



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:45 am GMT

PDB ID : 2RLA
Title : ALTERING THE BINUCLEAR MANGANESE CLUSTER OF ARGINASE
DIMINISHES THERMOSTABILITY AND CATALYTIC FUNCTION
Authors : Scolnick, L.R.; Kanyo, Z.F.; Christianson, D.W.
Deposited on : 1997-05-07
Resolution : 3.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

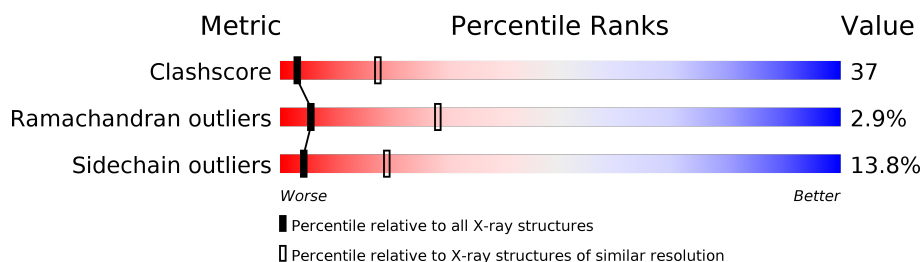
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6933 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 ARGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2302	1471	389	435	7			
1	B	303	Total	C	N	O	S	0	0	0
			2302	1471	389	435	7			
1	C	303	Total	C	N	O	S	0	0	0
			2302	1471	389	435	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

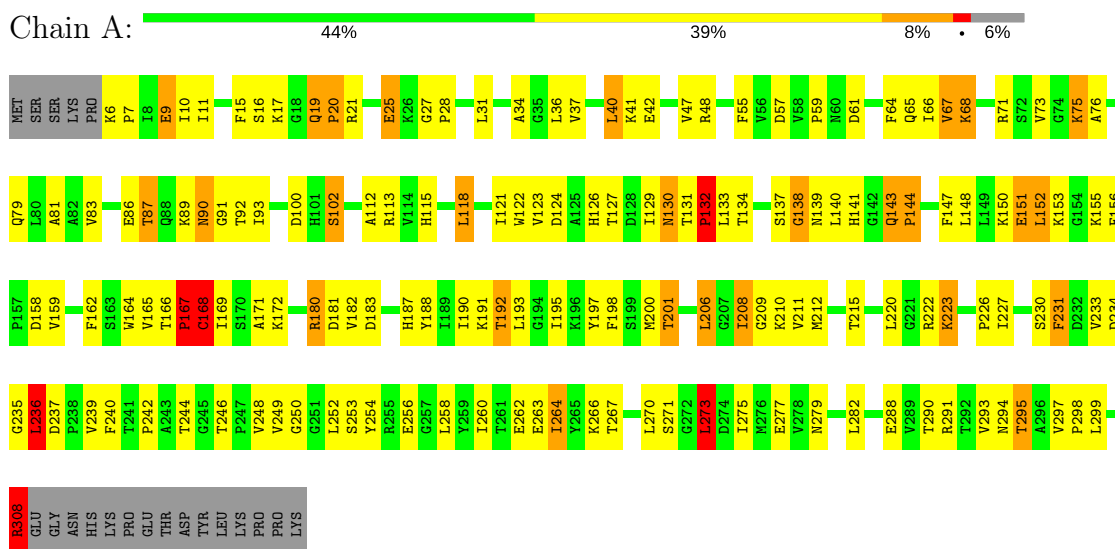
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	7	Total	O	0	0
			7	7		
3	C	6	Total	O	0	0
			6	6		

3 Residue-property plots

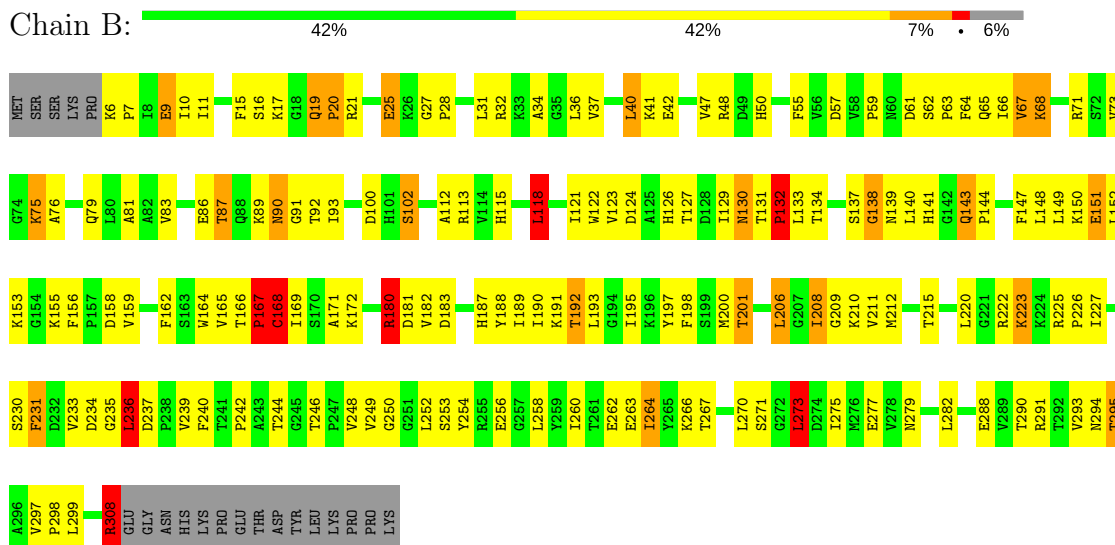
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

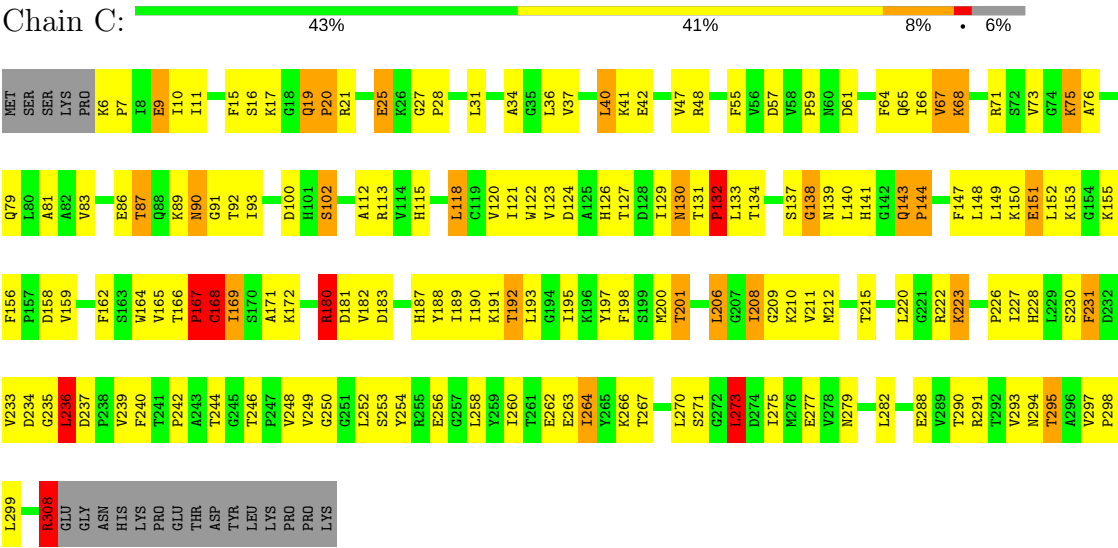
• Molecule 1: ARGINASE



• Molecule 1: ARGINASE



● Molecule 1: ARGINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.50Å 88.50Å 106.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	80.1 (20.00-3.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.78	1/2353 (0.0%)	1.03	8/3198 (0.3%)
1	B	0.78	1/2353 (0.0%)	1.03	10/3198 (0.3%)
1	C	0.79	1/2353 (0.0%)	1.02	7/3198 (0.2%)
All	All	0.78	3/7059 (0.0%)	1.03	25/9594 (0.3%)

