



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:49 AM GMT

PDB ID : 2IBM  
Title : A novel dimer interface and conformational changes revealed by an X-ray structure of B. subtilis SecA  
Authors : Zimmer, J.; Li, W.; Rapoport, T.A.  
Deposited on : 2006-09-11  
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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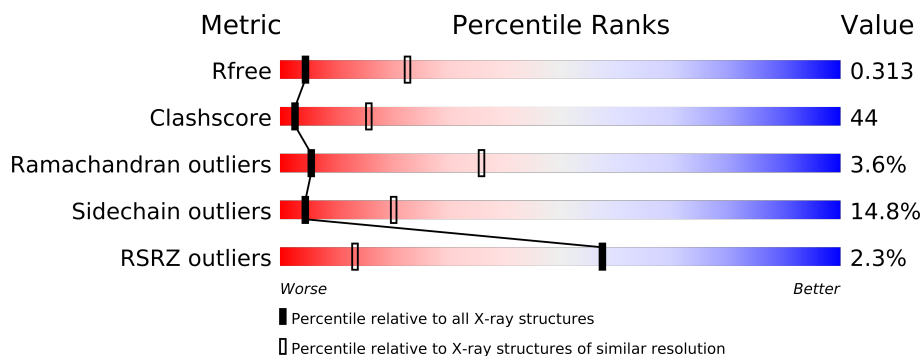
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	780	
1	B	780	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ADP	A	781	-	X

## 2 Entry composition i

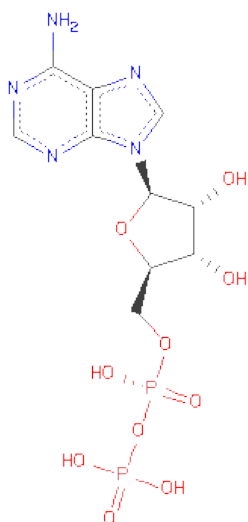
There are 2 unique types of molecules in this entry. The entry contains 12403 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	0	0
			6228	3899	1084	1210	35			
1	B	770	Total	C	N	O	S	0	0	0
			6148	3846	1072	1197	33			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



Chain B: 

M776	R709	A638	I569	M486	M411	R327	Q260	L191	A91
I780	E710	T639	I569	A487	E412	R328	R328	Y192	L92
	F711	A640	Q570	A487	G413	Y329	L261	K193	
	E712	A641	S571	I493	K414	Y329	T262	E194	E99
	K713	Y642	K572	K494	F415	E331	E263	Q195	M100
	W714	T643	M573	L495	K416	G332	E264	M196	K101
	I715	P644	V574		A417	L333	G265	M197	T102
	W716	R645	S575	K500	V418		K266	Q198	G103
	L717	E646	E579	G504	A419	A336	T267	K199	E104
	R718	E647	S580	L505	E420	I337	K268	P200	PHE
	A719	L648	S581	A506	D421	E338	A269	L201	ASP
	W720	P649	S582		V422	A339	E270		P11
	D721	E650	Q582	G509	A423	K340		A204	T12
	W722	E651	R583	T510	Q424	E341	I275	V205	K13
	K723	W652	R584	E511	R425		D276	I206	R14
	W724	K653	V585	R512	Y426	E344	I277		T15
	M725	L654	E586	H513	Q430	I345	L278	V209	L16
	D726	D655	G587	E514	F431	Q346	F279	D210	N17
	H727	G656	N588	S515	V432	N347	D280	S211	R18
	I728	L657		R516	V433	E348	V281	I212	Y19
			S592	R517	V434		K282	L213	V114
	M731	D659	R593			A353	H283	I214	
	D732		K594	L522	V439	T354	V284	D215	D27
	Q733	T663	Q595	R523		F357	L286	E216	A28
	L734	T664	L596	G524	S442	Q358	I287	A217	I29
	R735	L666	Q598	R525	E443		H288	R218	R30
		D667	Y599	G526	L444	M363	H289	T219	Y33
	H738	E668		G527	I445			L221	L36
	I739		V602	R528	S446	L367	Q292	I222	S37
	L740	K673	L603		K447	A368	A293	E135	D38
	R741		Q606	I534	E347	G369	L294	Q226	R39
	A742	T676	R607	T535	V458	F377	K302	A227	E146
	Y743	K679	E608	Q536	L459	M370	D295	K229	F147
	Q745	E680	V609	F537	K450	T371	K296	K229	L148
	T746	P681	I610	Y538	I454	G372	H297	S230	L41
	N747	D682	G612	L539		T373			K42
	P748	E683	Q613	S540	Q457		K300	T231	L45
	R750	M684	R614	M541	L459	E378	Q301	K232	F48
		L685	Q614	E544	M460	E379	D303	L233	
	M754	E686	F615	L545	A461	E380	D305	N238	E53
	E755	L687	E616	M546	K462	F381	Y306	A239	S160
		T688	V617	R547	N463	R382	V307	F240	
	M759	I692	I618	R548		N383	V308	K164	L61
	F760	L693	D619	F549	E467		T243	Y168	L62
		T694	S620	G550		M387	Q312	T244	V68
	M763	K695	E621	A551	I470	Q388		K244	V69
	I764	Y696	N622	E552		V389	T315	A246	R70
	S766	E766	L623	E553	E473	V390	D317	K247	
	I767	E700	R624	T554	A474	T391	V316	E248	S73
	E768	E701	E625	M555	G475		D317	K248	R74
	D769	Q702	I626	A556	Q476	V399	S318	D249	R75
		E703	V627	M557	K477	R400	F319	Y250	
				L558			T320	T251	L180
				D559			G321	Y252	K83
			M630		T481	R403	R322	D253	
			I631		L482	P404	L323	I254	M87
			K705	M563	A483	D405	K324	K255	G88
				D564	A484	L406	K325	D187	G89
			E636	D565	T484		K326	V257	
			R637		V485			V190	

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.83Å 166.83Å 211.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.53 – 3.20 40.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (40.53-3.20) 90.9 (40.53-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.321 , 0.323 0.304 , 0.313	Depositor DCC
$R_{free}$ test set	3431 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 17.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39716 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	12403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: ADP

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	0.63	2/6316 (0.0%)	0.88	9/8492 (0.1%)
1	B	0.68	1/6235 (0.0%)	0.90	19/8384 (0.2%)
All	All	0.65	3/12551 (0.0%)	0.89	28/16876 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	THR	CB-OG1	-13.18	1.16	1.43
1	A	279	PHE	C-N	6.88	1.49	1.34
1	A	701	GLU	N-CA	5.04	1.56	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	LEU	C-N-CA	10.24	147.31	121.70
1	B	247	GLU	CA-C-N	-9.45	96.40	117.20
1	B	353	ALA	N-CA-CB	8.80	122.42	110.10
1	B	244	LEU	CA-C-N	-8.14	99.29	117.20
1	A	11	PRO	N-CA-C	7.27	130.99	112.10
1	B	354	THR	CA-CB-OG1	6.79	123.26	109.00
1	A	14	ARG	N-CA-C	-6.36	93.82	111.00
1	B	711	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	B	650	GLU	N-CA-CB	-6.24	99.36	110.60
1	B	247	GLU	O-C-N	6.21	132.64	122.70
1	B	353	ALA	CB-CA-C	-6.14	100.89	110.10
1	B	704	GLY	N-CA-C	5.99	128.08	113.10
1	B	244	LEU	N-CA-C	5.94	127.04	111.00
1	A	252	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	B	623	LEU	CA-C-N	-5.94	104.14	117.20
1	B	624	ARG	CA-CB-CG	5.90	126.39	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	624	ARG	CB-CA-C	5.85	122.10	110.40
1	B	244	LEU	O-C-N	5.75	131.90	122.70
1	A	704	GLY	N-CA-C	5.61	127.12	113.10
1	A	280	ASP	C-N-CA	5.54	135.54	121.70
1	A	230	SER	N-CA-C	5.43	125.67	111.00
1	A	280	ASP	N-CA-CB	5.20	119.96	110.60
1	B	711	PHE	CB-CA-C	-5.18	100.04	110.40
1	B	247	GLU	CA-C-O	5.17	130.95	120.10
1	A	620	SER	N-CA-C	5.07	124.69	111.00
1	B	717	LEU	C-N-CA	-5.05	109.08	121.70
1	A	280	ASP	CA-C-N	-5.01	106.18	117.20
1	B	650	GLU	CB-CA-C	5.00	120.41	110.40

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	6228	0	6227	545	0
1	B	6148	0	6139	578	0
2	A	27	0	12	3	0
All	All	12403	0	12378	1092	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 44.

