



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:44 PM GMT

PDB ID : 2A4M
Title : Structure of Trprs II bound to ATP
Authors : Buddha, M.R.; Crane, B.R.
Deposited on : 2005-06-29
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

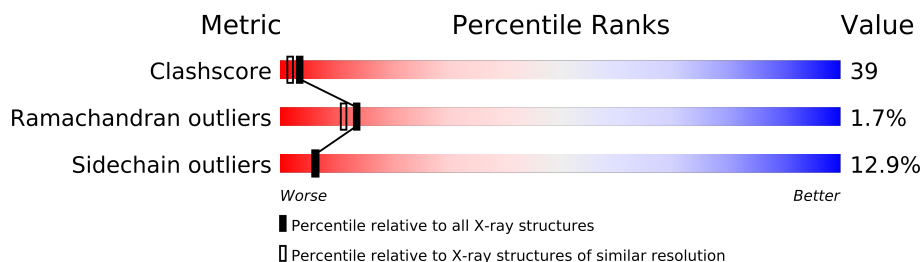
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	331	
1	B	331	
1	C	331	

2 Entry composition i

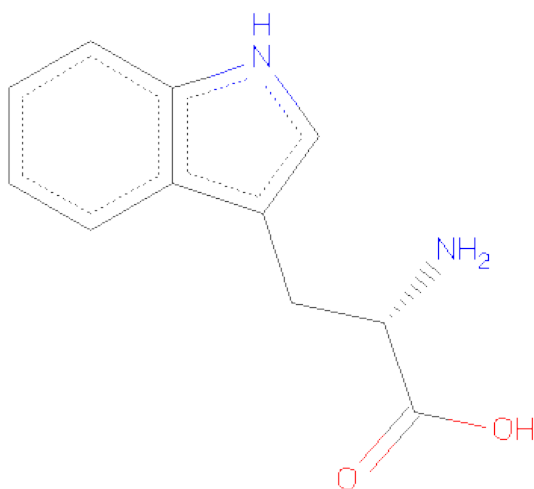
There are 3 unique types of molecules in this entry. The entry contains 8788 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tryptophanyl-tRNA synthetase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	2	0	0
			2544	1599	468	471	6			
1	B	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2527	1591	462	468	6			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total 382	O 382	0	0
3	B	395	Total 395	O 395	0	0
3	C	414	Total 414	O 414	0	0

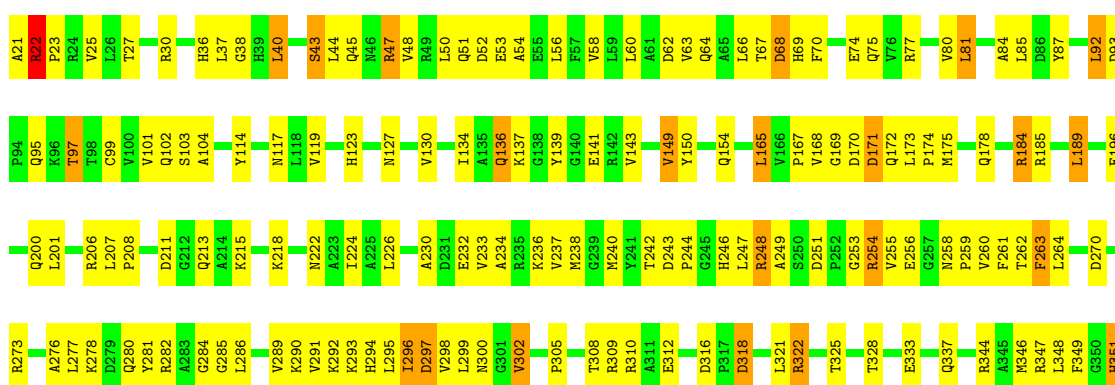
3 Residue-property plots

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.

Note EDS was not executed.

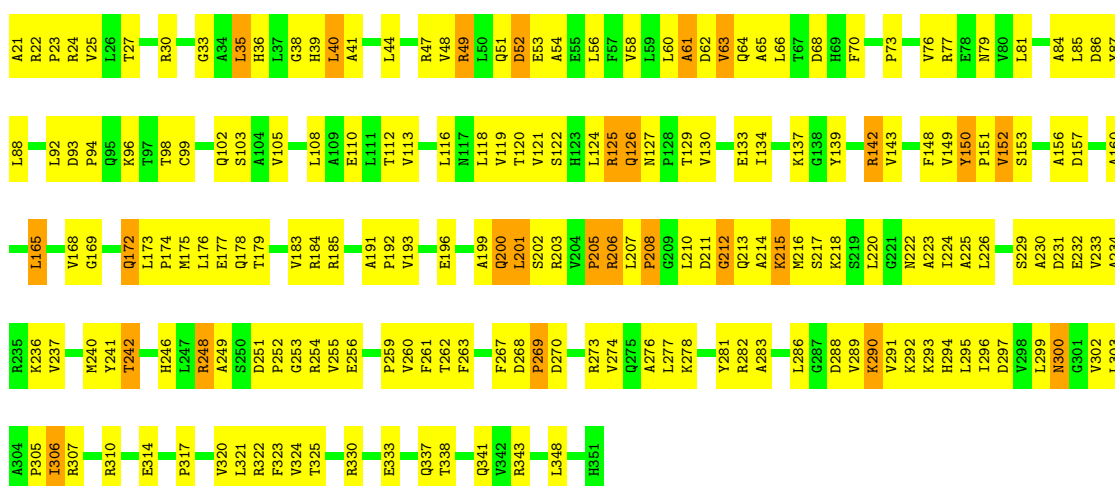
- Molecule 1: Tryptophanyl-tRNA synthetase II

Chain A:



- Molecule 1: Tryptophanyl-tRNA synthetase II

Chain B:



- Molecule 1: Tryptophanyl-tRNA synthetase II

Chain C:



P271	L173	K96	A21
A272	P174	T97	R22
R273	M175	T98	P23
A276	L176	C99	R24
L277	E177	V100	V25
K278	Q178	V101	L26
D279	T179	Q102	T27
Q280	R180	S103	
		A104	R30
	R185	V105	P31
		F106	T32
L286	L189	E107	T33
G287	V193	L108	L35
V289		A109	H36
K290	E196	E110	L37
V291	P197	L111	
K292		T112	L40
R293	Q200	V113	A41
H294	L201	L116	G42
L295	S202	N117	S43
V298	R203	T120	L44
L299	V204	H123	Q45
N300	P205		N46
			R47
L303	L210	N127	Q51
A304	M216	P128	E55
R307	A223	T129	L56
T308	I224	V130	F57
R309	S229	K131	V58
R310	A230	A132	L59
A311	R235	E133	L60
E314	D231	Q136	V63
R315	E232	K137	Q64
	V233		A65
L321	A234	P144	
	R235	A145	D68
T325	M238	G146	H69
E326			F70
G327	D243	V149	D71
T328	P244	Y150	
A329	R248	P151	E74
R330	L247	V152	Q75
G331	R248	S153	V76
R332		Q154	R77
		A155	E78
		A156	N79
Q337	R254	D157	V80
T338	V255	I158	L81
L339	E256		
G340	N258	L165	A82
Q341	P259	V166	V83
V342	V260	P167	A84
R343		V168	L85
R347	F267	G169	L92
	D268	D170	D93
H351	P269	D171	P94
	D270	O172	Q95