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
1	B	0	1
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	CYS	CB-SG	5.58	1.91	1.82
1	A	168	CYS	CB-SG	5.54	1.91	1.82
1	C	168	CYS	CB-SG	5.33	1.91	1.82

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	A	308	ARG	NE-CZ-NH2	-10.99	114.81	120.30
1	C	308	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	273	LEU	CA-CB-CG	9.96	138.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LEU	CA-CB-CG	9.83	137.92	115.30
1	B	273	LEU	CA-CB-CG	9.83	137.90	115.30
1	C	299	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	299	LEU	CA-CB-CG	6.46	130.16	115.30
1	B	299	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	277	GLU	N-CA-C	6.03	127.27	111.00
1	B	234	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	277	GLU	N-CA-C	6.01	127.24	111.00
1	C	234	ASP	CB-CG-OD1	5.98	123.69	118.30
1	C	277	GLU	N-CA-C	5.94	127.03	111.00
1	A	308	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	234	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	236	LEU	N-CA-C	-5.23	96.87	111.00
1	C	236	LEU	N-CA-C	-5.18	97.02	111.00
1	B	118	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	B	236	LEU	N-CA-C	-5.17	97.03	111.00
1	A	9	GLU	N-CA-C	-5.14	97.11	111.00
1	B	308	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	9	GLU	N-CA-C	-5.13	97.15	111.00
1	C	9	GLU	N-CA-C	-5.13	97.16	111.00
1	B	32	ARG	NE-CZ-NH1	-5.11	117.75	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ARG	Sidechain
1	B	308	ARG	Sidechain
1	C	308	ARG	Sidechain

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	2302	0	2332	172	0
1	B	2302	0	2332	180	0
1	C	2302	0	2332	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	11	0	0	0	0
3	B	7	0	0	2	0
3	C	6	0	0	0	0
All	All	6933	0	6996	519	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 37.