All (1092) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:620:SER:HB3	1:B:625:GLU:CG	1.49	1.39
1:A:723:LYS:HD3	1:A:763:MET:SD	1.67	1.35
1:A:747:ASN:H	1:A:748:PRO:CD	1.39	1.31
1:A:10:ASP:HB3	1:A:11:PRO:CD	1.61	1.29
1:A:303:ASP:O	1:A:304:VAL:HG23	1.10	1.28

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:747:ASN:N	1:A:748:PRO:HD2	1.34	1.27
1:B:723:LYS:CE	1:B:767:ILE:HD11	1.66	1.25
1:B:620:SER:HB3	1:B:625:GLU:CB	1.67	1.25
1:A:10:ASP:CB	1:A:11:PRO:HD2	1.57	1.25
1:B:723:LYS:HE3	1:B:767:ILE:CD1	1.65	1.25
1:B:650:GLU:OE1	1:B:650:GLU:C	1.78	1.22
1:A:723:LYS:CD	1:A:763:MET:SD	2.31	1.18
1:A:303:ASP:O	1:A:304:VAL:CG2	1.93	1.16
1:B:245:LYS:HE3	1:B:247:GLU:OE1	1.40	1.16
1:B:624:ARG:HH21	1:B:707:GLN:CB	1.57	1.16
1:B:248:LYS:HB2	1:B:265:GLY:CA	1.76	1.15
1:B:650:GLU:OE1	1:B:650:GLU:O	1.63	1.14
1:B:248:LYS:HB2	1:B:265:GLY:HA3	1.15	1.14
1:B:718:ARG:HG3	1:B:770:GLU:OE2	1.48	1.13
1:B:624:ARG:HH21	1:B:707:GLN:HB3	0.96	1.13
1:A:278:LEU:HB3	1:A:283:HIS:CG	1.83	1.11
1:A:281:VAL:HB	1:A:283:HIS:CD2	1.86	1.11
1:A:661:ILE:HG22	1:A:666:LEU:HD21	1.23	1.10
1:B:750:ARG:HG2	1:B:750:ARG:HH11	1.07	1.09
1:B:620:SER:HB3	1:B:625:GLU:HG2	1.13	1.08
1:B:630:MET:SD	1:B:775:VAL:HG21	1.93	1.07
1:B:620:SER:CB	1:B:625:GLU:HG2	1.85	1.06
1:A:661:ILE:HG22	1:A:666:LEU:CD2	1.85	1.06
1:B:620:SER:CB	1:B:625:GLU:CG	2.33	1.05
1:A:349:SER:HB3	1:B:557:MET:HG3	1.37	1.05
1:A:349:SER:CB	1:B:557:MET:HG3	1.86	1.05
1:A:207:ASP:HB2	1:A:370:MET:HE1	1.34	1.05
1:A:558:LEU:HG	1:A:563:MET:CE	1.87	1.04
1:A:558:LEU:HG	1:A:563:MET:HE1	1.35	1.04
1:B:516:ARG:CZ	1:B:582:GLN:HG2	1.86	1.04
1:B:723:LYS:HB2	1:B:763:MET:CG	1.87	1.04
1:B:647:GLU:CB	1:B:652:TRP:CZ3	2.42	1.03
1:B:647:GLU:C	1:B:652:TRP:HH2	1.61	1.03
1:A:254:ILE:HG22	1:A:255:LYS:H	0.86	1.03
1:A:284:VAL:HG21	1:A:717:LEU:HD21	1.35	1.01
1:B:637:ARG:HH21	1:B:769:ASP:HB3	1.21	1.01
1:A:279:PHE:HA	1:A:778:ALA:HB1	1.42	1.01
1:B:620:SER:CB	1:B:625:GLU:HB3	1.89	1.01
1:A:254:ILE:HG22	1:A:255:LYS:N	1.66	1.00
1:A:708:MET:SD	1:A:711:PHE:HE1	1.84	1.00
1:A:254:ILE:CG2	1:A:255:LYS:H	1.72	0.99
1:A:563:MET:O	1:A:564:ASP:OD1	1.80	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:723:LYS:HD3	1:A:763:MET:CE	1.92	0.99
1:B:275:ILE:HD11	1:B:283:HIS:CD2	1.98	0.99
1:A:553:ARG:HH21	1:A:560:ARG:HH21	1.02	0.99
1:A:661:ILE:CG2	1:A:666:LEU:HD21	1.93	0.99
1:B:295:LYS:HE2	1:B:333:LEU:HD22	1.39	0.99
1:A:226:GLN:HE21	1:A:228:ALA:H	1.11	0.98
1:B:718:ARG:HG3	1:B:770:GLU:CD	1.82	0.98
1:B:248:LYS:CB	1:B:265:GLY:CA	2.41	0.98
1:B:218:ARG:HD3	1:B:592:SER:HB3	1.44	0.98
1:A:485:ASN:O	1:A:486:MET:HG2	1.63	0.98
1:B:620:SER:HB3	1:B:625:GLU:HB3	1.39	0.97
1:A:457:GLN:HE21	1:A:470:ILE:HD12	1.27	0.97
1:B:243:THR:C	1:B:244:LEU:HD23	1.85	0.97
1:B:624:ARG:NH2	1:B:707:GLN:HB3	1.79	0.97
1:B:647:GLU:HB3	1:B:652:TRP:CZ3	1.98	0.97
1:B:637:ARG:HE	1:B:769:ASP:CB	1.77	0.96
1:B:647:GLU:CA	1:B:652:TRP:CH2	2.48	0.96
1:B:12:THR:O	1:B:16:LEU:HD22	1.63	0.96
1:B:637:ARG:NH2	1:B:769:ASP:HB3	1.80	0.96
1:A:278:LEU:HB3	1:A:283:HIS:CB	1.95	0.96
1:A:746:THR:O	1:A:746:THR:HG22	1.64	0.96
1:A:337:ILE:HD12	1:A:346:GLN:NE2	1.79	0.96
1:A:275:ILE:CG2	1:A:276:ASP:H	1.78	0.96
1:A:221:LEU:HD11	1:A:357:PHE:CZ	2.01	0.96
1:B:418:VAL:O	1:B:422:VAL:HG23	1.66	0.95
1:B:625:GLU:HG3	1:B:625:GLU:O	1.65	0.95
1:B:603:LEU:HD11	1:B:731:MET:HG2	1.47	0.95
1:A:666:LEU:CD1	1:A:691:ARG:HB3	1.96	0.95
1:A:708:MET:SD	1:A:711:PHE:CE1	2.59	0.95
1:B:647:GLU:HB3	1:B:652:TRP:HZ3	1.31	0.94
1:A:610:ILE:HG13	1:A:723:LYS:HE3	1.47	0.94
1:A:275:ILE:HG23	1:A:276:ASP:H	1.31	0.94
1:B:626:ILE:HD12	1:B:715:ILE:HD12	1.49	0.94
1:A:627:VAL:O	1:A:631:ILE:HG12	1.66	0.94
1:B:248:LYS:HZ3	1:B:268:LYS:HB2	1.33	0.94
1:A:278:LEU:HB3	1:A:283:HIS:HB3	1.48	0.93
1:A:5:LEU:HB3	1:A:383:ASN:OD1	1.69	0.93
1:B:647:GLU:N	1:B:652:TRP:CH2	2.37	0.92
1:B:331:GLU:OE2	1:B:722:SER:HB2	1.69	0.92
1:B:245:LYS:HE3	1:B:247:GLU:CD	1.90	0.92
1:B:647:GLU:C	1:B:652:TRP:CH2	2.43	0.92
1:B:620:SER:CB	1:B:625:GLU:CB	2.48	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LEU:CB	1:A:283:HIS:HB3	2.00	0.91