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.58Å 58.57Å 85.15Å 90.00° 96.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	0.3 (30.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8788	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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	0.36	0/2591	0.64	0/3519
1	B	0.32	0/2558	0.61	0/3478
1	C	0.43	0/2574	0.71	2/3499 (0.1%)
All	All	0.37	0/7723	0.65	2/10496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLN	N-CA-C	-5.79	95.36	111.00
1	C	44	LEU	CB-CA-C	5.71	121.05	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2544	0	2568	183	0
1	B	2511	0	2507	236	0
1	C	2527	0	2539	190	0
2	C	15	0	9	6	0
3	A	382	0	0	12	0
3	B	395	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	414	0	0	11	0
All	All	8788	0	7623	599	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (599) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:VAL:HG21	1:B:341:GLN:HB3	1.20	1.14
1:C:120:THR:HG23	1:C:123:HIS:H	1.13	1.08
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.21	1.06
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.16	1.05
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.11	1.05
1:B:207:LEU:HD23	1:B:216:MET:HE1	1.36	1.04
1:C:216:MET:HE3	1:C:224:ILE:H	1.17	1.03
1:B:226:LEU:HB3	1:B:306:ILE:HD11	1.39	1.03
1:C:204:VAL:HG12	1:C:205:PRO:HD2	1.41	1.02
1:C:77:ARG:O	1:C:80:VAL:HG12	1.64	0.97
1:A:51:GLN:HE22	1:A:93:ASP:H	1.06	0.97
1:A:51:GLN:HE21	1:A:97:THR:HG22	1.27	0.96
1:C:180:ARG:HD3	1:C:197:PRO:O	1.66	0.95
1:C:26:LEU:HD23	1:C:158:ILE:HD13	1.48	0.93
1:A:255:VAL:HG21	1:A:278:LYS:HG3	1.51	0.93
1:C:166:VAL:HG21	1:C:176:LEU:HD23	1.49	0.92
1:A:322:ARG:HH21	1:A:322:ARG:HG2	1.35	0.91
1:C:51:GLN:HE22	1:C:93:ASP:H	1.19	0.91
1:A:240:MET:HE3	1:A:260:VAL:HG12	1.54	0.90
1:B:226:LEU:HD12	1:B:226:LEU:H	1.38	0.89
1:C:337:GLN:HA	1:C:337:GLN:NE2	1.87	0.88
1:C:254:ARG:HD3	1:C:256:GLU:HG2	1.56	0.88
1:C:180:ARG:CG	1:C:180:ARG:HH11	1.86	0.86
1:B:52:ASP:HB3	1:B:96:LYS:NZ	1.91	0.85
1:A:51:GLN:HE22	1:A:93:ASP:N	1.75	0.85
1:C:108:LEU:O	1:C:112:THR:HG23	1.76	0.84
1:A:68:ASP:HB3	1:A:69:HIS:HD2	1.42	0.84
1:B:108:LEU:O	1:B:112:THR:HG23	1.77	0.84
1:B:230:ALA:HB1	1:B:300:ASN:HD21	1.40	0.84
1:A:295:LEU:O	1:A:298:VAL:HG12	1.75	0.84
1:C:255:VAL:HG21	1:C:278:LYS:HG2	1.59	0.84
1:B:73:PRO:O	1:B:76:VAL:HG12	1.76	0.84
1:A:189:LEU:HD21	1:C:71:ASP:HA	1.59	0.84
1:A:254:ARG:HD3	1:A:256:GLU:HG2	1.60	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:VAL:CG2	1:B:172:GLN:HB2	2.08	0.82
1:A:68:ASP:OD1	1:A:137:LYS:HE2	1.80	0.82
1:B:218:LYS:HE2	1:B:218:LYS:HA	1.62	0.81
1:B:127:ASN:HB3	1:B:130:VAL:HG12	1.62	0.81
1:B:36:HIS:HD2	1:B:38:GLY:H	1.28	0.80
1:C:35:LEU:HD23	1:C:44:LEU:HD11	1.63	0.79
1:A:43:SER:O	1:A:47:ARG:HD2	1.82	0.79
1:B:116:LEU:HD21	1:B:149:VAL:HG11	1.65	0.79
1:A:36:HIS:HD2	1:A:38:GLY:H	1.27	0.79
1:A:247:LEU:HB2	1:A:248:ARG:HH21	1.47	0.78
1:C:136:GLN:NE2	1:C:137:LYS:HD2	1.99	0.78
1:B:30:ARG:HD2	1:B:65:ALA:HA	1.65	0.78
1:B:30:ARG:HH22	1:B:68:ASP:HB3	1.48	0.77
1:B:33:GLY:HA2	1:B:79:ASN:ND2	1.99	0.77
1:B:333:GLU:O	1:B:337:GLN:HG2	1.84	0.77
1:C:120:THR:CG2	1:C:123:HIS:H	1.93	0.77
1:A:184:ARG:HE	1:A:196:GLU:CD	1.88	0.77
1:C:234:ALA:O	1:C:238:MET:HG2	1.85	0.77
1:C:168:VAL:HG22	1:C:172:GLN:HB2	1.67	0.76
1:C:216:MET:HE2	1:C:223:ALA:HB1	1.67	0.76
1:B:259:PRO:HA	1:B:262:THR:CG2	2.15	0.76
1:C:92:LEU:HG	1:C:97:THR:HG21	1.67	0.76
1:A:50:LEU:HD11	1:A:56:LEU:HD13	1.68	0.75
1:A:277:LEU:HD12	1:A:286:LEU:HD11	1.68	0.75
1:A:22:ARG:CB	1:A:23:PRO:HD3	2.17	0.75
1:B:193:VAL:HG21	1:B:341:GLN:CB	2.09	0.75
1:A:22:ARG:HB2	1:A:23:PRO:HD3	1.68	0.74
1:A:47:ARG:HA	1:A:50:LEU:HG	1.68	0.74
1:C:180:ARG:NH1	1:C:180:ARG:HG3	1.92	0.74
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.53	0.74
1:C:127:ASN:HB3	1:C:130:VAL:HG22	1.70	0.74
1:A:280:GLN:HB2	1:A:286:LEU:HD12	1.70	0.74
1:B:226:LEU:HB3	1:B:306:ILE:CD1	2.17	0.74
1:B:133:GLU:O	1:B:137:LYS:HG3	1.86	0.74
1:A:51:GLN:NE2	1:A:93:ASP:H	1.84	0.73
1:B:176:LEU:O	1:B:176:LEU:HD13	1.87	0.73
1:C:56:LEU:HD11	1:C:58:VAL:HG13	1.68	0.73
1:C:56:LEU:HD12	1:C:97:THR:HB	1.69	0.73
1:B:52:ASP:HB3	1:B:96:LYS:HZ1	1.54	0.73
1:B:149:VAL:HG13	1:B:152:VAL:HG13	1.70	0.73
1:B:121:VAL:O	1:B:125:ARG:HB2	1.89	0.73
1:A:168:VAL:HG23	1:A:172:GLN:HB2	1.71	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:GLY:H	1:B:172:GLN:HG3	1.55	0.72
1:B:134:ILE:HG23	1:B:139:TYR:HB2	1.71	0.72
1:C:171:ASP:HB2	1:C:172:GLN:NE2	2.05	0.71
1:C:260:VAL:HG13	1:C:295:LEU:HD12	1.71	0.71
1:A:40:LEU:HD23	1:A:226:LEU:HD21	1.73	0.71
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.72	0.71
1:A:51:GLN:HE21	1:A:97:THR:CG2	2.01	0.71
1:C:276:ALA:O	1:C:280:GLN:HG3	1.91	0.70
1:B:168:VAL:HG23	1:B:172:GLN:CB	2.12	0.70
1:C:22:ARG:HB2	1:C:23:PRO:HD3	1.73	0.70
1:B:274:VAL:HG12	1:B:278:LYS:HE3	1.72	0.70
1:A:22:ARG:HH21	1:A:53:GLU:HG3	1.57	0.70
1:C:30:ARG:HG2	3:C:1939:HOH:O	1.89	0.70
1:C:120:THR:HG23	1:C:123:HIS:N	1.98	0.70
1:C:216:MET:HE3	1:C:224:ILE:N	2.02	0.70
1:C:171:ASP:HB2	1:C:172:GLN:HE22	1.56	0.70
1:C:56:LEU:CD1	1:C:58:VAL:HG13	2.23	0.69
1:C:22:ARG:HB2	1:C:23:PRO:CD	2.23	0.69
1:C:233:VAL:HG21	1:C:307:ARG:HH21	1.58	0.69
1:A:36:HIS:HD2	1:A:38:GLY:N	1.91	0.68
1:A:101:VAL:HG13	1:A:104:ALA:HB3	1.74	0.68
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.76	0.68
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.74	0.68
1:A:305:PRO:HB2	1:A:309:ARG:NH2	2.09	0.68
1:A:237:VAL:HG13	1:A:240:MET:HE2	1.76	0.68
1:A:40:LEU:O	1:A:45:GLN:HG2	1.93	0.68
1:A:127:ASN:HB3	1:A:130:VAL:CG1	2.23	0.68
1:B:21:ALA:HB3	1:B:53:GLU:O	1.93	0.68