All (519) 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:61:ASP:HB2	1:B:71:ARG:HB2	1.41	1.01
1:A:61:ASP:HB2	1:A:71:ARG:HB2	1.41	0.99
1:C:61:ASP:HB2	1:C:71:ARG:HB2	1.42	0.97
1:C:81:ALA:HB1	1:C:113:ARG:HH12	1.30	0.97
1:B:81:ALA:HB1	1:B:113:ARG:HH12	1.29	0.95
1:A:81:ALA:HB1	1:A:113:ARG:HH12	1.29	0.95
1:C:19:GLN:HB3	1:C:141:HIS:ND1	1.89	0.87
1:A:19:GLN:HB3	1:A:141:HIS:ND1	1.89	0.87
1:C:79:GLN:O	1:C:83:VAL:HG23	1.75	0.86
1:B:19:GLN:HB3	1:B:141:HIS:ND1	1.90	0.86
1:B:79:GLN:O	1:B:83:VAL:HG23	1.75	0.86
1:B:61:ASP:CB	1:B:71:ARG:HB2	2.05	0.86
1:A:79:GLN:O	1:A:83:VAL:HG23	1.74	0.85
1:C:61:ASP:CB	1:C:71:ARG:HB2	2.05	0.85
1:A:61:ASP:CB	1:A:71:ARG:HB2	2.05	0.85
1:A:147:PHE:HZ	1:A:159:VAL:HG21	1.41	0.85
1:B:147:PHE:HZ	1:B:159:VAL:HG21	1.42	0.85
1:C:147:PHE:HZ	1:C:159:VAL:HG21	1.42	0.84
1:A:201:THR:HG22	1:B:308:ARG:HD3	1.58	0.83
1:C:112:ALA:HA	1:C:115:HIS:O	1.79	0.82
1:A:112:ALA:HA	1:A:115:HIS:O	1.80	0.82
1:C:15:PHE:CE2	1:C:17:LYS:HB2	2.15	0.82
1:B:112:ALA:HA	1:B:115:HIS:O	1.79	0.81
1:A:15:PHE:CE2	1:A:17:LYS:HB2	2.15	0.81
1:B:15:PHE:CE2	1:B:17:LYS:HB2	2.16	0.81
1:B:81:ALA:HB1	1:B:113:ARG:NH1	1.98	0.79
1:B:201:THR:HG22	1:C:308:ARG:HD3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:HB1	1:C:113:ARG:NH1	1.98	0.78
1:A:81:ALA:HB1	1:A:113:ARG:NH1	1.98	0.77
1:C:262:GLU:OE2	1:C:308:ARG:HD2	1.86	0.76
1:A:308:ARG:HD3	1:C:201:THR:HG22	1.66	0.76
1:A:208:ILE:HD12	1:A:209:GLY:H	1.51	0.76
1:C:208:ILE:HD12	1:C:209:GLY:H	1.51	0.76
1:A:262:GLU:OE2	1:A:308:ARG:HD2	1.86	0.75
1:B:294:ASN:O	1:B:298:PRO:HD3	1.86	0.75
1:C:291:ARG:O	1:C:295:THR:HG22	1.87	0.75
1:B:262:GLU:OE2	1:B:308:ARG:HD2	1.86	0.75
1:B:291:ARG:O	1:B:295:THR:HG22	1.87	0.75
1:A:294:ASN:O	1:A:298:PRO:HD3	1.87	0.74
1:B:208:ILE:HD12	1:B:209:GLY:H	1.51	0.74
1:C:294:ASN:O	1:C:298:PRO:HD3	1.86	0.74
1:C:37:VAL:O	1:C:41:LYS:HG2	1.88	0.73
1:A:37:VAL:O	1:A:41:LYS:HG2	1.89	0.73
1:A:291:ARG:O	1:A:295:THR:HG22	1.88	0.73
1:B:37:VAL:O	1:B:41:LYS:HG2	1.88	0.73
1:C:129:ILE:HG12	1:C:129:ILE:O	1.90	0.71
1:C:148:LEU:HD12	1:C:148:LEU:O	1.91	0.70
1:A:148:LEU:HD12	1:A:148:LEU:O	1.92	0.70
1:C:208:ILE:HD12	1:C:209:GLY:N	2.06	0.70
1:A:129:ILE:O	1:A:129:ILE:HG12	1.90	0.70
1:B:129:ILE:HG12	1:B:129:ILE:O	1.90	0.70
1:A:208:ILE:HD12	1:A:209:GLY:N	2.07	0.70
1:A:68:LYS:O	1:A:140:LEU:HD11	1.92	0.69
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.73	0.69
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.73	0.69
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.73	0.69
1:C:68:LYS:O	1:C:140:LEU:HD11	1.93	0.69
1:B:68:LYS:O	1:B:140:LEU:HD11	1.92	0.69
1:B:208:ILE:HD12	1:B:209:GLY:N	2.07	0.68
1:C:220:LEU:HD11	1:C:227:ILE:HD11	1.76	0.68
1:B:212:MET:CE	1:B:260:ILE:HG12	2.23	0.68
1:B:48:ARG:HH12	1:B:90:ASN:ND2	1.92	0.68
1:C:147:PHE:CZ	1:C:159:VAL:HG21	2.28	0.68
1:C:152:LEU:O	1:C:155:LYS:HB2	1.94	0.68
1:A:201:THR:CG2	1:B:308:ARG:HD3	2.23	0.68
1:A:48:ARG:HH12	1:A:90:ASN:ND2	1.92	0.68
1:C:48:ARG:HH12	1:C:90:ASN:ND2	1.92	0.68
1:C:212:MET:CE	1:C:260:ILE:HG12	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:CE	1:A:260:ILE:HG12	2.24	0.67
1:B:148:LEU:O	1:B:148:LEU:HD12	1.93	0.67
1:B:143:GLN:H	1:B:144:PRO:HD3	1.59	0.67
1:A:152:LEU:O	1:A:155:LYS:HB2	1.94	0.67
1:B:198:PHE:HE2	1:B:215:THR:HG22	1.59	0.67
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.76	0.67
1:C:143:GLN:H	1:C:144:PRO:HD3	1.59	0.67
1:A:198:PHE:HE2	1:A:215:THR:HG22	1.60	0.66
1:A:220:LEU:HD11	1:A:227:ILE:HD11	1.76	0.66
1:B:152:LEU:O	1:B:155:LYS:HB2	1.95	0.66
1:C:198:PHE:HE2	1:C:215:THR:HG22	1.59	0.66
1:A:147:PHE:CZ	1:A:159:VAL:HG21	2.27	0.66
1:B:143:GLN:N	1:B:144:PRO:HD3	2.11	0.65
1:C:140:LEU:H	1:C:140:LEU:HD12	1.61	0.65
1:A:180:ARG:NH1	1:A:248:VAL:HG23	2.11	0.65
1:B:147:PHE:CZ	1:B:159:VAL:HG21	2.28	0.65
1:A:143:GLN:N	1:A:144:PRO:HD3	2.12	0.65
1:A:143:GLN:H	1:A:144:PRO:HD3	1.60	0.65
1:B:143:GLN:N	1:B:144:PRO:CD	2.60	0.65
1:B:132:PRO:HD2	1:B:156:PHE:CG	2.32	0.65
1:B:140:LEU:H	1:B:140:LEU:HD12	1.62	0.65
1:C:180:ARG:NH1	1:C:248:VAL:HG23	2.12	0.65
1:A:121:ILE:HD12	1:A:264:ILE:HD11	1.79	0.65
1:A:132:PRO:HD2	1:A:156:PHE:CG	2.32	0.65
1:A:9:GLU:OE1	1:A:48:ARG:HD2	1.97	0.65
1:C:143:GLN:N	1:C:144:PRO:HD3	2.11	0.65
1:C:121:ILE:HD12	1:C:264:ILE:HD11	1.79	0.65
1:B:180:ARG:NH1	1:B:248:VAL:HG23	2.12	0.64
1:C:9:GLU:OE1	1:C:48:ARG:HD2	1.97	0.64
1:A:212:MET:HE3	1:A:260:ILE:HG12	1.78	0.64
1:A:143:GLN:N	1:A:144:PRO:CD	2.61	0.64
1:B:295:THR:C	1:B:298:PRO:HD2	2.18	0.64
1:C:132:PRO:HD2	1:C:156:PHE:CG	2.32	0.64
1:A:140:LEU:H	1:A:140:LEU:HD12	1.62	0.64
1:B:258:LEU:O	1:B:262:GLU:HG3	1.97	0.64
1:B:180:ARG:HA	1:C:308:ARG:HB3	1.80	0.64
1:A:295:THR:C	1:A:298:PRO:HD2	2.18	0.64
1:C:198:PHE:CE2	1:C:215:THR:HG22	2.33	0.64
1:A:198:PHE:CE2	1:A:215:THR:HG22	2.33	0.64
1:A:258:LEU:O	1:A:262:GLU:HG3	1.98	0.64
1:B:121:ILE:HD12	1:B:264:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:THR:C	1:C:298:PRO:HD2	2.18	0.64
1:B:9:GLU:OE1	1:B:48:ARG:HD2	1.97	0.63
1:C:212:MET:HE3	1:C:260:ILE:HG12	1.78	0.63
1:C:258:LEU:O	1:C:262:GLU:HG3	1.98	0.63
1:C:143:GLN:N	1:C:144:PRO:CD	2.60	0.63
1:C:48:ARG:HH22	1:C:90:ASN:HD22	1.48	0.62
1:B:198:PHE:CE2	1:B:215:THR:HG22	2.33	0.62
1:B:212:MET:HE3	1:B:260:ILE:HG12	1.80	0.62
1:A:19:GLN:HB3	1:A:141:HIS:CE1	2.34	0.62
1:B:153:LYS:HG3	1:B:167:PRO:HG2	1.82	0.62
1:A:48:ARG:HH22	1:A:90:ASN:HD22	1.48	0.61
1:C:19:GLN:HB3	1:C:141:HIS:CE1	2.34	0.61
1:B:131:THR:HB	1:B:156:PHE:HB3	1.83	0.61
1:C:131:THR:HB	1:C:156:PHE:HB3	1.83	0.61
1:A:131:THR:HB	1:A:156:PHE:HB3	1.83	0.61
1:B:10:ILE:HD12	1:B:37:VAL:HG22	1.83	0.61
1:C:66:ILE:HG13	1:C:66:ILE:O	2.00	0.61
1:A:66:ILE:HG13	1:A:66:ILE:O	2.00	0.61
1:C:153:LYS:HG3	1:C:167:PRO:HG2	1.82	0.61
1:A:222:ARG:CB	1:A:223:LYS:HD3	2.31	0.61