1:B:647:GLU:O	1:B:652:TRP:CH2	2.23	0.91
1:B:614:ARG:HH12	1:B:720:VAL:CG2	1.84	0.90
1:A:182:PHE:HB3	1:A:186:ARG:HH21	1.36	0.90
1:A:275:ILE:CG2	1:A:276:ASP:N	2.34	0.90
1:B:336:ALA:O	1:B:340:LYS:HD3	1.72	0.90
1:B:248:LYS:CD	1:B:265:GLY:HA2	2.02	0.90
1:A:660:LEU:HD23	1:A:661:ILE:HG13	1.52	0.90
1:B:636:GLU:HA	1:B:636:GLU:OE1	1.69	0.89
1:B:647:GLU:O	1:B:652:TRP:HH2	1.52	0.89
1:A:232:LYS:H	1:A:232:LYS:HD2	1.37	0.89
1:B:324:MET:HA	1:B:741:ARG:HD2	1.53	0.89
1:A:749:LEU:O	1:A:753:GLN:HG2	1.73	0.89
1:A:244:LEU:O	1:A:248:LYS:HB2	1.72	0.89
1:B:750:ARG:HG2	1:B:750:ARG:NH1	1.82	0.89
1:B:750:ARG:CG	1:B:750:ARG:HH11	1.86	0.88
1:A:228:ALA:HB3	1:A:230:SER:OG	1.74	0.88
1:A:317:ASP:HB3	1:A:320:THR:HG22	1.55	0.88
1:A:313:VAL:HG22	1:A:337:ILE:HD13	1.56	0.88
1:A:338:GLU:HG2	1:A:345:ILE:HG13	1.55	0.87
1:A:666:LEU:HD12	1:A:691:ARG:HB3	1.55	0.87
1:B:713:LYS:O	1:B:717:LEU:HB2	1.72	0.87
1:A:485:ASN:O	1:A:486:MET:CG	2.23	0.87
1:A:640:ALA:O	1:A:644:PRO:HD3	1.74	0.87
1:A:647:GLU:HG3	1:A:649:PRO:CD	2.05	0.87
1:A:226:GLN:HB2	1:A:350:MET:HB2	1.54	0.87
1:A:722:SER:O	1:A:726:ASP:HB2	1.74	0.86
1:A:673:LYS:HB2	1:A:677:PHE:HB3	1.54	0.86
1:A:561:PHE:O	1:A:569:ILE:HG13	1.76	0.85
1:B:248:LYS:CB	1:B:265:GLY:HA2	2.05	0.85
1:A:281:VAL:O	1:A:281:VAL:HG12	1.74	0.85
1:B:522:LEU:O	1:B:525:ARG:HG3	1.76	0.85
1:A:647:GLU:HG3	1:A:649:PRO:HD3	1.59	0.85
1:B:229:LYS:HB3	1:B:289:HIS:NE2	1.92	0.84
1:A:755:GLU:O	1:A:759:MET:HG3	1.75	0.84
1:B:718:ARG:CG	1:B:770:GLU:OE2	2.24	0.84
1:B:614:ARG:HH12	1:B:720:VAL:HG23	1.43	0.84
1:B:152:VAL:HG13	1:B:172:ILE:HG22	1.58	0.84
1:A:576:ARG:HH22	1:B:346:GLN:CD	1.80	0.83
1:A:723:LYS:HD2	1:A:763:MET:SD	2.16	0.83
1:A:657:LEU:HD12	1:A:660:LEU:HD22	1.59	0.83
1:B:12:THR:O	1:B:16:LEU:CD2	2.26	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:700:GLU:O	1:A:704:GLY:HA3	1.78	0.83
1:B:703:PHE:CE1	1:B:707:GLN:NE2	2.45	0.83
1:B:723:LYS:HB2	1:B:763:MET:HG3	1.61	0.83
1:A:249:ASP:OD2	1:A:294:LEU:HD21	1.78	0.83
1:A:741:ARG:HH22	1:B:376:THR:HG22	1.43	0.83
1:A:673:LYS:HB2	1:A:677:PHE:CB	2.08	0.82
1:B:626:ILE:CG2	1:B:715:ILE:HD11	2.09	0.82
1:B:459:LEU:HD22	1:B:487:ALA:HB1	1.61	0.82
1:B:706:GLU:O	1:B:709:ARG:HB2	1.79	0.82
1:B:637:ARG:HE	1:B:769:ASP:HB3	1.45	0.82
1:A:338:GLU:HG2	1:A:345:ILE:HA	1.61	0.82
1:B:514:GLU:OE1	1:B:514:GLU:HA	1.79	0.82
1:A:630:MET:HE3	1:A:775:VAL:HG11	1.58	0.82
1:B:295:LYS:HE2	1:B:333:LEU:CD2	2.10	0.82
1:B:637:ARG:HE	1:B:769:ASP:CA	1.92	0.81
1:A:599:TYR:HD2	1:A:735:ARG:HG3	1.45	0.81
1:A:351:THR:HG22	1:A:728:ILE:HG22	1.62	0.81
1:A:255:LYS:CD	1:A:762:HIS:HE1	1.93	0.81
1:B:217:ALA:HB1	1:B:358:GLN:HE22	1.45	0.81
1:A:348:GLU:OE2	1:B:573:MET:CB	2.29	0.81
1:B:624:ARG:NH2	1:B:707:GLN:CB	2.41	0.81
1:B:348:GLU:OE1	1:B:348:GLU:HA	1.81	0.81
1:B:647:GLU:CB	1:B:652:TRP:HZ3	1.88	0.81
1:A:253:ASP:OD2	1:A:645:ARG:HG2	1.81	0.80
1:A:611:TYR:O	1:A:615:PHE:HD1	1.65	0.80
1:A:5:LEU:CD2	1:A:5:LEU:H	1.94	0.80
1:B:248:LYS:CB	1:B:265:GLY:HA3	2.01	0.80
1:B:248:LYS:HD2	1:B:265:GLY:HA2	1.62	0.80
1:A:221:LEU:HD11	1:A:357:PHE:CE2	2.17	0.80
1:B:256:THR:HG21	1:B:295:LYS:HD2	1.63	0.79
1:B:720:VAL:O	1:B:725:MET:HG3	1.82	0.79
1:A:557:MET:HG2	1:B:226:GLN:NE2	1.97	0.79
1:A:610:ILE:HG13	1:A:723:LYS:CE	2.12	0.79
1:A:255:LYS:HD3	1:A:762:HIS:CE1	2.18	0.79
1:A:218:ARG:O	1:B:549:PHE:HB3	1.83	0.79
1:A:744:ALA:O	1:A:748:PRO:HD3	1.83	0.79
1:B:637:ARG:HB3	1:B:665:TYR:OH	1.82	0.79
1:B:368:ALA:HA	1:B:387:MET:CE	2.12	0.79
1:B:275:ILE:HD11	1:B:283:HIS:NE2	1.98	0.79
1:A:626:ILE:HG23	1:A:711:PHE:CD1	2.18	0.79
1:A:110:SER:O	1:A:114:VAL:HG23	1.82	0.78
1:B:248:LYS:HZ3	1:B:268:LYS:CB	1.97	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:THR:O	1:A:243:THR:HG22	1.84	0.78
1:A:400:ARG:HD2	1:A:526:SER:HB3	1.65	0.78
1:B:626:ILE:HG21	1:B:715:ILE:HD11	1.64	0.78
1:B:626:ILE:HD12	1:B:715:ILE:CD1	2.13	0.78
1:A:275:ILE:HG22	1:A:276:ASP:N	1.99	0.78
1:A:553:ARG:HH21	1:A:560:ARG:NH2	1.81	0.78
1:B:695:LYS:HD3	1:B:776:MET:CE	2.12	0.78
1:B:703:PHE:O	1:B:703:PHE:CD1	2.37	0.78
1:A:278:LEU:N	1:A:278:LEU:HD23	1.99	0.78