1:A:232:GLU:O	1:A:236:LYS:HG2	1.94	0.67
1:C:166:VAL:HG23	1:C:166:VAL:O	1.95	0.67
1:B:259:PRO:HA	1:B:262:THR:HG22	1.74	0.67
1:B:160:ALA:HA	1:B:338:THR:HG21	1.76	0.67
1:B:229:SER:OG	1:B:232:GLU:HB2	1.94	0.67
1:C:201:LEU:HD23	1:C:202:SER:H	1.60	0.67
1:A:25:VAL:HG22	1:A:165:LEU:HB3	1.77	0.67
1:A:240:MET:CE	1:A:260:VAL:HG12	2.25	0.67
1:B:130:VAL:O	1:B:134:ILE:HG13	1.95	0.66
1:B:232:GLU:O	1:B:236:LYS:HB2	1.96	0.66
1:C:204:VAL:HG12	1:C:205:PRO:CD	2.23	0.66
1:B:35:LEU:HD12	1:B:226:LEU:HD13	1.77	0.66
1:C:158:ILE:HD11	2:C:500:TRP:HH2	1.61	0.66
1:B:321:LEU:O	1:B:325:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:VAL:HG12	1:A:328:THR:OG1	1.96	0.66
1:B:208:PRO:HG3	1:B:262:THR:HG23	1.78	0.66
1:C:36:HIS:HB2	1:C:216:MET:CE	2.26	0.66
1:C:216:MET:CE	1:C:224:ILE:H	2.02	0.65
1:C:79:ASN:O	1:C:83:VAL:HG22	1.95	0.65
1:A:68:ASP:HB3	1:A:69:HIS:CD2	2.30	0.65
1:B:288:ASP:HA	1:B:291:VAL:HG12	1.79	0.65
1:A:184:ARG:HH21	1:A:184:ARG:HG2	1.61	0.65
1:C:295:LEU:O	1:C:298:VAL:HG13	1.97	0.65
1:B:149:VAL:HG12	1:B:149:VAL:O	1.95	0.65
1:A:273:ARG:NH2	1:A:294:HIS:NE2	2.45	0.65
1:B:35:LEU:HD11	1:B:86:ASP:HB3	1.79	0.65
1:C:254:ARG:CD	1:C:256:GLU:HG2	2.27	0.65
1:C:175:MET:SD	1:C:175:MET:C	2.75	0.65
1:B:119:VAL:HG21	1:B:178:GLN:OE1	1.96	0.65
1:C:36:HIS:HB2	1:C:216:MET:HE1	1.79	0.65
1:A:349:PHE:CD2	1:C:80:VAL:HG11	2.32	0.64
1:B:317:PRO:O	1:B:320:VAL:HG12	1.97	0.64
1:A:211:ASP:OD1	1:A:222:ASN:HB3	1.96	0.64
1:B:168:VAL:HG11	1:B:199:ALA:HB1	1.79	0.64
1:B:36:HIS:HD2	1:B:38:GLY:N	1.96	0.64
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.28	0.64
1:A:22:ARG:HH21	1:A:53:GLU:CG	2.10	0.64
1:A:22:ARG:H	1:A:54:ALA:HA	1.61	0.64
1:B:52:ASP:HB3	1:B:96:LYS:HZ3	1.62	0.64
1:B:230:ALA:CB	1:B:300:ASN:HD21	2.11	0.64
1:B:110:GLU:O	1:B:113:VAL:HG12	1.98	0.64
1:B:229:SER:O	1:B:233:VAL:HG23	1.97	0.64
1:C:290:LYS:HA	1:C:290:LYS:HE2	1.80	0.63
1:A:173:LEU:N	1:A:174:PRO:HD2	2.13	0.63
1:C:120:THR:HG21	3:C:1438:HOH:O	1.98	0.63
1:B:296:ILE:O	1:B:300:ASN:HB2	1.99	0.63
1:B:207:LEU:HD12	1:B:208:PRO:HD2	1.81	0.62
1:A:322:ARG:NH2	1:A:322:ARG:HG2	2.11	0.62
1:C:110:GLU:O	1:C:113:VAL:HG12	1.99	0.62
1:C:176:LEU:HD13	1:C:176:LEU:C	2.20	0.62
1:A:30:ARG:HH22	1:A:68:ASP:HB2	1.65	0.62
1:B:108:LEU:HD13	1:B:157:ASP:OD1	2.00	0.62
1:B:30:ARG:NH2	1:B:68:ASP:HB3	2.14	0.62
1:B:105:VAL:HG13	1:B:108:LEU:HG	1.82	0.62
1:B:149:VAL:HG13	1:B:152:VAL:CG1	2.29	0.62
1:B:208:PRO:HG3	1:B:262:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:ARG:N	1:A:248:ARG:HD3	2.14	0.61
1:B:201:LEU:HD22	1:B:202:SER:H	1.64	0.61
1:B:173:LEU:O	1:B:177:GLU:HB2	1.99	0.61
1:C:180:ARG:HD2	1:C:196:GLU:CG	2.30	0.61
1:C:60:LEU:HD22	1:C:83:VAL:CG2	2.30	0.61
1:A:298:VAL:O	1:A:302:VAL:HG12	2.00	0.61
1:B:127:ASN:HB3	1:B:130:VAL:CG1	2.30	0.61
1:B:215:LYS:NZ	1:B:215:LYS:HB2	2.16	0.61
1:B:226:LEU:HD12	1:B:226:LEU:N	2.14	0.61
1:C:32:THR:O	1:C:32:THR:HG22	2.00	0.61
1:C:294:HIS:O	1:C:298:VAL:HG12	2.00	0.61
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.64	0.60
1:B:23:PRO:O	1:B:54:ALA:HB1	2.01	0.60
1:C:37:LEU:HD13	3:C:2057:HOH:O	2.00	0.60
1:B:173:LEU:N	1:B:174:PRO:HD2	2.16	0.60
1:B:41:ALA:CB	1:B:207:LEU:HD22	2.31	0.60
1:A:22:ARG:CG	1:A:23:PRO:HD3	2.31	0.60
1:C:41:ALA:HB2	1:C:267:PHE:CZ	2.35	0.60
1:C:56:LEU:HD11	1:C:58:VAL:CG1	2.30	0.60
1:C:105:VAL:HG13	1:C:108:LEU:HG	1.82	0.60
1:C:268:ASP:OD1	1:C:294:HIS:HE1	1.84	0.60
1:A:77:ARG:NH2	1:C:351:HIS:O	2.33	0.60
1:B:291:VAL:HG13	1:B:292:LYS:N	2.16	0.60
1:A:62:ASP:O	1:A:66:LEU:HD23	2.02	0.60
1:B:303:LEU:O	1:B:306:ILE:HG23	2.02	0.60
1:B:253:GLY:O	1:B:282:ARG:HA	2.00	0.60
1:B:295:LEU:O	1:B:299:LEU:HG	2.02	0.59
1:B:139:TYR:O	1:B:142:ARG:HG3	2.02	0.59
1:A:44:LEU:O	1:A:48:VAL:HG23	2.02	0.59
1:C:120:THR:HG22	1:C:123:HIS:HB2	1.83	0.59
1:A:44:LEU:HA	1:A:47:ARG:CD	2.31	0.59
1:C:107:GLU:OE2	1:C:332:ARG:NH1	2.35	0.59
1:B:201:LEU:CD2	1:B:202:SER:H	2.16	0.59
1:C:230:ALA:HB1	1:C:300:ASN:HD21	1.68	0.59
1:B:288:ASP:O	1:B:291:VAL:HG12	2.01	0.59
1:A:316:ASP:OD1	1:A:318:ASP:OD2	2.21	0.59
1:A:64:GLN:NE2	1:A:154:GLN:HG3	2.18	0.58
2:C:500:TRP:CG	2:C:500:TRP:OXT	2.55	0.58
1:B:142:ARG:HD3	1:B:142:ARG:O	2.03	0.58
1:B:36:HIS:CD2	1:B:38:GLY:H	2.17	0.58
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.17	0.58
1:C:175:MET:HB2	3:C:1000:HOH:O	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:116:LEU:CD2	1:C:152:VAL:HG21	2.33	0.58
1:B:125:ARG:HG3	1:B:125:ARG:HH21	1.68	0.58
1:A:264:LEU:HG	1:A:295:LEU:HD12	1.86	0.57
1:C:201:LEU:HD23	1:C:202:SER:N	2.19	0.57
1:C:98:THR:HG21	1:C:330:ARG:HG2	1.86	0.57
1:B:112:THR:HG22	1:B:156:ALA:CB	2.34	0.57
1:C:255:VAL:HG21	1:C:278:LYS:CG	2.34	0.57
1:B:274:VAL:O	1:B:278:LYS:HG3	2.04	0.57
1:C:116:LEU:HD23	1:C:152:VAL:HG21	1.85	0.57
1:B:112:THR:O	1:B:116:LEU:HG	2.03	0.57
1:B:36:HIS:H	1:B:39:HIS:HD2	1.52	0.57
1:C:258:ASN:HD22	1:C:258:ASN:C	2.07	0.57
1:B:27:THR:O	1:B:58:VAL:HA	2.04	0.57
1:B:172:GLN:C	1:B:174:PRO:HD2	2.25	0.56
1:B:193:VAL:O	1:B:193:VAL:HG22	2.04	0.56
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.18	0.56
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.33	0.56
1:A:22:ARG:HB2	1:A:23:PRO:CD	2.35	0.56
1:A:63:VAL:H	1:A:102:GLN:HE21	1.53	0.56
1:B:179:THR:O	1:B:183:VAL:HG23	2.04	0.56
1:B:220:LEU:C	1:B:222:ASN:N	2.59	0.56
1:B:60:LEU:O	1:B:62:ASP:N	2.38	0.56
1:B:220:LEU:C	1:B:222:ASN:H	2.07	0.56
1:C:154:GLN:CD	2:C:500:TRP:OXT	2.43	0.56
1:C:295:LEU:HA	1:C:298:VAL:CG1	2.36	0.56
1:A:64:GLN:H	1:A:102:GLN:HE22	1.54	0.56
1:C:315:ARG:HB2	3:C:1506:HOH:O	2.06	0.56
1:A:248:ARG:H	1:A:248:ARG:HD3	1.71	0.56
3:A:1267:HOH:O	1:C:103:SER:HB3	2.06	0.56
1:B:63:VAL:HG13	1:B:102:GLN:CD	2.25	0.56