1:A:153:LYS:HG3	1:A:167:PRO:HG2	1.82	0.61
1:B:222:ARG:CB	1:B:223:LYS:HD3	2.31	0.61
1:B:66:ILE:O	1:B:66:ILE:HG13	2.00	0.61
1:C:64:PHE:O	1:C:67:VAL:HG13	2.01	0.61
1:B:19:GLN:HB3	1:B:141:HIS:CE1	2.34	0.61
1:A:64:PHE:O	1:A:67:VAL:HG13	2.01	0.60
1:B:220:LEU:HD23	3:B:507:HOH:O	2.01	0.60
1:B:48:ARG:HH22	1:B:90:ASN:HD22	1.48	0.60
1:A:61:ASP:HB2	1:A:71:ARG:CB	2.25	0.60
1:B:41:LYS:HD3	1:B:47:VAL:HB	1.83	0.60
1:B:127:THR:HG23	1:B:182:VAL:HG22	1.83	0.60
1:B:15:PHE:HE2	1:B:73:VAL:HG22	1.67	0.60
1:B:64:PHE:O	1:B:67:VAL:HG13	2.01	0.60
1:A:10:ILE:HD12	1:A:37:VAL:HG22	1.83	0.60
1:A:41:LYS:HD3	1:A:47:VAL:HB	1.83	0.60
1:C:222:ARG:CB	1:C:223:LYS:HD3	2.31	0.60
1:C:15:PHE:HE2	1:C:73:VAL:HG22	1.66	0.60
1:A:127:THR:HG23	1:A:182:VAL:HG22	1.83	0.59
1:B:48:ARG:NH2	1:B:92:THR:HG21	2.17	0.59
1:B:212:MET:HE3	1:B:260:ILE:HG23	1.83	0.59
1:C:41:LYS:HD3	1:C:47:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH2	1:A:92:THR:HG21	2.17	0.59
1:A:131:THR:O	1:A:133:LEU:N	2.35	0.59
1:C:10:ILE:HD12	1:C:37:VAL:HG22	1.83	0.59
1:C:48:ARG:NH2	1:C:92:THR:HG21	2.17	0.59
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.66	0.59
1:C:127:THR:HG23	1:C:182:VAL:HG22	1.84	0.59
1:C:131:THR:O	1:C:133:LEU:N	2.35	0.59
1:B:212:MET:CE	1:B:260:ILE:HG23	2.33	0.59
1:C:61:ASP:HB2	1:C:71:ARG:CB	2.25	0.59
1:A:75:LYS:HZ3	1:A:79:GLN:HG3	1.68	0.58
1:B:263:GLU:O	1:B:267:THR:HG23	2.03	0.58
1:B:75:LYS:HZ3	1:B:79:GLN:HG3	1.69	0.58
1:B:61:ASP:HB2	1:B:71:ARG:CB	2.24	0.58
1:C:75:LYS:HZ3	1:C:79:GLN:HG3	1.67	0.58
1:A:263:GLU:O	1:A:267:THR:HG23	2.03	0.58
1:B:131:THR:O	1:B:133:LEU:N	2.35	0.58
1:C:263:GLU:O	1:C:267:THR:HG23	2.04	0.58
1:B:19:GLN:HG3	1:B:100:ASP:OD1	2.04	0.57
1:B:172:LYS:N	1:B:172:LYS:HD2	2.20	0.57
1:B:16:SER:H	1:B:17:LYS:HZ3	1.53	0.57
1:B:180:ARG:HD3	1:B:200:MET:HG2	1.87	0.57
1:C:212:MET:CE	1:C:260:ILE:HG23	2.34	0.57
1:C:55:PHE:CE1	1:C:76:ALA:O	2.58	0.57
1:A:212:MET:CE	1:A:260:ILE:HG23	2.34	0.57
1:C:240:PHE:O	1:C:291:ARG:HG2	2.05	0.57
1:A:180:ARG:HD3	1:A:200:MET:HG2	1.87	0.56
1:C:172:LYS:N	1:C:172:LYS:HD2	2.20	0.56
1:A:19:GLN:HG3	1:A:100:ASP:OD1	2.04	0.56
1:C:190:ILE:HA	1:C:195:ILE:HD12	1.86	0.56
1:B:190:ILE:HA	1:B:195:ILE:HD12	1.87	0.56
1:C:16:SER:H	1:C:17:LYS:HZ3	1.53	0.56
1:C:19:GLN:HG3	1:C:100:ASP:OD1	2.04	0.56
1:C:212:MET:HE3	1:C:260:ILE:HG23	1.88	0.56
1:A:240:PHE:O	1:A:291:ARG:HG2	2.06	0.56
1:B:21:ARG:HH11	1:B:282:LEU:HD11	1.71	0.56
1:B:55:PHE:CE1	1:B:76:ALA:O	2.58	0.56
1:A:21:ARG:HH11	1:A:282:LEU:HD11	1.70	0.56
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.41	0.56
1:C:187:HIS:HD2	1:C:191:LYS:HB2	1.71	0.56
1:A:172:LYS:HD2	1:A:172:LYS:N	2.20	0.56
1:A:190:ILE:HA	1:A:195:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:PHE:O	1:B:291:ARG:HG2	2.06	0.56
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.40	0.55
1:A:55:PHE:CE1	1:A:76:ALA:O	2.59	0.55
1:B:201:THR:CG2	1:C:308:ARG:HD3	2.35	0.55
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.41	0.55
1:B:187:HIS:HD2	1:B:191:LYS:HB2	1.72	0.55
1:B:254:TYR:CE1	1:B:258:LEU:HD11	2.41	0.55
1:C:21:ARG:HH11	1:C:282:LEU:HD11	1.70	0.55
1:C:180:ARG:HD3	1:C:200:MET:HG2	1.87	0.55
1:A:126:HIS:HD2	1:A:181:ASP:HB3	1.72	0.55
1:A:222:ARG:HB2	1:A:223:LYS:HD3	1.89	0.55
1:A:254:TYR:CE1	1:A:258:LEU:HD11	2.41	0.55
1:B:222:ARG:HB2	1:B:223:LYS:HD3	1.89	0.55
1:C:126:HIS:HD2	1:C:181:ASP:HB3	1.72	0.55
1:C:222:ARG:HB2	1:C:223:LYS:HD3	1.89	0.55
1:B:133:LEU:HD12	1:B:155:LYS:O	2.08	0.54
1:B:188:TYR:O	1:B:192:THR:HB	2.07	0.54
1:A:16:SER:OG	1:A:25:GLU:HG3	2.08	0.54
1:C:254:TYR:CE1	1:C:258:LEU:HD11	2.42	0.54
1:C:133:LEU:HD12	1:C:155:LYS:O	2.07	0.54
1:B:115:HIS:O	1:B:118:LEU:HD12	2.08	0.54
1:B:182:VAL:HG12	1:B:183:ASP:O	2.07	0.54
1:B:86:GLU:O	1:B:87:THR:C	2.46	0.54
1:C:16:SER:OG	1:C:25:GLU:HG3	2.07	0.54
1:A:133:LEU:HD12	1:A:155:LYS:O	2.08	0.54
1:C:115:HIS:O	1:C:118:LEU:HD12	2.08	0.54
1:A:188:TYR:O	1:A:192:THR:HB	2.07	0.54
1:B:200:MET:HA	1:B:200:MET:HE3	1.89	0.54
1:C:182:VAL:HG12	1:C:183:ASP:O	2.08	0.54
1:C:55:PHE:HE1	1:C:76:ALA:O	1.91	0.54
1:A:182:VAL:HG12	1:A:183:ASP:O	2.08	0.54
1:A:187:HIS:HD2	1:A:191:LYS:HB2	1.72	0.54
1:A:212:MET:HE3	1:A:260:ILE:HG23	1.88	0.53
1:B:55:PHE:HE1	1:B:76:ALA:O	1.91	0.53
1:C:188:TYR:O	1:C:192:THR:HB	2.08	0.53
1:B:16:SER:OG	1:B:25:GLU:HG3	2.08	0.53
1:B:291:ARG:O	1:B:295:THR:CG2	2.57	0.53
1:A:86:GLU:O	1:A:87:THR:C	2.46	0.53
1:B:126:HIS:HD2	1:B:181:ASP:HB3	1.73	0.53
1:A:222:ARG:HB2	1:A:223:LYS:HZ2	1.73	0.53
1:B:100:ASP:HB2	1:B:102:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:HIS:O	1:A:118:LEU:HD12	2.08	0.53
1:C:100:ASP:HB2	1:C:102:SER:OG	2.09	0.53
1:B:222:ARG:HB2	1:B:223:LYS:HZ2	1.74	0.53
1:C:291:ARG:O	1:C:295:THR:CG2	2.56	0.53
1:A:55:PHE:HE1	1:A:76:ALA:O	1.92	0.52
1:B:48:ARG:NH1	1:B:90:ASN:ND2	2.56	0.52
1:A:100:ASP:HB2	1:A:102:SER:OG	2.09	0.52
1:B:118:LEU:N	1:B:118:LEU:HD13	2.24	0.52
1:B:36:LEU:HD12	1:B:36:LEU:O	2.10	0.52
1:C:162:PHE:O	1:C:165:VAL:HB	2.10	0.52
1:A:162:PHE:O	1:A:165:VAL:HB	2.09	0.52
1:A:48:ARG:NH1	1:A:90:ASN:ND2	2.56	0.52
1:B:118:LEU:H	1:B:118:LEU:HD13	1.74	0.52
1:C:86:GLU:O	1:C:87:THR:C	2.46	0.52
1:C:48:ARG:NH1	1:C:90:ASN:ND2	2.56	0.52
1:A:36:LEU:O	1:A:36:LEU:HD12	2.10	0.52
1:C:118:LEU:HD13	1:C:118:LEU:N	2.25	0.52
1:A:118:LEU:HD13	1:A:118:LEU:N	2.25	0.52
1:B:295:THR:O	1:B:298:PRO:HD2	2.10	0.52
1:C:200:MET:HA	1:C:200:MET:HE3	1.91	0.52
1:C:36:LEU:HD12	1:C:36:LEU:O	2.10	0.52
1:C:48:ARG:NH2	1:C:90:ASN:HD22	2.08	0.52
1:B:66:ILE:O	1:B:138:GLY:HA2	2.10	0.51
1:B:162:PHE:O	1:B:165:VAL:HB	2.10	0.51
1:B:150:LYS:HA	1:B:167:PRO:HB3	1.92	0.51
1:C:118:LEU:H	1:C:118:LEU:HD13	1.75	0.51
1:A:118:LEU:H	1:A:118:LEU:HD13	1.76	0.51
1:A:150:LYS:HA	1:A:167:PRO:HB3	1.92	0.51
1:C:150:LYS:HA	1:C:167:PRO:HB3	1.92	0.51