1:B:582:GLN:HE21	1:B:586:GLU:HG3	1.48	0.78
1:B:637:ARG:NE	1:B:769:ASP:HB3	1.99	0.77
1:A:226:GLN:HE21	1:A:228:ALA:N	1.81	0.77
1:A:740:LEU:H	1:A:740:LEU:HD23	1.49	0.77
1:B:448:LEU:HD12	1:B:449:LEU:N	1.98	0.77
1:B:301:GLN:HB3	1:B:304:VAL:HB	1.66	0.77
1:A:284:VAL:HG21	1:A:717:LEU:CD2	2.14	0.77
1:A:279:PHE:CA	1:A:778:ALA:HB1	2.14	0.77
1:A:279:PHE:CD1	1:A:778:ALA:O	2.37	0.77
1:A:278:LEU:HD11	1:A:286:LEU:HB2	1.67	0.76
1:A:10:ASP:CB	1:A:11:PRO:CD	2.36	0.76
1:B:245:LYS:CE	1:B:247:GLU:OE1	2.28	0.76
1:B:650:GLU:CD	1:B:650:GLU:O	2.24	0.76
1:B:241:VAL:O	1:B:244:LEU:HG	1.86	0.76
1:B:463:ASN:O	1:B:467:GLU:HG3	1.85	0.76
1:A:210:ASP:OD2	1:A:371:THR:HG21	1.84	0.76
1:B:425:ARG:HD2	1:B:430:GLN:OE1	1.85	0.76
1:B:711:PHE:O	1:B:715:ILE:HG13	1.86	0.76
1:A:9:PHE:CD2	1:A:10:ASP:N	2.53	0.75
1:B:250:TYR:HE2	1:B:659:ASP:HB3	1.49	0.75
1:A:217:ALA:HB1	1:A:358:GLN:NE2	2.01	0.75
1:B:516:ARG:NE	1:B:582:GLN:HG2	2.00	0.75
1:B:647:GLU:HB2	1:B:652:TRP:CZ3	2.20	0.75
1:B:552:GLU:HA	1:B:555:MET:HG3	1.67	0.75
1:A:654:LEU:HD12	1:A:657:LEU:HB3	1.68	0.75
1:B:307:VAL:HG12	1:B:308:VAL:N	2.01	0.75
1:B:637:ARG:HE	1:B:769:ASP:HA	1.51	0.74
1:A:276:ASP:O	1:A:278:LEU:HD23	1.88	0.74
1:B:206:ILE:HG21	1:B:209:VAL:HG23	1.70	0.74
1:B:723:LYS:HB2	1:B:763:MET:HG2	1.70	0.74
1:A:626:ILE:CG2	1:A:711:PHE:HD1	2.00	0.74
1:B:354:THR:CG2	1:B:735:ARG:HH22	2.00	0.74
1:B:637:ARG:CZ	1:B:769:ASP:HB3	2.17	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:655:ASP:O	1:B:659:ASP:HB2	1.86	0.73
1:A:654:LEU:HB3	1:A:675:ASP:HB2	1.69	0.73
1:A:194:GLU:HG3	1:A:195:GLN:N	2.02	0.73
1:B:414:LYS:O	1:B:418:VAL:HG23	1.88	0.73
1:B:650:GLU:CD	1:B:650:GLU:C	2.46	0.73
1:A:654:LEU:HD22	1:A:677:PHE:HE2	1.53	0.73
1:A:747:ASN:N	1:A:748:PRO:CD	2.10	0.73
1:A:182:PHE:HB3	1:A:186:ARG:NH2	2.03	0.73
1:B:514:GLU:OE1	1:B:585:VAL:HG11	1.88	0.73
1:B:199:ARG:HB3	1:B:200:PRO:CD	2.18	0.73
1:B:610:ILE:CD1	1:B:723:LYS:HZ3	2.01	0.73
1:A:351:THR:HG22	1:A:728:ILE:CG2	2.17	0.73
1:A:666:LEU:HD11	1:A:691:ARG:HB3	1.70	0.73
1:A:291:ASN:O	1:A:295:LYS:HG3	1.89	0.73
1:A:207:ASP:HB2	1:A:370:MET:CE	2.18	0.73
1:A:654:LEU:HD23	1:A:675:ASP:HA	1.71	0.72
1:A:382:ARG:CZ	1:A:388:GLN:HG2	2.18	0.72
1:A:255:LYS:HD3	1:A:762:HIS:HE1	1.49	0.72
1:A:349:SER:HB2	1:B:557:MET:HG3	1.69	0.72
1:A:315:ILE:HD12	1:A:327:ARG:HB3	1.71	0.72
1:B:295:LYS:CE	1:B:333:LEU:HD22	2.18	0.72
1:A:142:GLY:HA2	1:A:152:VAL:HG21	1.72	0.72
1:A:562:GLY:CA	1:A:569:ILE:HG13	2.19	0.72
1:B:722:SER:OG	1:B:723:LYS:N	2.12	0.72
1:A:348:GLU:OE2	1:B:573:MET:HB2	1.89	0.71
1:B:288:HIS:CD2	1:B:718:ARG:HH12	2.06	0.71
1:B:198:GLN:O	1:B:199:ARG:HD2	1.91	0.71
1:B:190:VAL:HG22	1:B:195:GLN:HG3	1.72	0.71
1:B:243:THR:HG22	1:B:243:THR:O	1.90	0.71
1:B:636:GLU:CA	1:B:636:GLU:OE1	2.38	0.71
1:A:348:GLU:OE2	1:B:573:MET:HB3	1.90	0.71
1:B:39:ASP:HA	1:B:42:LYS:HB3	1.73	0.71
1:A:246:ALA:HB1	1:A:264:GLU:HB3	1.73	0.71
1:B:654:LEU:O	1:B:657:LEU:N	2.23	0.70
1:B:459:LEU:HD21	1:B:467:GLU:HB3	1.72	0.70
1:B:368:ALA:HA	1:B:387:MET:HE1	1.73	0.70
1:A:213:LEU:HD22	1:A:385:TYR:CZ	2.27	0.70
1:B:354:THR:HG21	1:B:735:ARG:HH22	1.54	0.70
1:A:279:PHE:HD1	1:A:779:GLU:CA	2.03	0.70
1:A:706:GLU:O	1:A:709:ARG:HB3	1.92	0.70
1:B:642:TYR:HE1	1:B:685:LEU:HA	1.56	0.70
1:A:662:ASN:HA	1:A:666:LEU:O	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:TYR:HE1	1:A:455:PRO:HG2	1.56	0.70
1:A:66:PHE:CE2	1:A:112:LEU:HB3	2.26	0.70
1:A:662:ASN:HB3	1:A:670:ALA:HB3	1.72	0.70
1:A:279:PHE:HA	1:A:778:ALA:CB	2.20	0.70
1:A:627:VAL:O	1:A:631:ILE:CG1	2.38	0.69
1:B:626:ILE:CG2	1:B:715:ILE:CD1	2.70	0.69
1:A:258:ALA:HB3	1:A:295:LYS:HG2	1.74	0.69
1:B:626:ILE:HG21	1:B:715:ILE:CD1	2.22	0.69
1:A:647:GLU:HG3	1:A:649:PRO:HD2	1.74	0.69
1:A:744:ALA:O	1:A:748:PRO:CD	2.40	0.69
1:A:677:PHE:HZ	1:A:684:MET:HE2	1.57	0.69
1:A:562:GLY:HA2	1:A:569:ILE:HG13	1.75	0.69
1:B:246:ALA:HB3	1:B:248:LYS:HG2	1.73	0.69
1:B:233:LEU:HB3	1:B:289:HIS:HD1	1.58	0.69
1:A:746:THR:O	1:A:746:THR:CG2	2.37	0.68
1:B:325:LYS:H	1:B:741:ARG:HD3	1.57	0.68
1:A:426:TYR:CD1	1:A:454:ILE:HG23	2.27	0.68