1:A:321:LEU:O	1:A:325:THR:HG23	2.06	0.56
1:A:40:LEU:CD2	1:A:226:LEU:HD21	2.36	0.56
1:B:35:LEU:HD12	1:B:226:LEU:CD1	2.36	0.56
1:B:36:HIS:HA	1:B:225:ALA:HA	1.86	0.56
1:B:168:VAL:HG22	1:B:169:GLY:N	2.21	0.55
1:B:241:TYR:O	1:B:259:PRO:HD2	2.06	0.55
1:B:254:ARG:HD3	1:B:256:GLU:HB2	1.88	0.55
1:A:259:PRO:HA	1:A:262:THR:CG2	2.37	0.55
1:B:40:LEU:HD13	1:B:267:PHE:HE2	1.71	0.55
1:B:149:VAL:CG1	1:B:149:VAL:O	2.54	0.55
1:A:292:LYS:O	1:A:296:ILE:HG23	2.07	0.55
1:B:98:THR:OG1	1:B:330:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:203:ARG:C	1:C:204:VAL:HG23	2.27	0.55
1:B:269:PRO:HD2	1:B:273:ARG:NH1	2.22	0.55
1:B:215:LYS:HB2	1:B:215:LYS:HZ3	1.72	0.54
1:A:93:ASP:O	1:A:97:THR:HG23	2.07	0.54
1:A:137:LYS:HE3	3:A:1401:HOH:O	2.07	0.54
1:C:40:LEU:O	1:C:45:GLN:HG3	2.07	0.54
1:B:207:LEU:CD1	1:B:208:PRO:HD2	2.37	0.54
1:C:64:GLN:OE1	1:C:154:GLN:HG3	2.06	0.54
1:A:322:ARG:CG	1:A:322:ARG:HH21	2.11	0.54
1:B:52:ASP:OD2	1:B:52:ASP:N	2.36	0.54
1:C:24:ARG:HD3	1:C:55:GLU:OE2	2.08	0.54
1:B:293:LYS:HZ2	1:B:296:ILE:HD11	1.71	0.54
1:B:255:VAL:HG13	1:B:261:PHE:HB3	1.90	0.54
1:B:242:THR:HG23	1:B:292:LYS:CE	2.37	0.54
1:A:58:VAL:HG23	1:A:99:CYS:HA	1.89	0.54
1:C:133:GLU:O	1:C:137:LYS:HD3	2.07	0.54
1:B:129:THR:O	1:B:133:GLU:HG3	2.08	0.54
1:B:201:LEU:HD22	1:B:202:SER:N	2.23	0.54
1:B:226:LEU:HD23	1:B:306:ILE:CD1	2.37	0.54
1:B:254:ARG:HH11	1:B:256:GLU:HB2	1.73	0.54
1:B:259:PRO:O	1:B:263:PHE:HB2	2.08	0.54
1:C:254:ARG:HD2	1:C:256:GLU:O	2.08	0.54
1:A:237:VAL:HG13	1:A:240:MET:CE	2.38	0.54
1:A:58:VAL:HG23	1:A:58:VAL:O	2.07	0.54
1:B:289:VAL:O	1:B:293:LYS:HB2	2.08	0.53
1:B:299:LEU:O	1:B:303:LEU:HD13	2.08	0.53
1:A:22:ARG:NH2	1:A:53:GLU:HG3	2.24	0.53
1:C:154:GLN:OE1	2:C:500:TRP:OXT	2.26	0.53
1:B:116:LEU:HD23	1:B:152:VAL:HG21	1.91	0.53
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.71	0.53
1:B:119:VAL:HG22	1:B:120:THR:N	2.24	0.53
1:A:318:ASP:HA	3:A:2065:HOH:O	2.08	0.53
1:A:244:PRO:C	1:A:246:HIS:H	2.12	0.53
1:C:60:LEU:HD22	1:C:83:VAL:HG23	1.91	0.53
1:A:233:VAL:O	1:A:237:VAL:HG23	2.09	0.53
1:A:40:LEU:HD22	1:A:44:LEU:HD12	1.90	0.53
1:C:286:LEU:HD12	1:C:291:VAL:HG23	1.91	0.53
1:A:189:LEU:CD2	1:C:71:ASP:HA	2.35	0.52
1:A:206:ARG:NH1	1:A:215:LYS:HE2	2.24	0.52
1:C:51:GLN:HE22	1:C:93:ASP:N	1.98	0.52
1:B:47:ARG:O	1:B:51:GLN:HB2	2.09	0.52
1:C:180:ARG:CG	1:C:180:ARG:NH1	2.56	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:254:ARG:HH11	1:B:256:GLU:CB	2.22	0.52
1:B:61:ALA:HB1	1:B:64:GLN:HB3	1.91	0.52
1:A:346:MET:HE3	1:A:348:LEU:HD11	1.91	0.52
1:C:180:ARG:HD2	1:C:196:GLU:HG3	1.91	0.52
1:A:27:THR:OG1	1:A:47:ARG:NH1	2.43	0.52
1:B:293:LYS:NZ	1:B:296:ILE:HD11	2.23	0.52
1:A:168:VAL:HG22	1:A:169:GLY:O	2.10	0.52
1:B:149:VAL:CG1	1:B:152:VAL:HG13	2.40	0.52
1:B:202:SER:OG	1:B:205:PRO:HB3	2.09	0.52
1:C:339:LEU:O	1:C:343:ARG:HG3	2.10	0.52
1:C:60:LEU:CD2	1:C:83:VAL:HG23	2.40	0.51
1:A:248:ARG:NE	1:A:251:ASP:OD2	2.43	0.51
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.94	0.51
1:C:26:LEU:HD23	1:C:158:ILE:CD1	2.31	0.51
1:C:310:ARG:O	1:C:314:GLU:HG2	2.10	0.51
1:A:218:LYS:HE3	3:A:1289:HOH:O	2.09	0.51
1:B:207:LEU:CD2	1:B:216:MET:HE1	2.26	0.51
1:B:110:GLU:O	1:B:113:VAL:CG1	2.57	0.51
1:A:296:ILE:HD12	1:A:300:ASN:ND2	2.25	0.51
1:B:273:ARG:O	1:B:277:LEU:HD23	2.09	0.51
1:A:74:GLU:OE2	1:C:347:ARG:NH1	2.43	0.51
1:A:270:ASP:O	1:A:273:ARG:HB3	2.10	0.51
1:C:74:GLU:HB2	3:C:2059:HOH:O	2.09	0.51
1:B:299:LEU:HA	1:B:302:VAL:HG12	1.93	0.51
1:C:158:ILE:HD11	2:C:500:TRP:CH2	2.45	0.51
1:B:44:LEU:O	1:B:48:VAL:HG23	2.11	0.51
1:A:175:MET:C	1:A:175:MET:SD	2.89	0.51
1:B:261:PHE:CD1	1:B:278:LYS:HG2	2.46	0.51
1:A:149:VAL:O	1:A:149:VAL:CG1	2.58	0.51
1:C:105:VAL:O	1:C:105:VAL:HG13	2.11	0.50
1:A:296:ILE:HG13	1:A:297:ASP:N	2.25	0.50
1:B:49:ARG:O	1:B:52:ASP:OD2	2.29	0.50
1:B:99:CYS:HB2	1:B:323:PHE:CZ	2.46	0.50
1:B:226:LEU:CB	1:B:306:ILE:HD11	2.27	0.50
1:A:74:GLU:OE1	1:C:347:ARG:NH1	2.44	0.50
1:B:168:VAL:CG2	1:B:169:GLY:N	2.74	0.50
1:B:76:VAL:HG13	1:B:77:ARG:N	2.27	0.50
1:A:253:GLY:O	1:A:282:ARG:HA	2.11	0.50
1:B:149:VAL:O	1:B:152:VAL:HG13	2.11	0.50
1:B:41:ALA:HB2	1:B:207:LEU:HD22	1.94	0.49
1:B:168:VAL:HG22	1:B:169:GLY:O	2.12	0.49
1:A:137:LYS:HD3	1:A:139:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:121:VAL:HG13	1:B:148:PHE:CE1	2.47	0.49
1:C:170:ASP:HA	1:C:173:LEU:HD12	1.94	0.49
1:A:254:ARG:HH11	1:A:256:GLU:CG	2.26	0.49
1:A:22:ARG:CB	1:A:23:PRO:CD	2.90	0.49
1:B:98:THR:CG2	1:B:330:ARG:HD2	2.43	0.49
1:B:175:MET:C	1:B:175:MET:SD	2.91	0.49
1:B:261:PHE:CE1	1:B:278:LYS:HG2	2.48	0.49
1:C:32:THR:HG23	1:C:75:GLN:NE2	2.27	0.49
1:B:66:LEU:O	1:B:70:PHE:HB3	2.11	0.49
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.37	0.49
1:A:277:LEU:CD1	1:A:286:LEU:HD11	2.41	0.49
1:A:259:PRO:HA	1:A:262:THR:HG22	1.94	0.49
1:A:286:LEU:HD22	1:A:291:VAL:CG2	2.42	0.49
1:B:125:ARG:HG3	1:B:125:ARG:NH2	2.28	0.49
1:B:58:VAL:HG13	1:B:58:VAL:O	2.13	0.49
1:B:248:ARG:HD3	1:B:248:ARG:N	2.28	0.49
1:C:180:ARG:HD2	1:C:196:GLU:HG2	1.94	0.49
1:B:215:LYS:HZ3	1:B:215:LYS:CB	2.25	0.49
1:B:215:LYS:NZ	1:B:217:SER:OG	2.45	0.49
1:A:258:ASN:OD1	1:A:260:VAL:HG22	2.12	0.49
1:C:149:VAL:O	1:C:152:VAL:HG22	2.13	0.49
1:A:21:ALA:HB1	1:A:54:ALA:C	2.32	0.49
1:B:220:LEU:O	1:B:222:ASN:N	2.46	0.48
1:A:127:ASN:CB	1:A:130:VAL:HG12	2.40	0.48
1:C:256:GLU:CD	1:C:256:GLU:H	2.15	0.48
1:A:50:LEU:C	1:A:50:LEU:HD12	2.33	0.48
1:B:288:ASP:CA	1:B:291:VAL:HG12	2.42	0.48
1:B:122:SER:O	1:B:126:GLN:HB2	2.13	0.48
1:B:255:VAL:HG13	1:B:261:PHE:CB	2.44	0.48
1:B:291:VAL:CG1	1:B:292:LYS:N	2.75	0.48
1:B:290:LYS:HA	1:B:290:LYS:HE2	1.95	0.48
1:C:25:VAL:HG22	1:C:165:LEU:HB3	1.95	0.48