1:A:181:ASP:HB2	1:A:248:VAL:HG11	1.93	0.51
1:C:181:ASP:HB2	1:C:248:VAL:HG11	1.93	0.51
1:C:66:ILE:O	1:C:138:GLY:HA2	2.11	0.50
1:A:291:ARG:O	1:A:295:THR:CG2	2.57	0.50
1:A:66:ILE:O	1:A:138:GLY:HA2	2.11	0.50
1:B:181:ASP:HB2	1:B:248:VAL:HG11	1.94	0.50
1:A:180:ARG:CD	1:A:200:MET:HG2	2.41	0.50
1:B:225:ARG:NE	3:B:507:HOH:O	2.45	0.50
1:C:180:ARG:CD	1:C:200:MET:HG2	2.42	0.50
1:C:131:THR:OG1	1:C:133:LEU:HB2	2.12	0.50
1:A:15:PHE:HA	1:A:17:LYS:HZ1	1.76	0.50
1:A:249:VAL:CG1	1:A:250:GLY:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:OG1	1:A:133:LEU:HB2	2.11	0.50
1:A:295:THR:O	1:A:298:PRO:HD2	2.11	0.50
1:B:48:ARG:NH2	1:B:90:ASN:HD22	2.08	0.50
1:C:123:VAL:HG11	1:C:231:PHE:CZ	2.46	0.50
1:B:180:ARG:CD	1:B:200:MET:HG2	2.42	0.50
1:A:48:ARG:NH2	1:A:90:ASN:HD22	2.09	0.49
1:C:197:TYR:CD1	1:C:197:TYR:N	2.80	0.49
1:A:197:TYR:N	1:A:197:TYR:CD1	2.81	0.49
1:A:200:MET:HE3	1:A:200:MET:HA	1.94	0.49
1:B:290:THR:O	1:B:294:ASN:HB2	2.13	0.49
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.95	0.49
1:A:249:VAL:HG12	1:A:250:GLY:N	2.28	0.49
1:A:308:ARG:HD3	1:C:201:THR:CG2	2.39	0.49
1:A:180:ARG:HA	1:B:308:ARG:HB3	1.95	0.49
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.95	0.49
1:C:249:VAL:CG1	1:C:250:GLY:N	2.75	0.49
1:C:275:ILE:O	1:C:275:ILE:HG22	2.12	0.49
1:C:295:THR:O	1:C:298:PRO:HD2	2.11	0.49
1:B:131:THR:C	1:B:133:LEU:H	2.16	0.49
1:B:171:ALA:C	1:B:172:LYS:HD2	2.33	0.49
1:B:190:ILE:HG13	1:B:191:LYS:N	2.27	0.49
1:B:123:VAL:HG11	1:B:231:PHE:CZ	2.47	0.49
1:C:190:ILE:HG13	1:C:191:LYS:N	2.27	0.49
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.94	0.49
1:B:147:PHE:CE1	1:B:162:PHE:CD2	3.01	0.49
1:B:275:ILE:HG22	1:B:275:ILE:O	2.12	0.48
1:A:127:THR:OG1	1:A:129:ILE:HG22	2.13	0.48
1:A:171:ALA:C	1:A:172:LYS:HD2	2.33	0.48
1:A:275:ILE:HG22	1:A:275:ILE:O	2.13	0.48
1:B:172:LYS:CD	1:B:172:LYS:N	2.76	0.48
1:A:212:MET:HE3	1:A:260:ILE:HA	1.95	0.48
1:C:171:ALA:C	1:C:172:LYS:HD2	2.34	0.48
1:C:249:VAL:HG12	1:C:250:GLY:N	2.28	0.48
1:A:190:ILE:HG13	1:A:191:LYS:N	2.27	0.48
1:A:123:VAL:HG11	1:A:231:PHE:CZ	2.48	0.48
1:C:212:MET:HE3	1:C:260:ILE:HA	1.96	0.48
1:A:172:LYS:N	1:A:172:LYS:CD	2.76	0.48
1:B:166:THR:O	1:B:168:CYS:N	2.46	0.48
1:B:249:VAL:CG1	1:B:250:GLY:N	2.76	0.48
1:C:153:LYS:HE2	1:C:167:PRO:HG2	1.95	0.48
1:C:172:LYS:N	1:C:172:LYS:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:O	1:C:168:CYS:N	2.47	0.48
1:A:152:LEU:HD13	1:A:193:LEU:CD2	2.44	0.48
1:A:16:SER:H	1:A:17:LYS:HZ3	1.61	0.48
1:B:127:THR:OG1	1:B:129:ILE:HG22	2.13	0.48
1:B:153:LYS:HE2	1:B:167:PRO:HG2	1.95	0.48
1:B:197:TYR:N	1:B:197:TYR:CD1	2.81	0.48
1:C:147:PHE:CE1	1:C:162:PHE:CD2	3.01	0.48
1:C:222:ARG:HB2	1:C:223:LYS:HZ2	1.79	0.48
1:A:36:LEU:C	1:A:36:LEU:HD12	2.34	0.48
1:B:131:THR:OG1	1:B:133:LEU:HB2	2.14	0.48
1:C:210:LYS:O	1:C:211:VAL:C	2.52	0.48
1:A:147:PHE:CE1	1:A:162:PHE:CD2	3.02	0.47
1:B:152:LEU:HD13	1:B:193:LEU:CD2	2.44	0.47
1:B:40:LEU:HB3	1:B:47:VAL:HG21	1.96	0.47
1:C:236:LEU:HA	1:C:236:LEU:HD23	1.59	0.47
1:A:166:THR:O	1:A:168:CYS:N	2.47	0.47
1:C:131:THR:C	1:C:133:LEU:H	2.17	0.47
1:C:127:THR:OG1	1:C:129:ILE:HG22	2.14	0.47
1:B:48:ARG:CZ	1:B:92:THR:HG21	2.45	0.47
1:A:131:THR:C	1:A:133:LEU:H	2.17	0.47
1:B:36:LEU:HD12	1:B:36:LEU:C	2.34	0.47
1:C:187:HIS:CD2	1:C:191:LYS:HB2	2.49	0.47
1:C:290:THR:O	1:C:294:ASN:HB2	2.13	0.47
1:A:11:ILE:HD11	1:A:87:THR:HG21	1.96	0.47
1:B:212:MET:HE3	1:B:260:ILE:HA	1.97	0.47
1:C:40:LEU:HB3	1:C:47:VAL:HG21	1.97	0.47
1:C:193:LEU:HA	1:C:193:LEU:HD12	1.57	0.47
1:C:11:ILE:HD11	1:C:87:THR:HG21	1.97	0.46
1:C:36:LEU:HD12	1:C:36:LEU:C	2.34	0.46
1:A:187:HIS:CD2	1:A:191:LYS:HB2	2.50	0.46
1:C:152:LEU:HD13	1:C:193:LEU:CD2	2.44	0.46
1:C:6:LYS:CB	1:C:7:PRO:HD3	2.45	0.46
1:A:131:THR:C	1:A:133:LEU:N	2.69	0.46
1:B:122:TRP:CD1	1:B:124:ASP:HB2	2.51	0.46
1:B:131:THR:C	1:B:133:LEU:N	2.68	0.46
1:B:64:PHE:CE1	1:B:65:GLN:HG3	2.51	0.46
1:B:11:ILE:HD11	1:B:87:THR:HG21	1.97	0.46
1:C:236:LEU:HD23	1:C:252:LEU:HB2	1.98	0.46
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.58	0.46
1:A:290:THR:O	1:A:294:ASN:HB2	2.14	0.46
1:B:193:LEU:HA	1:B:193:LEU:HD12	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TRP:CD1	1:A:124:ASP:HB2	2.50	0.46
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.58	0.46
1:A:236:LEU:HD23	1:A:252:LEU:HB2	1.98	0.46
1:C:131:THR:C	1:C:133:LEU:N	2.69	0.46
1:C:237:ASP:HB3	1:C:240:PHE:CE2	2.51	0.46
1:C:64:PHE:CE1	1:C:65:GLN:HG3	2.50	0.46
1:A:151:GLU:HG2	1:A:151:GLU:H	1.52	0.46
1:A:237:ASP:HB3	1:A:240:PHE:CE2	2.51	0.46
1:A:48:ARG:CZ	1:A:92:THR:HG21	2.45	0.46
1:B:147:PHE:CD1	1:B:162:PHE:HD2	2.34	0.46
1:B:180:ARG:HH21	1:B:235:GLY:HA2	1.81	0.46
1:A:40:LEU:HB3	1:A:47:VAL:HG21	1.97	0.46
1:B:294:ASN:O	1:B:298:PRO:CD	2.62	0.46
1:A:64:PHE:CE1	1:A:65:GLN:HG3	2.51	0.45
1:A:210:LYS:O	1:A:211:VAL:C	2.53	0.45
1:B:249:VAL:HG12	1:B:250:GLY:N	2.30	0.45
1:C:48:ARG:CZ	1:C:92:THR:HG21	2.45	0.45
1:A:153:LYS:HE2	1:A:167:PRO:HG2	1.96	0.45
1:A:75:LYS:NZ	1:A:79:GLN:HG3	2.31	0.45
1:C:21:ARG:NH1	1:C:282:LEU:HD11	2.31	0.45
1:C:89:LYS:O	1:C:91:GLY:N	2.50	0.45
1:A:253:SER:H	1:A:256:GLU:HB2	1.81	0.45
1:B:187:HIS:CD2	1:B:191:LYS:HB2	2.50	0.45
1:B:236:LEU:HD23	1:B:252:LEU:HB2	1.99	0.45
1:B:237:ASP:HB3	1:B:240:PHE:CE2	2.51	0.45
1:B:75:LYS:HE2	1:B:75:LYS:HA	1.98	0.45
1:B:89:LYS:O	1:B:91:GLY:N	2.50	0.45
1:C:147:PHE:CD1	1:C:162:PHE:HD2	2.35	0.45
1:C:206:LEU:HB2	1:C:210:LYS:HB3	1.98	0.45
1:C:180:ARG:HH21	1:C:235:GLY:HA2	1.82	0.45
1:A:6:LYS:CB	1:A:7:PRO:HD3	2.46	0.45
1:C:122:TRP:CD1	1:C:124:ASP:HB2	2.51	0.45
1:C:253:SER:H	1:C:256:GLU:HB2	1.82	0.45
1:A:147:PHE:CD1	1:A:162:PHE:HD2	2.35	0.45
1:A:237:ASP:HB3	1:A:240:PHE:CD2	2.52	0.45
1:C:294:ASN:O	1:C:298:PRO:CD	2.62	0.45
1:B:81:ALA:CB	1:B:113:ARG:HH12	2.15	0.45