1:A:627:VAL:HG11	1:A:696:TYR:OH	1.93	0.68
1:B:36:LEU:H	1:B:75:ARG:HH22	1.42	0.68
1:B:246:ALA:HB1	1:B:268:LYS:NZ	2.08	0.68
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.59	0.68
1:A:279:PHE:O	1:A:778:ALA:HB1	1.94	0.68
1:A:254:ILE:CG2	1:A:255:LYS:N	2.42	0.68
1:B:626:ILE:HB	1:B:711:PHE:CD1	2.29	0.68
1:A:278:LEU:H	1:A:278:LEU:HD23	1.58	0.68
1:A:553:ARG:NH2	1:A:560:ARG:HH21	1.85	0.68
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.59	0.68
1:B:380:GLU:OE2	1:B:593:ARG:NH1	2.27	0.67
1:A:300:MET:SD	1:A:306:TYR:CE2	2.87	0.67
1:A:303:ASP:C	1:A:304:VAL:HG23	2.10	0.67
1:A:255:LYS:CD	1:A:762:HIS:CE1	2.75	0.67
1:B:301:GLN:HA	1:B:301:GLN:OE1	1.94	0.67
1:B:206:ILE:O	1:B:369:GLY:HA2	1.94	0.67
1:A:406:LEU:CD2	1:A:570:GLN:HE21	2.07	0.67
1:B:647:GLU:CB	1:B:652:TRP:CH2	2.78	0.67
1:A:337:ILE:HD12	1:A:346:GLN:HE22	1.55	0.67
1:A:249:ASP:OD2	1:A:294:LEU:CD2	2.42	0.67
1:A:717:LEU:HG	1:A:718:ARG:N	2.09	0.67
1:A:182:PHE:CB	1:A:186:ARG:HH21	2.06	0.67
1:B:610:ILE:CD1	1:B:723:LYS:NZ	2.57	0.67
1:B:218:ARG:CD	1:B:592:SER:HB3	2.23	0.67
1:A:677:PHE:CZ	1:A:684:MET:HE2	2.30	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:627:VAL:HG22	1:B:711:PHE:CZ	2.30	0.67
1:B:769:ASP:OD1	1:B:770:GLU:N	2.28	0.67
1:B:307:VAL:CG1	1:B:308:VAL:N	2.57	0.66
1:A:544:GLU:O	1:A:545:LEU:HB2	1.95	0.66
1:B:476:GLN:HE22	1:B:494:LYS:HZ3	1.43	0.66
1:B:261:LEU:HD12	1:B:262:THR:HB	1.75	0.66
1:A:599:TYR:CD2	1:A:735:ARG:HG3	2.28	0.66
1:B:206:ILE:HG23	1:B:212:ILE:HD12	1.77	0.66
1:B:248:LYS:NZ	1:B:268:LYS:HB2	2.08	0.66
1:B:400:ARG:HD2	1:B:535:THR:HG23	1.76	0.66
1:A:458:VAL:HA	1:A:482:ILE:HG23	1.77	0.66
1:B:248:LYS:HA	1:B:261:LEU:HB3	1.78	0.66
1:A:611:TYR:O	1:A:615:PHE:CD1	2.49	0.66
1:A:246:ALA:O	1:A:262:THR:HB	1.96	0.66
1:B:302:LYS:O	1:B:302:LYS:CG	2.43	0.66
1:A:561:PHE:HD1	1:A:561:PHE:O	1.78	0.66
1:B:16:LEU:H	1:B:16:LEU:CD2	2.07	0.66
1:B:344:GLU:O	1:B:346:GLN:N	2.29	0.66
1:A:421:ASP:O	1:A:425:ARG:HG2	1.95	0.66
1:A:313:VAL:HG22	1:A:337:ILE:CD1	2.25	0.66
1:B:206:ILE:CG2	1:B:209:VAL:HG23	2.25	0.66
1:A:361:PHE:HB3	1:A:367:LEU:HD21	1.78	0.66
1:A:485:ASN:C	1:A:485:ASN:OD1	2.34	0.66
1:B:720:VAL:HG12	1:B:721:ASP:N	2.09	0.65
1:A:576:ARG:HH12	1:B:346:GLN:HE22	1.44	0.65
1:B:582:GLN:NE2	1:B:586:GLU:HG3	2.11	0.65
1:B:368:ALA:HA	1:B:387:MET:HE3	1.77	0.65
1:A:724:TRP:HA	1:A:724:TRP:CE3	2.31	0.65
1:B:516:ARG:HH11	1:B:516:ARG:N	1.94	0.65
1:A:206:ILE:HG23	1:A:212:ILE:HD12	1.78	0.65
1:A:761:GLU:O	1:A:765:GLU:HG3	1.97	0.65
1:A:433:LEU:HD21	1:A:525:ARG:HD3	1.78	0.65
1:A:274:GLY:O	1:A:275:ILE:HG13	1.96	0.65
1:A:317:ASP:HB3	1:A:320:THR:CG2	2.26	0.65
1:A:654:LEU:HD22	1:A:677:PHE:CE2	2.33	0.64
1:B:554:THR:O	1:B:558:LEU:HG	1.98	0.64
1:B:620:SER:HB2	1:B:625:GLU:HB3	1.75	0.64
1:A:278:LEU:HB2	1:A:283:HIS:HB3	1.79	0.64
1:A:637:ARG:NE	1:A:769:ASP:HB2	2.13	0.64
1:A:680:GLU:HB2	1:A:683:GLU:HB2	1.80	0.64
1:A:279:PHE:HD1	1:A:779:GLU:HA	1.61	0.64
1:B:439:VAL:HA	1:B:442:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:637:ARG:HH21	1:B:769:ASP:CB	2.05	0.64
1:B:248:LYS:HB3	1:B:265:GLY:CA	2.28	0.64
1:B:630:MET:SD	1:B:775:VAL:CG2	2.79	0.64
1:B:649:PRO:O	1:B:652:TRP:CH2	2.50	0.64
1:A:426:TYR:CE1	1:A:455:PRO:HG2	2.32	0.64
1:A:667:ASP:OD1	1:A:777:LYS:HE2	1.97	0.64
1:B:254:ILE:HG23	1:B:255:LYS:H	1.61	0.64
1:B:135:SER:OG	1:B:154:LEU:HD21	1.98	0.64
1:B:110:SER:O	1:B:114:VAL:HG23	1.97	0.64
1:B:270:GLU:HA	1:B:275:ILE:HG22	1.79	0.64
1:B:233:LEU:HB2	1:B:289:HIS:CE1	2.34	0.63
1:B:379:GLU:HG2	1:B:383:ASN:HD22	1.63	0.63
1:B:246:ALA:HB1	1:B:268:LYS:HZ1	1.63	0.63
1:A:471:ILE:HG21	1:A:491:THR:HB	1.81	0.63
1:A:637:ARG:HE	1:A:769:ASP:HB2	1.63	0.63
1:A:654:LEU:CD1	1:A:657:LEU:HB3	2.28	0.63
1:B:325:LYS:N	1:B:741:ARG:HD3	2.13	0.63
1:B:377:GLU:HG2	1:B:517:ARG:HD3	1.81	0.63
1:B:380:GLU:CD	1:B:593:ARG:HH12	2.02	0.63
1:A:645:ARG:O	1:A:646:GLU:HG3	1.98	0.63
1:B:238:ASN:HD21	1:B:340:LYS:HA	1.63	0.63
1:A:249:ASP:HB2	1:A:260:GLN:HG2	1.78	0.63
1:A:410:THR:HG21	1:B:462:LYS:HE3	1.81	0.63
1:A:627:VAL:HA	1:A:630:MET:SD	2.39	0.63
1:A:5:LEU:HD22	1:A:5:LEU:H	1.63	0.63