1:B:22:ARG:N	1:B:23:PRO:CD	2.77	0.48
1:B:210:LEU:HB2	1:B:222:ASN:OD1	2.14	0.48
1:B:242:THR:HG23	1:B:292:LYS:HE2	1.95	0.48
1:B:288:ASP:HA	1:B:291:VAL:CG1	2.44	0.48
1:A:81:LEU:HB2	3:A:1075:HOH:O	2.13	0.48
1:B:231:ASP:HB2	3:B:1702:HOH:O	2.13	0.48
1:A:51:GLN:NE2	1:A:93:ASP:N	2.51	0.48
1:B:218:LYS:CE	1:B:218:LYS:HA	2.40	0.48
1:A:119:VAL:HG23	3:A:1011:HOH:O	2.14	0.48
1:B:177:GLU:HG3	3:B:2105:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:HIS:HA	1:B:297:ASP:OD2	2.13	0.48
1:A:23:PRO:O	1:A:54:ALA:HB1	2.14	0.48
1:C:110:GLU:O	1:C:113:VAL:CG1	2.61	0.48
1:B:314:GLU:HA	3:B:2012:HOH:O	2.14	0.48
1:C:120:THR:CG2	1:C:123:HIS:HB2	2.44	0.47
1:C:80:VAL:HG13	1:C:81:LEU:H	1.78	0.47
1:A:351:HIS:N	1:A:351:HIS:CD2	2.81	0.47
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.96	0.47
1:A:322:ARG:CG	1:A:322:ARG:NH2	2.72	0.47
1:C:32:THR:CG2	1:C:32:THR:O	2.63	0.47
1:C:165:LEU:HD22	1:C:200:GLN:HB2	1.95	0.47
1:C:193:VAL:HG11	1:C:341:GLN:HB3	1.96	0.47
1:B:241:TYR:CD1	1:B:241:TYR:O	2.67	0.47
1:B:112:THR:HG22	1:B:156:ALA:HB3	1.96	0.47
1:A:211:ASP:HB3	1:A:213:GLN:HG3	1.96	0.47
1:A:114:TYR:CD1	1:A:346:MET:HE1	2.49	0.47
1:C:64:GLN:H	1:C:102:GLN:HE22	1.62	0.47
1:C:127:ASN:OD1	1:C:129:THR:CG2	2.62	0.47
1:B:63:VAL:CG1	1:B:102:GLN:HG2	2.44	0.47
1:B:84:ALA:O	1:B:87:TYR:HB2	2.15	0.47
1:A:255:VAL:CG2	1:A:278:LYS:HG3	2.33	0.47
1:B:269:PRO:HG2	1:B:270:ASP:H	1.80	0.47
1:C:58:VAL:HG23	1:C:58:VAL:O	2.14	0.47
1:A:47:ARG:CG	1:A:47:ARG:HH11	2.26	0.47
1:C:127:ASN:OD1	1:C:129:THR:HG22	2.15	0.47
1:C:229:SER:O	1:C:233:VAL:HG23	2.15	0.47
1:A:62:ASP:OD1	1:A:103:SER:OG	2.28	0.47
1:A:296:ILE:HG21	3:A:1058:HOH:O	2.14	0.47
1:B:88:LEU:HD21	1:B:323:PHE:CD1	2.49	0.47
1:C:95:GLN:NE2	1:C:95:GLN:HA	2.30	0.47
1:B:216:MET:HG3	1:B:223:ALA:HA	1.96	0.47
1:A:36:HIS:CD2	1:A:38:GLY:H	2.18	0.47
1:B:129:THR:HG22	1:B:133:GLU:OE1	2.15	0.47
1:B:120:THR:O	1:B:124:LEU:HB2	2.15	0.47
1:A:292:LYS:O	1:A:296:ILE:CG2	2.62	0.47
1:B:24:ARG:CB	3:B:1811:HOH:O	2.61	0.47
1:C:77:ARG:O	1:C:80:VAL:CG1	2.50	0.47
1:C:175:MET:O	1:C:175:MET:SD	2.73	0.47
1:C:321:LEU:O	1:C:325:THR:HG23	2.15	0.47
1:A:66:LEU:HD12	1:A:70:PHE:HA	1.96	0.47
1:C:56:LEU:HD13	1:C:56:LEU:C	2.35	0.46
1:A:243:ASP:OD1	1:A:244:PRO:O	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:326:GLU:HG2	3:C:1724:HOH:O	2.15	0.46
1:C:81:LEU:HB2	3:C:1064:HOH:O	2.15	0.46
1:A:273:ARG:O	1:A:277:LEU:HD22	2.15	0.46
1:A:206:ARG:CZ	1:A:215:LYS:HE2	2.45	0.46
1:A:175:MET:HB2	3:A:1149:HOH:O	2.15	0.46
1:B:35:LEU:CD1	1:B:86:ASP:HB3	2.46	0.46
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.80	0.46
1:B:222:ASN:CG	1:B:222:ASN:O	2.54	0.46
1:C:166:VAL:CG2	1:C:176:LEU:HD23	2.33	0.46
1:A:230:ALA:O	1:A:233:VAL:HG12	2.15	0.46
1:B:116:LEU:HD21	1:B:149:VAL:CG1	2.41	0.46
1:A:295:LEU:HD23	1:A:295:LEU:O	2.15	0.46
1:B:184:ARG:HD2	1:B:196:GLU:OE1	2.16	0.46
1:B:23:PRO:HG2	1:B:54:ALA:HB2	1.96	0.46
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.51	0.46
1:A:211:ASP:OD1	1:A:213:GLN:NE2	2.49	0.46
1:C:25:VAL:HG13	1:C:167:PRO:HD3	1.97	0.46
1:C:154:GLN:NE2	2:C:500:TRP:OXT	2.49	0.46
1:C:258:ASN:HD22	1:C:260:VAL:H	1.62	0.46
1:A:289:VAL:O	1:A:293:LYS:HG3	2.15	0.46
1:B:207:LEU:CG	1:B:208:PRO:HD2	2.46	0.46
1:A:255:VAL:HG21	1:A:278:LYS:CG	2.34	0.46
1:A:277:LEU:H	1:A:277:LEU:HD22	1.81	0.46
1:B:234:ALA:HA	1:B:296:ILE:CG2	2.46	0.46
1:A:263:PHE:HB3	1:A:295:LEU:HD11	1.97	0.46
1:A:149:VAL:O	1:A:149:VAL:HG13	2.17	0.45
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.98	0.45
1:B:260:VAL:HG13	1:B:295:LEU:HD22	1.99	0.45
1:C:102:GLN:HG3	1:C:108:LEU:HD12	1.97	0.45
1:A:25:VAL:HG13	1:A:167:PRO:HD3	1.98	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD2	1.82	0.45
1:C:268:ASP:OD1	1:C:294:HIS:CE1	2.69	0.45
1:A:123:HIS:HE1	3:A:1860:HOH:O	1.97	0.45
1:B:208:PRO:HG2	1:B:263:PHE:HE2	1.81	0.45
1:B:208:PRO:HG2	1:B:263:PHE:CE2	2.52	0.45
1:B:35:LEU:HG	1:B:86:ASP:OD2	2.17	0.45
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.32	0.45
1:A:255:VAL:HG13	1:A:261:PHE:CD2	2.52	0.45
1:C:254:ARG:CG	1:C:256:GLU:HG2	2.45	0.45
1:C:85:LEU:CD1	1:C:310:ARG:CZ	2.94	0.45
1:B:254:ARG:HB2	1:B:256:GLU:OE1	2.16	0.45
1:A:171:ASP:N	1:A:171:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:ALA:O	1:A:87:TYR:HB2	2.17	0.45
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.82	0.45
1:B:86:ASP:OD1	1:B:310:ARG:NH1	2.49	0.44
1:C:60:LEU:HD22	1:C:83:VAL:HG21	1.99	0.44
1:B:105:VAL:O	1:B:105:VAL:HG13	2.18	0.44
1:A:273:ARG:O	1:A:276:ALA:HB3	2.16	0.44
1:C:102:GLN:O	1:C:105:VAL:HG12	2.17	0.44
1:A:43:SER:C	1:A:47:ARG:HD2	2.37	0.44
1:C:168:VAL:O	1:C:202:SER:N	2.49	0.44
1:C:258:ASN:ND2	1:C:260:VAL:H	2.15	0.44
1:B:324:VAL:HG23	1:B:325:THR:N	2.32	0.44
1:C:150:TYR:N	1:C:151:PRO:CD	2.80	0.44
3:A:2166:HOH:O	1:B:322:ARG:HD2	2.16	0.44
1:B:241:TYR:O	1:B:259:PRO:CD	2.66	0.44
1:C:127:ASN:O	1:C:131:LYS:HB2	2.17	0.44
1:C:30:ARG:HB2	1:C:65:ALA:HB2	2.00	0.44
1:C:304:ALA:O	1:C:308:THR:HG23	2.17	0.44
1:B:212:GLY:O	1:B:213:GLN:C	2.55	0.44
1:C:51:GLN:NE2	1:C:97:THR:CG2	2.79	0.44
1:B:320:VAL:HG13	1:B:321:LEU:N	2.33	0.44
1:B:23:PRO:HG2	1:B:54:ALA:CB	2.47	0.44
1:B:40:LEU:HA	1:B:44:LEU:HB3	1.99	0.44
1:B:269:PRO:HD2	1:B:273:ARG:HH11	1.83	0.44
1:A:333:GLU:O	1:A:337:GLN:HG3	2.18	0.44
1:A:44:LEU:HA	1:A:47:ARG:HD2	2.00	0.44
1:C:165:LEU:CD2	1:C:200:GLN:HB2	2.48	0.44
1:B:207:LEU:HG	1:B:208:PRO:HD2	2.00	0.44
1:C:136:GLN:NE2	1:C:137:LYS:CD	2.77	0.44
1:A:296:ILE:CD1	1:A:300:ASN:ND2	2.80	0.44
1:C:273:ARG:O	1:C:277:LEU:CD2	2.66	0.44
1:C:231:ASP:CG	1:C:232:GLU:N	2.71	0.44
1:A:277:LEU:O	1:A:281:TYR:HB2	2.18	0.44
1:B:237:VAL:O	1:B:240:MET:N	2.45	0.44