1:B:21:ARG:NH1	1:B:282:LEU:HD11	2.31	0.45
1:B:237:ASP:HB3	1:B:240:PHE:CD2	2.52	0.44
1:A:21:ARG:NH1	1:A:282:LEU:HD11	2.31	0.44
1:B:132:PRO:HG3	1:B:143:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HB3	1:B:223:LYS:HD3	1.99	0.44
1:A:127:THR:CB	1:A:129:ILE:HG22	2.47	0.44
1:B:210:LYS:O	1:B:211:VAL:C	2.54	0.44
1:B:75:LYS:NZ	1:B:79:GLN:HG3	2.31	0.44
1:A:132:PRO:HG3	1:A:143:GLN:OE1	2.17	0.44
1:A:180:ARG:HH21	1:A:235:GLY:HA2	1.82	0.44
1:B:6:LYS:CB	1:B:7:PRO:HD3	2.46	0.44
1:C:75:LYS:HE2	1:C:75:LYS:HA	1.99	0.44
1:A:75:LYS:HA	1:A:75:LYS:HE2	2.00	0.44
1:B:89:LYS:C	1:B:91:GLY:H	2.21	0.44
1:C:222:ARG:HB3	1:C:223:LYS:HD3	1.99	0.44
1:A:206:LEU:HB2	1:A:210:LYS:HB3	1.98	0.44
1:C:127:THR:CB	1:C:129:ILE:HG22	2.48	0.44
1:B:127:THR:CB	1:B:129:ILE:HG22	2.48	0.44
1:B:253:SER:H	1:B:256:GLU:HB2	1.82	0.44
1:B:279:ASN:CG	1:B:282:LEU:HD23	2.38	0.44
1:C:86:GLU:O	1:C:89:LYS:N	2.51	0.44
1:A:27:GLY:N	1:A:28:PRO:HD2	2.33	0.44
1:A:89:LYS:O	1:A:91:GLY:N	2.51	0.44
1:B:206:LEU:HB2	1:B:210:LYS:HB3	1.98	0.44
1:C:237:ASP:HB3	1:C:240:PHE:CD2	2.52	0.44
1:C:89:LYS:C	1:C:91:GLY:H	2.22	0.44
1:C:279:ASN:CG	1:C:282:LEU:HD23	2.39	0.44
1:C:75:LYS:NZ	1:C:79:GLN:HG3	2.31	0.44
1:C:132:PRO:HG3	1:C:143:GLN:OE1	2.17	0.43
1:B:129:ILE:CG1	1:B:129:ILE:O	2.62	0.43
1:C:118:LEU:H	1:C:118:LEU:CD1	2.31	0.43
1:A:118:LEU:CD1	1:A:118:LEU:H	2.32	0.43
1:A:279:ASN:CG	1:A:282:LEU:HD23	2.39	0.43
1:B:118:LEU:H	1:B:118:LEU:CD1	2.31	0.43
1:B:189:ILE:O	1:B:193:LEU:N	2.48	0.43
1:A:89:LYS:C	1:A:91:GLY:H	2.22	0.43
1:B:27:GLY:N	1:B:28:PRO:HD2	2.34	0.43
1:A:254:TYR:CE1	1:A:258:LEU:CD1	3.02	0.43
1:A:93:ILE:HG23	1:A:271:SER:C	2.39	0.43
1:A:86:GLU:O	1:A:89:LYS:N	2.50	0.43
1:C:189:ILE:O	1:C:193:LEU:N	2.48	0.43
1:B:270:LEU:HD11	1:B:273:LEU:HB2	2.01	0.43
1:B:62:SER:HA	1:B:63:PRO:HD2	1.74	0.43
1:C:15:PHE:HA	1:C:17:LYS:HZ1	1.83	0.43
1:C:240:PHE:O	1:C:242:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:HB3	1:A:200:MET:HG2	2.01	0.42
1:B:86:GLU:O	1:B:89:LYS:N	2.51	0.42
1:C:27:GLY:N	1:C:28:PRO:HD2	2.33	0.42
1:B:254:TYR:CE1	1:B:258:LEU:CD1	3.02	0.42
1:B:50:HIS:ND1	1:B:50:HIS:O	2.53	0.42
1:B:93:ILE:HG23	1:B:271:SER:C	2.40	0.42
1:C:81:ALA:CB	1:C:113:ARG:HH12	2.15	0.42
1:B:153:LYS:CG	1:B:167:PRO:HG2	2.49	0.42
1:B:212:MET:HE2	1:B:260:ILE:HG12	2.00	0.42
1:A:222:ARG:HB3	1:A:223:LYS:HD3	1.99	0.42
1:A:262:GLU:O	1:A:266:LYS:HB2	2.19	0.42
1:A:297:VAL:N	1:A:298:PRO:HD2	2.35	0.42
1:B:15:PHE:HA	1:B:17:LYS:HZ1	1.83	0.42
1:C:151:GLU:HG2	1:C:151:GLU:H	1.52	0.42
1:A:153:LYS:CG	1:A:167:PRO:HG2	2.50	0.42
1:A:226:PRO:HB3	1:A:271:SER:OG	2.20	0.42
1:C:127:THR:HB	1:C:129:ILE:HG22	2.01	0.42
1:C:180:ARG:HB3	1:C:200:MET:HG2	2.02	0.42
1:C:262:GLU:O	1:C:266:LYS:HB2	2.20	0.42
1:B:262:GLU:O	1:B:266:LYS:HB2	2.19	0.42
1:B:297:VAL:N	1:B:298:PRO:HD2	2.35	0.42
1:A:137:SER:O	1:A:139:ASN:N	2.53	0.42
1:A:34:ALA:HB2	1:A:293:VAL:HG11	2.02	0.42
1:B:48:ARG:NH2	1:B:92:THR:CG2	2.83	0.42
1:A:130:ASN:ND2	1:A:134:THR:C	2.73	0.42
1:A:126:HIS:CD2	1:A:181:ASP:HB3	2.53	0.42
1:C:288:GLU:HG2	1:C:291:ARG:NH2	2.35	0.42
1:A:127:THR:HB	1:A:129:ILE:HG22	2.01	0.41
1:C:270:LEU:HD11	1:C:273:LEU:HB2	2.02	0.41
1:B:137:SER:O	1:B:139:ASN:N	2.53	0.41
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.87	0.41
1:C:147:PHE:CZ	1:C:159:VAL:CG2	3.03	0.41
1:C:254:TYR:CE1	1:C:258:LEU:CD1	3.03	0.41
1:C:10:ILE:CD1	1:C:37:VAL:HG22	2.50	0.41
1:A:48:ARG:NH2	1:A:92:THR:CG2	2.83	0.41
1:B:127:THR:HB	1:B:129:ILE:HG22	2.01	0.41
1:B:235:GLY:O	1:B:252:LEU:HD12	2.20	0.41
1:C:137:SER:O	1:C:139:ASN:N	2.53	0.41
1:C:297:VAL:N	1:C:298:PRO:HD2	2.35	0.41
1:A:240:PHE:O	1:A:242:PRO:HD2	2.20	0.41
1:B:180:ARG:HB3	1:B:200:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:HE1	1:A:260:ILE:HG23	2.02	0.41
1:C:126:HIS:CD2	1:C:181:ASP:HB3	2.53	0.41
1:A:288:GLU:HG2	1:A:291:ARG:NH2	2.36	0.41
1:B:240:PHE:O	1:B:242:PRO:HD2	2.20	0.41
1:B:226:PRO:HB3	1:B:271:SER:OG	2.20	0.41
1:C:226:PRO:HB3	1:C:271:SER:OG	2.20	0.41
1:A:164:TRP:CH2	1:A:165:VAL:HG22	2.56	0.41
1:A:270:LEU:HD11	1:A:273:LEU:HB2	2.02	0.41
1:B:61:ASP:HB2	1:B:71:ARG:HD2	2.03	0.41
1:C:93:ILE:HG23	1:C:271:SER:C	2.41	0.41
1:C:34:ALA:HB2	1:C:293:VAL:HG11	2.02	0.41
1:A:129:ILE:O	1:A:129:ILE:CG1	2.61	0.41
1:B:149:LEU:HD23	1:B:149:LEU:HA	1.92	0.41
1:B:288:GLU:HG2	1:B:291:ARG:NH2	2.36	0.41
1:C:120:VAL:HA	1:C:228:HIS:O	2.21	0.41
1:A:235:GLY:O	1:A:252:LEU:HD12	2.21	0.41
1:A:87:THR:HA	1:A:90:ASN:OD1	2.21	0.41
1:B:151:GLU:H	1:B:151:GLU:HG2	1.51	0.41
1:C:130:ASN:ND2	1:C:134:THR:C	2.75	0.41
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.86	0.41
1:A:61:ASP:HB2	1:A:71:ARG:HD2	2.03	0.41
1:B:100:ASP:HB3	1:B:141:HIS:HB2	2.03	0.41
1:A:100:ASP:HB3	1:A:141:HIS:HB2	2.03	0.41
1:B:130:ASN:ND2	1:B:134:THR:C	2.75	0.41
1:B:126:HIS:CD2	1:B:181:ASP:HB3	2.54	0.41
1:C:48:ARG:NH2	1:C:92:THR:CG2	2.83	0.41
1:B:164:TRP:CH2	1:B:165:VAL:HG22	2.56	0.40
1:C:153:LYS:CG	1:C:167:PRO:HG2	2.50	0.40
1:A:16:SER:H	1:A:17:LYS:NZ	2.19	0.40
1:B:147:PHE:CZ	1:B:159:VAL:CG2	3.02	0.40
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.86	0.40
1:C:87:THR:HA	1:C:90:ASN:OD1	2.21	0.40
1:A:227:ILE:HG21	1:A:264:ILE:HD12	2.03	0.40
1:B:87:THR:HA	1:B:90:ASN:OD1	2.21	0.40
1:C:129:ILE:O	1:C:129:ILE:CG1	2.62	0.40
1:C:100:ASP:HB3	1:C:141:HIS:HB2	2.03	0.40
1:A:227:ILE:HG21	1:A:264:ILE:CD1	2.52	0.40
1:B:16:SER:O	1:B:19:GLN:O	2.40	0.40
1:C:164:TRP:CH2	1:C:165:VAL:HG22	2.56	0.40
1:B:34:ALA:HB2	1:B:293:VAL:HG11	2.02	0.40
1:C:149:LEU:HA	1:C:169:ILE:O	2.21	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	301/323 (93%)	255 (85%)	38 (13%)	8 (3%)	6	30
1	B	301/323 (93%)	255 (85%)	37 (12%)	9 (3%)	5	27
1	C	301/323 (93%)	255 (85%)	37 (12%)	9 (3%)	5	27
All	All	903/969 (93%)	765 (85%)	112 (12%)	26 (3%)	5	28

