	437	LEU
1	B	448	LEU
1	B	459	SER
1	B	466	ASN
1	B	477	ASP
1	B	484	THR
1	B	508	PHE
1	B	522	ILE
1	B	527	ILE
1	B	537	LEU
1	B	540	LEU
1	B	550	LEU
1	B	564	SER
1	B	571	MET
1	B	583	GLU
1	B	588	LEU
1	B	638	LEU
1	B	639	ILE
1	B	643	LEU
1	B	655	SER
1	B	666	LEU
1	B	672	GLU
1	B	679	GLU
1	B	684	LEU

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Mol	Chain	Res	Type
1	B	689	THR
1	B	702	LEU
1	B	705	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	HIS
1	A	606	ASN
1	B	222	ASN

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	694/735 (94%)	0.35	70 (10%) 9 5	48, 84, 143, 186	0
1	B	707/735 (96%)	0.40	75 (10%) 8 5	49, 87, 145, 219	0
All	All	1401/1470 (95%)	0.38	145 (10%) 9 5	48, 86, 145, 219	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	VAL	8.6
1	A	599	CYS	7.7
1	B	581	ALA	7.6
1	A	224	ALA	7.1
1	B	585	PRO	6.0
1	A	117	PRO	5.8
1	A	27	ARG	5.7
1	B	584	ILE	5.5
1	B	209	GLY	5.4
1	B	268	GLN	5.0
1	A	35	MET	5.0
1	B	599	CYS	4.9
1	B	210	LYS	4.9
1	B	164	TRP	4.8
1	B	122	ALA	4.7
1	A	151	TRP	4.7
1	B	211	THR	4.6
1	B	347	LEU	4.5
1	B	346	ASP	4.5
1	A	474	CYS	4.3
1	B	103	VAL	4.3
1	A	388	TYR	4.2
1	B	587	LEU	4.2
1	A	392	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	378	PHE	4.1
1	A	250	GLY	4.1
1	B	588	LEU	4.1
1	A	342	PHE	4.1
1	B	35	MET	4.0
1	A	223	PRO	4.0
1	A	116	GLY	4.0
1	A	112	THR	4.0
1	A	29	PRO	3.9
1	B	586	GLY	3.9
1	B	267	VAL	3.9
1	B	205	ALA	3.9
1	A	254	SER	3.8
1	A	253	VAL	3.8
1	B	121	VAL	3.8
1	B	480	VAL	3.7
1	B	590	GLY	3.7
1	B	33	GLU	3.7
1	A	313	PRO	3.7
1	A	674	TYR	3.5
1	B	388	TYR	3.5
1	B	2	TYR	3.5
1	B	41	TYR	3.4
1	A	475	GLU	3.4
1	A	115	ILE	3.3
1	A	291	ILE	3.3
1	A	114	LYS	3.3
1	A	294	ALA	3.3
1	B	382	TYR	3.3
1	B	478	PRO	3.3
1	A	24	ALA	3.3
1	B	387	ARG	3.2
1	B	30	GLU	3.1
1	B	323	ILE	3.1
1	B	532	SER	3.0
1	A	177	SER	3.0
1	B	589	GLU	3.0
1	B	32	THR	3.0
1	A	38	ILE	3.0
1	A	671	LEU	3.0
1	A	28	LYS	3.0
1	B	307	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	3.0
1	B	34	ARG	2.9
1	B	31	GLY	2.9
1	A	30	GLU	2.9
1	A	600	ILE	2.9
1	A	287	ILE	2.9
1	A	470	ILE	2.8
1	B	580	GLN	2.8
1	B	454	SER	2.8
1	B	273	ASN	2.8
1	A	3	VAL	2.8
1	B	150	LYS	2.8
1	B	275	VAL	2.8
1	B	582	ARG	2.8
1	B	510	ALA	2.8
1	A	726	PHE	2.8
1	B	270	ILE	2.7
1	A	34	ARG	2.7
1	A	209	GLY	2.7
1	B	409	GLY	2.7
1	B	386	TYR	2.7
1	B	310	VAL	2.7
1	A	382	TYR	2.7
1	A	257	ILE	2.7
1	A	665	TYR	2.7
1	A	389	LYS	2.7
1	A	20	ALA	2.7
1	B	525	SER	2.7
1	A	208	VAL	2.7
1	A	338	PHE	2.6
1	B	342	PHE	2.6
1	B	366	ALA	2.6
1	B	156	ASP	2.6
1	A	574	VAL	2.6
1	B	3	VAL	2.6
1	B	313	PRO	2.6
1	B	27	ARG	2.5
1	A	33	GLU	2.5
1	A	391	THR	2.5
1	A	290	PRO	2.5
1	A	2	TYR	2.5
1	B	473	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	165	LEU	2.5
1	A	32	THR	2.5
1	A	524	PRO	2.4
1	B	685	VAL	2.4
1	B	408	ASN	2.4
1	A	5	ALA	2.4
1	A	673	GLY	2.4
1	A	255	SER	2.4
1	A	341	TYR	2.4
1	B	253	VAL	2.4
1	A	210	LYS	2.4
1	A	134	GLY	2.3
1	B	672	GLU	2.3
1	B	151	TRP	2.3
1	B	338	PHE	2.3
1	A	152	MET	2.3
1	A	563	ILE	2.3
1	A	22	PHE	2.3
1	A	476	LEU	2.2
1	A	596	TYR	2.2
1	B	349	GLY	2.2
1	A	288	SER	2.2
1	A	23	ALA	2.2
1	A	176	VAL	2.2
1	A	249	VAL	2.2
1	A	360	ILE	2.1
1	B	679	GLU	2.1
1	B	444	ALA	2.1
1	B	274	LEU	2.1
1	B	516	SER	2.1
1	B	166	GLY	2.1
1	B	277	GLN	2.1
1	A	141	LEU	2.0
1	B	527	ILE	2.0
1	A	381	GLU	2.0
1	B	314	SER	2.0
1	B	341	TYR	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(Å <sup>2</sup> )	Q<0.9
3	CA	A	728	1/1	0.93	0.14	-0.60	107,107,107,107	0
3	CA	B	728	1/1	0.79	0.15	-	98,98,98,98	0
2	MG	B	727	1/1	0.76	0.15	-	96,96,96,96	0
2	MG	A	727	1/1	0.91	0.35	-	105,105,105,105	0

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

There are no such residues in this entry.