1:C:238:MET:H	1:C:238:MET:HG2	1.61	0.43
1:C:112:THR:HG22	1:C:153:SER:HA	2.00	0.43
1:A:308:THR:O	1:A:312:GLU:HG3	2.18	0.43
1:A:37:LEU:HD22	1:A:224:ILE:HB	1.99	0.43
1:A:184:ARG:NH2	1:A:184:ARG:HG2	2.31	0.43
1:B:242:THR:HG21	1:B:288:ASP:HB3	2.01	0.43
1:A:173:LEU:N	1:A:174:PRO:CD	2.80	0.43
1:A:233:VAL:HG13	1:A:234:ALA:N	2.33	0.43
1:B:116:LEU:CD2	1:B:149:VAL:HG11	2.42	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:273:ARG:O	1:B:276:ALA:HB3	2.19	0.43
1:A:60:LEU:HD13	1:A:80:VAL:HG13	1.99	0.43
1:B:215:LYS:O	1:B:222:ASN:ND2	2.50	0.43
1:B:168:VAL:HG12	1:B:200:GLN:H	1.84	0.43
1:A:299:LEU:HA	1:A:302:VAL:CG1	2.47	0.43
1:B:142:ARG:O	1:B:142:ARG:CD	2.66	0.43
1:B:252:PRO:HG3	3:B:1440:HOH:O	2.18	0.43
1:C:288:ASP:O	1:C:292:LYS:HG3	2.19	0.43
1:B:193:VAL:CG2	1:B:341:GLN:HE21	2.31	0.43
1:B:281:TYR:C	1:B:283:ALA:H	2.21	0.43
1:C:230:ALA:HB1	1:C:300:ASN:ND2	2.31	0.43
1:B:256:GLU:CD	1:B:256:GLU:H	2.22	0.43
1:B:25:VAL:HA	1:B:165:LEU:O	2.18	0.43
1:B:150:TYR:N	1:B:151:PRO:CD	2.82	0.43
1:B:169:GLY:H	1:B:172:GLN:CG	2.29	0.43
1:A:184:ARG:HH21	1:A:184:ARG:CG	2.29	0.43
1:A:208:PRO:HG3	1:A:262:THR:HG21	2.01	0.43
1:C:247:LEU:CD1	1:C:247:LEU:N	2.82	0.43
1:C:100:VAL:HB	1:C:328:THR:HA	2.00	0.43
1:A:40:LEU:HA	1:A:44:LEU:HB2	1.99	0.43
1:A:101:VAL:O	1:A:101:VAL:HG13	2.19	0.42
1:A:310:ARG:HD3	3:A:1286:HOH:O	2.17	0.42
1:B:234:ALA:HA	1:B:296:ILE:HG22	2.01	0.42
1:B:134:ILE:HD13	1:B:143:VAL:HG21	2.01	0.42
1:C:133:GLU:O	1:C:136:GLN:HG3	2.19	0.42
1:C:129:THR:O	1:C:133:GLU:HG3	2.19	0.42
1:C:80:VAL:HG13	1:C:81:LEU:N	2.34	0.42
1:C:178:GLN:HA	3:C:1087:HOH:O	2.20	0.42
1:B:216:MET:HA	1:B:222:ASN:O	2.19	0.42
1:B:41:ALA:HB1	1:B:207:LEU:HD13	2.00	0.42
1:C:35:LEU:HD23	1:C:44:LEU:CD1	2.43	0.42
1:C:243:ASP:HA	1:C:244:PRO:HD2	1.87	0.42
1:B:193:VAL:HG21	1:B:341:GLN:HE21	1.84	0.42
1:B:211:ASP:O	1:B:213:GLN:N	2.43	0.42
1:C:108:LEU:HD13	1:C:157:ASP:OD1	2.20	0.42
1:B:40:LEU:HA	1:B:44:LEU:CB	2.49	0.42
1:A:117:ASN:HD22	1:C:146:GLY:HA3	1.83	0.42
1:B:226:LEU:CD1	1:B:226:LEU:H	2.16	0.42
1:A:299:LEU:O	1:A:302:VAL:HG13	2.19	0.42
1:B:119:VAL:HG22	1:B:120:THR:H	1.83	0.42
1:A:254:ARG:HH11	1:A:256:GLU:HG2	1.85	0.42
1:B:253:GLY:O	1:B:282:ARG:CA	2.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.95	0.42
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.20	0.42
1:B:213:GLN:O	1:B:215:LYS:N	2.53	0.42
1:A:349:PHE:HE2	1:C:81:LEU:HD22	1.85	0.41
1:A:66:LEU:O	1:A:70:PHE:HB3	2.19	0.41
1:C:112:THR:HG22	1:C:156:ALA:CB	2.50	0.41
1:A:127:ASN:O	1:A:130:VAL:HG12	2.19	0.41
1:A:74:GLU:CD	1:C:347:ARG:NH1	2.74	0.41
1:B:191:ALA:HA	1:B:192:PRO:HD3	1.89	0.41
1:C:93:ASP:HB3	1:C:96:LYS:HB2	2.02	0.41
1:B:118:LEU:HD13	1:B:185:ARG:HG3	2.02	0.41
1:B:289:VAL:HG12	1:B:290:LYS:HE3	2.01	0.41
1:A:165:LEU:HD21	1:A:200:GLN:HB2	2.02	0.41
1:A:136:GLN:HE21	1:A:136:GLN:CA	2.32	0.41
1:C:59:LEU:HD12	1:C:100:VAL:HG22	2.02	0.41
1:C:43:SER:O	1:C:47:ARG:HD3	2.21	0.41
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.85	0.41
1:A:230:ALA:O	1:A:233:VAL:CG1	2.68	0.41
1:A:22:ARG:HE	1:A:53:GLU:HG3	1.85	0.41
1:C:85:LEU:HD13	1:C:310:ARG:CZ	2.50	0.41
1:B:205:PRO:O	1:B:206:ARG:C	2.59	0.41
1:A:67:THR:HA	1:C:117:ASN:ND2	2.36	0.41
1:B:215:LYS:NZ	1:B:215:LYS:CB	2.79	0.41
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.33	0.41
1:B:105:VAL:HG13	1:B:108:LEU:CG	2.49	0.41
1:A:295:LEU:HD23	1:A:299:LEU:HG	2.03	0.41
1:A:22:ARG:CD	1:A:23:PRO:HD3	2.51	0.41
1:C:299:LEU:O	1:C:303:LEU:HB2	2.20	0.41
1:B:254:ARG:CD	1:B:256:GLU:HB2	2.51	0.41
1:A:136:GLN:NE2	1:A:136:GLN:HA	2.36	0.41
1:B:193:VAL:CG2	1:B:193:VAL:O	2.69	0.41
1:B:211:ASP:C	1:B:213:GLN:H	2.24	0.41
1:B:233:VAL:HG21	1:B:303:LEU:CD2	2.51	0.41
1:C:295:LEU:HD22	1:C:299:LEU:HG	2.03	0.41
1:A:305:PRO:HB2	1:A:309:ARG:HH22	1.79	0.41
1:C:185:ARG:HH11	1:C:189:LEU:CD2	2.34	0.41
1:C:144:PRO:HB2	3:C:1014:HOH:O	2.20	0.41
1:B:343:ARG:HD2	3:B:1116:HOH:O	2.21	0.41
1:B:296:ILE:HG13	1:B:297:ASP:N	2.36	0.40
1:A:247:LEU:CD1	1:A:247:LEU:N	2.83	0.40
1:A:22:ARG:HH21	1:A:53:GLU:HG2	1.85	0.40
1:B:173:LEU:N	1:B:174:PRO:CD	2.82	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:LEU:HD13	1:C:80:VAL:HG23	2.03	0.40
1:A:93:ASP:O	1:A:97:THR:CG2	2.69	0.40
1:B:105:VAL:HG13	1:B:108:LEU:CD1	2.51	0.40
1:B:253:GLY:HA3	1:B:281:TYR:CE2	2.56	0.40
1:B:62:ASP:OD1	1:B:103:SER:HB2	2.22	0.40
1:A:117:ASN:ND2	1:C:146:GLY:HA3	2.35	0.40
1:B:303:LEU:O	1:B:307:ARG:HB2	2.22	0.40
1:A:286:LEU:HD22	1:A:291:VAL:HG22	2.03	0.40
1:C:310:ARG:O	1:C:314:GLU:CG	2.69	0.40
1:A:211:ASP:CG	1:A:213:GLN:HE21	2.25	0.40
1:A:64:GLN:H	1:A:102:GLN:NE2	2.17	0.40
1:B:302:VAL:O	1:B:305:PRO:HD2	2.21	0.40
1:A:248:ARG:N	1:A:248:ARG:CD	2.81	0.40
1:C:167:PRO:HA	1:C:200:GLN:HB3	2.02	0.40
1:B:118:LEU:HB3	1:B:185:ARG:HG2	2.03	0.40
1:B:93:ASP:HA	1:B:94:PRO:HD3	2.00	0.40
1:A:178:GLN:HB3	3:A:1713:HOH:O	2.22	0.40
1:C:205:PRO:HB3	3:C:1637:HOH:O	2.21	0.40
1:B:321:LEU:O	1:B:324:VAL:HG22	2.21	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	329/331 (99%)	305 (93%)	19 (6%)	5 (2%)	15	13
1	B	329/331 (99%)	299 (91%)	21 (6%)	9 (3%)	8	5
1	C	329/331 (99%)	309 (94%)	17 (5%)	3 (1%)	25	26
All	All	987/993 (99%)	913 (92%)	57 (6%)	17 (2%)	14	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	ALA
1	C	202	SER
1	A	22	ARG
1	B	208	PRO
1	B	214	ALA
1	B	242	THR
1	A	249	ALA
1	B	206	ARG
1	B	269	PRO
1	C	22	ARG
1	A	43	SER
1	A	285	GLY
1	B	205	PRO
1	B	249	ALA
1	A	284	GLY
1	C	205	PRO
1	B	212	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/264 (100%)	228 (86%)	36 (14%)	5	5
1	B	256/264 (97%)	225 (88%)	31 (12%)	7	7
1	C	260/264 (98%)	226 (87%)	34 (13%)	6	6
All	All	780/792 (98%)	679 (87%)	101 (13%)	6	6