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	PRO
1	B	59	PRO
1	C	59	PRO
1	A	167	PRO
1	A	169	ILE
1	B	167	PRO
1	B	169	ILE
1	C	167	PRO
1	C	169	ILE
1	A	138	GLY
1	B	138	GLY
1	C	138	GLY
1	A	90	ASN
1	B	90	ASN
1	C	90	ASN
1	A	132	PRO
1	B	132	PRO
1	C	132	PRO
1	B	180	ARG
1	C	180	ARG
1	A	143	GLN

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Mol	Chain	Res	Type
1	B	143	GLN
1	C	143	GLN
1	B	208	ILE
1	A	208	ILE
1	C	208	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	254/274 (93%)	218 (86%)	36 (14%)	4	18
1	B	254/274 (93%)	220 (87%)	34 (13%)	4	20
1	C	254/274 (93%)	219 (86%)	35 (14%)	4	19
All	All	762/822 (93%)	657 (86%)	105 (14%)	4	19

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	20	PRO
1	A	25	GLU
1	A	31	LEU
1	A	40	LEU
1	A	42	GLU
1	A	57	ASP
1	A	67	VAL
1	A	68	LYS
1	A	75	LYS
1	A	87	THR
1	A	102	SER
1	A	118	LEU
1	A	130	ASN
1	A	132	PRO
1	A	144	PRO
1	A	151	GLU