1:A:206:ILE:HD12	1:A:206:ILE:H	1.61	0.63
1:B:723:LYS:HE2	1:B:763:MET:HG2	1.80	0.63
1:A:645:ARG:HG3	1:A:657:LEU:HD13	1.80	0.63
1:A:626:ILE:HG23	1:A:711:PHE:HD1	1.59	0.63
1:B:238:ASN:OD1	1:B:297:HIS:HE1	1.81	0.63
1:B:307:VAL:HG21	1:B:316:VAL:HG21	1.81	0.63
1:A:640:ALA:O	1:A:644:PRO:CD	2.47	0.62
1:A:106:LYS:HD3	1:A:370:MET:HB3	1.81	0.62
1:B:254:ILE:HG23	1:B:255:LYS:N	2.14	0.62
1:A:547:ARG:O	1:B:219:THR:HG22	1.99	0.62
1:B:261:LEU:C	1:B:261:LEU:CD1	2.67	0.62
1:A:261:LEU:HD23	1:A:266:MET:HG2	1.82	0.62
1:B:627:VAL:O	1:B:631:ILE:N	2.28	0.62
1:B:421:ASP:OD1	1:B:425:ARG:NH1	2.32	0.62
1:A:255:LYS:NZ	1:A:762:HIS:HE1	1.98	0.62
1:B:354:THR:HG21	1:B:735:ARG:HH12	1.65	0.62
1:A:420:GLU:O	1:A:424:GLN:HG3	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:190:VAL:HG22	1:B:195:GLN:CG	2.29	0.62
1:B:512:ARG:HG2	1:B:539:LEU:HD21	1.80	0.62
1:B:185:LEU:HD22	1:B:353:ALA:HB1	1.80	0.62
1:B:676:ILE:HG12	1:B:684:MET:HG2	1.80	0.62
1:B:354:THR:HG21	1:B:735:ARG:NH2	2.13	0.62
1:B:723:LYS:CB	1:B:763:MET:HG3	2.30	0.62
1:A:324:MET:HA	1:A:740:LEU:HD13	1.82	0.62
1:B:250:TYR:O	1:B:251:THR:HB	1.99	0.61
1:B:213:LEU:O	1:B:217:ALA:HB2	2.00	0.61
1:B:624:ARG:CZ	1:B:700:GLU:HG2	2.30	0.61
1:A:558:LEU:HG	1:A:563:MET:HE3	1.75	0.61
1:B:74:ARG:HH11	1:B:74:ARG:HG3	1.64	0.61
1:A:281:VAL:O	1:A:281:VAL:CG1	2.49	0.61
1:B:640:ALA:O	1:B:644:PRO:HD3	2.01	0.61
1:B:732:ASP:O	1:B:735:ARG:HB3	2.01	0.61
1:A:686:GLU:HG2	1:A:687:LEU:N	2.14	0.61
1:B:723:LYS:HG2	1:B:767:ILE:HG12	1.83	0.61
1:B:191:LEU:HD21	1:B:716:VAL:HG11	1.82	0.61
1:B:711:PHE:O	1:B:715:ILE:CG1	2.49	0.61
1:A:426:TYR:CD2	1:A:426:TYR:C	2.73	0.61
1:A:406:LEU:HG	1:A:536:GLN:NE2	2.15	0.61
1:B:760:PHE:CD1	1:B:763:MET:HE1	2.36	0.61
1:A:254:ILE:HG22	1:A:255:LYS:HG3	1.81	0.61
1:A:255:LYS:O	1:A:256:THR:HB	2.00	0.61
1:B:317:ASP:HB3	1:B:320:THR:HG23	1.83	0.61
1:B:238:ASN:ND2	1:B:340:LYS:HD2	2.15	0.60
1:A:541:MET:SD	1:A:561:PHE:HZ	2.25	0.60
1:A:404:PRO:O	1:A:536:GLN:NE2	2.34	0.60
1:A:288:HIS:O	1:A:292:GLN:HG2	2.00	0.60
1:A:610:ILE:HD12	1:A:723:LYS:NZ	2.17	0.60
1:B:718:ARG:HG3	1:B:770:GLU:OE1	2.01	0.60
1:A:259:VAL:HG21	1:A:769:ASP:OD2	1.99	0.60
1:A:217:ALA:HB1	1:A:358:GLN:HE21	1.66	0.60
1:A:312:GLN:NE2	1:B:572:LYS:HD3	2.17	0.60
1:A:724:TRP:HA	1:A:724:TRP:HE3	1.66	0.60
1:A:270:GLU:O	1:A:274:GLY:N	2.33	0.60
1:B:645:ARG:HG3	1:B:657:LEU:HB2	1.84	0.60
1:A:700:GLU:O	1:A:704:GLY:CA	2.48	0.60
1:A:418:VAL:O	1:A:422:VAL:HG23	2.02	0.60
1:B:243:THR:O	1:B:244:LEU:HD23	2.01	0.60
1:B:102:THR:HB	1:B:524:GLY:O	2.02	0.60
1:B:218:ARG:HD3	1:B:592:SER:CB	2.26	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:713:LYS:O	1:B:717:LEU:CB	2.49	0.60
1:B:494:LYS:H	1:B:494:LYS:HD3	1.65	0.60
1:B:288:HIS:O	1:B:292:GLN:HG2	2.01	0.60
1:A:723:LYS:HG2	1:A:767:ILE:HD11	1.84	0.60
1:A:661:ILE:CG2	1:A:666:LEU:CD2	2.65	0.60
1:A:747:ASN:H	1:A:748:PRO:HD2	0.51	0.60
1:A:646:GLU:HA	1:A:651:GLU:HA	1.84	0.60
1:A:142:GLY:O	1:A:146:GLU:HG3	2.02	0.60
1:B:627:VAL:HG12	1:B:631:ILE:HG13	1.84	0.60
1:B:627:VAL:HG22	1:B:711:PHE:HZ	1.66	0.60
1:A:325:LYS:HB2	1:A:740:LEU:HB3	1.82	0.59
1:A:401:ASP:OD2	1:A:403:ARG:HD3	2.02	0.59
1:A:284:VAL:HG13	1:A:718:ARG:HH21	1.67	0.59
1:A:255:LYS:NZ	1:A:762:HIS:CE1	2.69	0.59
1:A:560:ARG:O	1:A:561:PHE:CG	2.55	0.59
1:B:297:HIS:CE1	1:B:340:LYS:HB3	2.37	0.59
1:B:463:ASN:C	1:B:463:ASN:HD22	2.05	0.59
1:B:19:TYR:HE1	1:B:390:VAL:HG11	1.68	0.59
1:B:248:LYS:NZ	1:B:268:LYS:HD2	2.17	0.59
1:B:624:ARG:HH21	1:B:707:GLN:HB2	1.59	0.59
1:B:617:VAL:HG12	1:B:617:VAL:O	2.02	0.59
1:A:249:ASP:HB3	1:A:260:GLN:O	2.02	0.59
1:A:529:GLN:HA	1:A:529:GLN:OE1	2.00	0.59
1:A:554:THR:HG21	1:A:557:MET:O	2.02	0.59
1:A:358:GLN:HG3	1:A:385:TYR:OH	2.02	0.59
1:A:406:LEU:HD23	1:A:570:GLN:HE21	1.66	0.59
1:B:300:MET:HG3	1:B:337:ILE:HD11	1.84	0.59
1:B:442:SER:O	1:B:446:SER:HB3	2.03	0.59
1:B:187:ASP:OD1	1:B:196:MET:HA	2.02	0.59
1:A:374:ALA:O	1:A:389:VAL:HG21	2.02	0.59
1:B:417:ALA:HA	1:B:420:GLU:HB3	1.84	0.59
1:A:278:LEU:CD1	1:A:286:LEU:HB2	2.32	0.59
1:A:684:MET:SD	1:A:684:MET:N	2.75	0.59