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	40	LEU
1	A	47	ARG
1	A	52	ASP
1	A	68	ASP
1	A	75	GLN
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	85	LEU
1	A	92	LEU
1	A	95	GLN
1	A	97	THR
1	A	136	GLN
1	A	141	GLU
1	A	149	VAL
1	A	150	TYR
1	A	165	LEU
1	A	170	ASP
1	A	171	ASP
1	A	184	ARG
1	A	185	ARG
1	A	189	LEU
1	A	201	LEU
1	A	238	MET
1	A	242	THR
1	A	248	ARG
1	A	254	ARG
1	A	263	PHE
1	A	290	LYS
1	A	296	ILE
1	A	297	ASP
1	A	302	VAL
1	A	318	ASP
1	A	322	ARG
1	A	344	ARG
1	A	347	ARG
1	A	351	HIS
1	B	35	LEU
1	B	40	LEU
1	B	49	ARG
1	B	52	ASP
1	B	56	LEU
1	B	63	VAL
1	B	81	LEU
1	B	85	LEU
1	B	92	LEU
1	B	125	ARG
1	B	126	GLN
1	B	142	ARG
1	B	150	TYR

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Mol	Chain	Res	Type
1	B	152	VAL
1	B	153	SER
1	B	165	LEU
1	B	172	GLN
1	B	200	GLN
1	B	201	LEU
1	B	203	ARG
1	B	215	LYS
1	B	224	ILE
1	B	246	HIS
1	B	248	ARG
1	B	251	ASP
1	B	268	ASP
1	B	286	LEU
1	B	290	LYS
1	B	300	ASN
1	B	306	ILE
1	B	348	LEU
1	C	24	ARG
1	C	30	ARG
1	C	37	LEU
1	C	81	LEU
1	C	85	LEU
1	C	92	LEU
1	C	97	THR
1	C	103	SER
1	C	150	TYR
1	C	165	LEU
1	C	168	VAL
1	C	180	ARG
1	C	185	ARG
1	C	189	LEU
1	C	193	VAL
1	C	200	GLN
1	C	201	LEU
1	C	204	VAL
1	C	205	PRO
1	C	210	LEU
1	C	231	ASP
1	C	238	MET
1	C	247	LEU
1	C	248	ARG