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	158	ASP
1	A	167	PRO
1	A	168	CYS
1	A	180	ARG
1	A	192	THR
1	A	201	THR
1	A	206	LEU
1	A	223	LYS
1	A	230	SER
1	A	231	PHE
1	A	233	VAL
1	A	236	LEU
1	A	239	VAL
1	A	244	THR
1	A	246	THR
1	A	264	ILE
1	A	273	LEU
1	A	295	THR
1	B	19	GLN
1	B	20	PRO
1	B	25	GLU
1	B	31	LEU
1	B	40	LEU
1	B	42	GLU
1	B	57	ASP
1	B	67	VAL
1	B	68	LYS
1	B	75	LYS
1	B	87	THR
1	B	102	SER
1	B	118	LEU
1	B	130	ASN
1	B	132	PRO
1	B	151	GLU
1	B	158	ASP
1	B	167	PRO
1	B	168	CYS
1	B	180	ARG
1	B	192	THR
1	B	201	THR
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	223	LYS
1	B	230	SER
1	B	231	PHE
1	B	233	VAL
1	B	236	LEU
1	B	239	VAL
1	B	244	THR
1	B	246	THR
1	B	264	ILE
1	B	273	LEU
1	B	295	THR
1	C	19	GLN
1	C	20	PRO
1	C	25	GLU
1	C	31	LEU
1	C	40	LEU
1	C	42	GLU
1	C	57	ASP
1	C	67	VAL
1	C	68	LYS
1	C	75	LYS
1	C	87	THR
1	C	102	SER
1	C	118	LEU
1	C	130	ASN
1	C	132	PRO
1	C	144	PRO
1	C	151	GLU
1	C	158	ASP
1	C	167	PRO
1	C	168	CYS
1	C	180	ARG
1	C	192	THR
1	C	201	THR
1	C	206	LEU
1	C	223	LYS
1	C	230	SER
1	C	231	PHE
1	C	233	VAL
1	C	236	LEU
1	C	239	VAL
1	C	244	THR

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Mol	Chain	Res	Type
1	C	246	THR
1	C	264	ILE
1	C	273	LEU
1	C	295	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	88	GLN
1	A	90	ASN
1	A	111	HIS
1	A	126	HIS
1	A	130	ASN
1	A	187	HIS
1	B	79	GLN
1	B	88	GLN
1	B	90	ASN
1	B	111	HIS
1	B	130	ASN
1	B	187	HIS
1	C	79	GLN
1	C	88	GLN
1	C	90	ASN
1	C	111	HIS
1	C	126	HIS
1	C	130	ASN
1	C	187	HIS

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 3 ligands modelled in this entry, 3 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.