1:A:592:SER:O	1:A:595:GLN:HG2	2.03	0.59
1:B:614:ARG:NH1	1:B:720:VAL:HG23	2.14	0.59
1:B:686:GLU:OE1	1:B:686:GLU:HA	2.02	0.59
1:A:83:LYS:HA	1:A:86:LEU:HD12	1.85	0.59
1:B:244:LEU:HD22	1:B:248:LYS:HE3	1.84	0.58
1:A:328:ARG:NH1	1:A:328:ARG:HG2	2.14	0.58
1:A:626:ILE:O	1:A:630:MET:HB3	2.04	0.58
1:A:647:GLU:HG3	1:A:648:LEU:N	2.18	0.58
1:B:483:ALA:HB1	1:B:487:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:695:LYS:HD3	1:B:776:MET:HE3	1.83	0.58
1:B:206:ILE:CG2	1:B:209:VAL:HA	2.34	0.58
1:A:279:PHE:HD1	1:A:778:ALA:O	1.83	0.58
1:B:88:GLY:HA3	1:B:109:THR:HG21	1.86	0.58
1:B:245:LYS:CE	1:B:247:GLU:CD	2.69	0.58
1:A:764:ILE:O	1:A:768:GLU:HG3	2.03	0.58
1:B:703:PHE:CZ	1:B:707:GLN:NE2	2.71	0.58
1:B:476:GLN:HE22	1:B:494:LYS:NZ	2.00	0.58
1:B:100:MET:O	1:B:372:GLY:HA2	2.04	0.58
1:B:676:ILE:CG1	1:B:684:MET:HG2	2.34	0.58
1:B:87:MET:HA	1:B:90:VAL:HG12	1.86	0.58
1:A:257:LYS:NZ	1:A:660:LEU:HD12	2.18	0.58
1:A:510:THR:O	1:A:511:GLU:HB3	2.04	0.58
1:B:703:PHE:CG	1:B:703:PHE:O	2.57	0.58
1:A:626:ILE:CG2	1:A:711:PHE:CD1	2.81	0.58
1:B:741:ARG:HG3	1:B:742:ALA:N	2.17	0.58
1:B:460:ASN:ND2	1:B:462:LYS:HB2	2.19	0.57
1:B:302:LYS:O	1:B:302:LYS:HG3	2.04	0.57
1:A:279:PHE:HD1	1:A:778:ALA:C	2.07	0.57
1:A:610:ILE:HG21	1:A:723:LYS:HE2	1.85	0.57
1:A:426:TYR:C	1:A:426:TYR:HD2	2.08	0.57
1:A:5:LEU:CB	1:A:383:ASN:OD1	2.49	0.57
1:A:324:MET:HB3	1:A:327:ARG:HD2	1.86	0.57
1:A:561:PHE:C	1:A:561:PHE:CD1	2.77	0.57
1:B:718:ARG:HD2	1:B:722:SER:HB3	1.87	0.57
1:B:647:GLU:HB3	1:B:652:TRP:CH2	2.39	0.57
1:B:766:SER:O	1:B:769:ASP:OD1	2.21	0.57
1:A:561:PHE:O	1:A:561:PHE:CD1	2.57	0.57
1:A:649:PRO:O	1:A:650:GLU:HG3	2.04	0.57
1:A:723:LYS:HG3	1:A:724:TRP:N	2.20	0.57
1:B:307:VAL:CG2	1:B:316:VAL:HG21	2.35	0.57
1:B:152:VAL:HG13	1:B:172:ILE:CG2	2.34	0.56
1:A:301:GLN:O	1:A:306:TYR:HB2	2.05	0.56
1:B:168:TYR:CD1	1:B:197:VAL:HG12	2.39	0.56
1:A:329:TYR:HB3	1:A:333:LEU:HB2	1.86	0.56
1:A:637:ARG:NH2	1:A:769:ASP:HB2	2.20	0.56
1:B:696:TYR:OH	1:B:711:PHE:CE2	2.58	0.56
1:B:430:GLN:HG2	1:B:504:GLY:O	2.06	0.56
1:A:300:MET:SD	1:A:306:TYR:HE2	2.28	0.56
1:B:102:THR:HA	1:B:106:LYS:HZ3	1.70	0.56
1:B:403:ARG:HB3	1:B:536:GLN:OE1	2.05	0.56
1:A:668:GLU:C	1:A:670:ALA:H	2.09	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:VAL:CG1	1:A:192:TYR:O	2.53	0.56
1:A:747:ASN:O	1:A:750:ARG:HB2	2.05	0.56
1:B:249:ASP:H	1:B:261:LEU:HB2	1.70	0.56
1:A:358:GLN:CG	1:A:385:TYR:OH	2.54	0.56
1:B:27:ASP:O	1:B:30:ARG:HB3	2.04	0.56
1:A:610:ILE:CD1	1:A:723:LYS:HZ2	2.17	0.56
1:B:221:LEU:HD11	1:B:357:PHE:CE2	2.40	0.56
1:A:647:GLU:HG3	1:A:648:LEU:H	1.70	0.56
1:B:250:TYR:CE2	1:B:659:ASP:HB3	2.37	0.56
1:B:695:LYS:HD3	1:B:776:MET:HE1	1.86	0.56
1:A:438:ALA:HB1	1:A:440:GLU:OE1	2.06	0.56
1:B:723:LYS:HB2	1:B:763:MET:SD	2.46	0.56
1:B:626:ILE:O	1:B:627:VAL:C	2.44	0.56
1:B:233:LEU:HB3	1:B:289:HIS:ND1	2.19	0.56
1:A:348:GLU:OE1	1:B:573:MET:SD	2.63	0.56
1:A:512:ARG:HD2	1:A:519:ASP:OD1	2.05	0.56
1:A:426:TYR:HD1	1:A:454:ILE:HG23	1.68	0.56
1:B:642:TYR:O	1:B:646:GLU:HG3	2.06	0.56
1:B:637:ARG:NE	1:B:769:ASP:HA	2.19	0.55
1:A:279:PHE:CD1	1:A:778:ALA:C	2.80	0.55
1:B:17:ASN:O	1:B:20:GLU:HB2	2.06	0.55
1:A:373:THR:O	1:A:517:ARG:HD2	2.06	0.55
1:A:734:LEU:O	1:A:738:ILE:HB	2.06	0.55
1:A:270:GLU:OE2	1:A:278:LEU:HD21	2.07	0.55
1:B:626:ILE:HG23	1:B:715:ILE:CD1	2.36	0.55
1:B:252:TYR:HE2	1:B:254:ILE:HG22	1.71	0.55
1:A:641:ALA:HB1	1:A:660:LEU:HD11	1.87	0.55
1:B:16:LEU:H	1:B:16:LEU:HD22	1.72	0.55
1:A:300:MET:SD	1:A:306:TYR:CD2	2.99	0.55
1:A:626:ILE:HG21	1:A:711:PHE:HD1	1.71	0.55
1:A:541:MET:SD	1:A:561:PHE:CZ	3.00	0.55
1:A:43:HIS:HA	1:A:46:ILE:HD12	1.89	0.55
1:A:672:GLU:O	1:A:673:LYS:C	2.45	0.55
1:A:552:GLU:H	1:A:560:ARG:HH12	1.54	0.55
1:A:337:ILE:HD12	1:A:346:GLN:CD	2.27	0.55
1:B:720:VAL:CG1	1:B:721:ASP:N	2.69	0.55
1:B:315:ILE:HG13	1:B:327:ARG:HB2	1.88	0.55
1:A:561:PHE:O	1:A:569:ILE:CG1	2.53	0.55
1:B:354:THR:HG21	1:B:735:ARG:NH1	2.21	0.55
1:A:356:THR:HB	1:A:358:GLN:OE1	2.07	0.55
1:A:736:GLN:O	1:A:737:GLY:C	2.43	0.55
1:A:606:GLN:NE2	1:A:760:PHE:HB2	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:624:ARG:NH1	1:B:700:GLU:HG2	2.22	0.54