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Mol	Chain	Res	Type
1	C	256	GLU
1	C	258	ASN
1	C	286	LEU
1	C	295	LEU
1	C	298	VAL
1	C	321	LEU
1	C	326	GLU
1	C	330	ARG
1	C	332	ARG
1	C	337	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	46	ASN
1	A	51	GLN
1	A	64	GLN
1	A	69	HIS
1	A	102	GLN
1	A	117	ASN
1	A	123	HIS
1	A	126	GLN
1	A	136	GLN
1	A	178	GLN
1	A	200	GLN
1	A	213	GLN
1	A	351	HIS
1	B	36	HIS
1	B	39	HIS
1	B	46	ASN
1	B	69	HIS
1	B	117	ASN
1	B	172	GLN
1	B	200	GLN
1	B	280	GLN
1	B	300	ASN
1	B	341	GLN
1	C	51	GLN
1	C	69	HIS
1	C	95	GLN
1	C	102	GLN

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Mol	Chain	Res	Type
1	C	117	ASN
1	C	126	GLN
1	C	154	GLN
1	C	258	ASN
1	C	294	HIS
1	C	300	ASN
1	C	337	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRP	C	500	-	16,16,16	0.68	0	22,22,22	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	C	500	-	-	0/8/8/8	0/0/2/2

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.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.