1:B:711:PHE:O	1:B:715:ILE:CD1	2.55	0.54
1:A:301:GLN:O	1:A:306:TYR:CB	2.55	0.54
1:A:160:SER:C	1:A:162:ASP:H	2.09	0.54
1:B:647:GLU:O	1:B:652:TRP:CZ2	2.59	0.54
1:A:337:ILE:HG22	1:A:344:GLU:O	2.07	0.54
1:A:650:GLU:HB3	1:A:652:TRP:HB2	1.89	0.54
1:A:440:GLU:HB3	1:B:411:MET:HE1	1.88	0.54
1:B:646:GLU:OE1	1:B:681:PRO:HG3	2.08	0.54
1:B:706:GLU:O	1:B:709:ARG:CB	2.55	0.54
1:B:230:SER:C	1:B:232:LYS:H	2.10	0.54
1:B:614:ARG:HH12	1:B:720:VAL:HG22	1.69	0.54
1:B:344:GLU:O	1:B:344:GLU:CG	2.56	0.54
1:B:92:LEU:HB2	1:B:113:PRO:HG3	1.89	0.54
1:B:610:ILE:HG13	1:B:724:TRP:CZ3	2.42	0.54
1:A:279:PHE:CD1	1:A:779:GLU:HA	2.40	0.54
1:A:606:GLN:HG2	1:A:760:PHE:CE1	2.43	0.54
1:A:625:GLU:O	1:A:629:ASN:ND2	2.40	0.54
1:B:595:GLN:HE22	1:B:739:HIS:CE1	2.25	0.54
1:B:650:GLU:OE1	1:B:651:GLU:N	2.37	0.54
1:B:325:LYS:H	1:B:741:ARG:CD	2.20	0.54
1:A:50:GLU:O	1:A:54:LYS:HG3	2.07	0.54
1:B:723:LYS:O	1:B:727:HIS:HB2	2.07	0.54
1:B:217:ALA:HB1	1:B:358:GLN:NE2	2.20	0.54
1:A:723:LYS:CG	1:A:767:ILE:HD11	2.38	0.54
1:B:718:ARG:NH1	1:B:770:GLU:OE1	2.35	0.54
1:B:642:TYR:CD2	1:B:642:TYR:N	2.73	0.54
1:B:231:THR:HB	1:B:348:GLU:HG3	1.88	0.54
1:B:177:ASN:HD22	1:B:212:ILE:HG23	1.73	0.54
1:B:476:GLN:NE2	1:B:494:LYS:NZ	2.56	0.54
1:A:606:GLN:HE21	1:A:760:PHE:HB2	1.72	0.54
1:B:595:GLN:HE22	1:B:739:HIS:HE1	1.56	0.54
1:A:676:ILE:O	1:A:676:ILE:HG22	2.08	0.54
1:B:718:ARG:HD2	1:B:722:SER:CB	2.38	0.54
1:B:760:PHE:CE1	1:B:763:MET:HE1	2.43	0.54
1:B:238:ASN:HD21	1:B:340:LYS:CA	2.21	0.54
1:B:447:LYS:HD3	1:B:450:LYS:HE3	1.90	0.54
1:A:604:ARG:O	1:A:608:GLU:HG2	2.08	0.54
1:A:322:ARG:NH1	1:A:743:TYR:HE1	2.06	0.54
1:B:209:VAL:HG13	1:B:210:ASP:N	2.22	0.54
1:B:652:TRP:HB2	1:B:654:LEU:HG	1.89	0.53
1:B:523:ARG:HB3	1:B:535:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:541:MET:HE1	1:B:559:ASP:OD2	2.07	0.53
1:A:671:LEU:HD11	1:A:674:SER:HA	1.90	0.53
1:A:695:LYS:O	1:A:698:GLU:HG2	2.08	0.53
1:A:548:ARG:HH12	1:B:735:ARG:HD3	1.73	0.53
1:B:494:LYS:HD3	1:B:494:LYS:N	2.21	0.53
1:A:459:LEU:HD22	1:A:467:GLU:HB3	1.89	0.53
1:B:610:ILE:HG13	1:B:724:TRP:CE3	2.44	0.53
1:A:284:VAL:CG1	1:A:718:ARG:HH21	2.21	0.53
1:A:105:GLY:HA2	2:A:781:ADP:PA	2.48	0.53
1:A:302:LYS:HG2	1:A:303:ASP:N	2.23	0.53
1:A:259:VAL:HA	1:A:291:ASN:OD1	2.08	0.53
1:A:252:TYR:CD2	1:A:257:LYS:O	2.62	0.53
1:A:610:ILE:CD1	1:A:723:LYS:NZ	2.71	0.53
1:B:244:LEU:HD22	1:B:248:LYS:CE	2.39	0.53
1:B:248:LYS:NZ	1:B:268:LYS:CB	2.70	0.53
1:B:336:ALA:O	1:B:340:LYS:CD	2.53	0.53
1:B:647:GLU:HA	1:B:647:GLU:OE1	2.09	0.53
1:A:127:VAL:HB	1:A:206:ILE:HA	1.91	0.53
1:B:206:ILE:HG22	1:B:209:VAL:HA	1.91	0.53
1:B:210:ASP:OD1	1:B:371:THR:HG21	2.09	0.53
1:B:199:ARG:HB3	1:B:200:PRO:HD3	1.90	0.53
1:A:206:ILE:CG2	1:A:212:ILE:HD12	2.39	0.52
1:A:630:MET:O	1:A:634:SER:OG	2.25	0.52
1:B:447:LYS:HB3	1:B:450:LYS:HG3	1.90	0.52
1:A:279:PHE:CD1	1:A:779:GLU:CA	2.89	0.52
1:B:221:LEU:O	1:B:354:THR:HA	2.09	0.52
1:A:93:HIS:CD2	1:A:116:LEU:HD23	2.45	0.52
1:A:210:ASP:OD2	1:A:371:THR:CG2	2.57	0.52
1:A:576:ARG:HE	1:B:312:GLN:HE21	1.56	0.52
1:B:434:VAL:HB	1:B:482:ILE:HG13	1.92	0.52
1:A:637:ARG:HH21	1:A:769:ASP:HB2	1.75	0.52
1:A:644:PRO:C	1:A:646:GLU:H	2.13	0.52
1:A:317:ASP:CB	1:A:320:THR:HG22	2.34	0.52
1:B:522:LEU:O	1:B:525:ARG:CG	2.55	0.52
1:A:686:GLU:OE2	1:A:687:LEU:HG	2.10	0.52
1:A:27:ASP:O	1:A:30:ARG:HB3	2.10	0.52
1:A:5:LEU:HD23	1:A:5:LEU:H	1.75	0.52
1:A:637:ARG:CZ	1:A:769:ASP:HB2	2.40	0.52
1:A:407:ILE:HB	1:A:569:ILE:HG22	1.92	0.52
1:B:322:ARG:HG3	1:B:742:ALA:HB3	1.92	0.52
1:A:91:ALA:O	1:A:96:ASN:HB2	2.10	0.52
1:A:643:THR:N	1:A:644:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:GLN:NE2	1:A:470:ILE:HD12	2.10	0.51
1:B:612:LYS:O	1:B:613:GLN:C	2.48	0.51
1:B:625:GLU:O	1:B:625:GLU:CG	2.42	0.51
1:A:283:HIS:O	1:A:284:VAL:C	2.48	0.51
1:B:418:VAL:O	1:B:422:VAL:CG2	2.51	0.51
1:A:221:LEU:O	1:A:354:THR:HA	2.10	0.51
1:A:206:ILE:N	1:A:206:ILE:HD12	2.24	0.51
1:B:246:ALA:CB	1:B:268:LYS:HZ2	2.24	0.51
1:B:13:LYS:HA	1:B:16:LEU:HD21	1.93	0.51
1:B:39:ASP:HA	1:B:42:LYS:CB	2.39	0.51
1:B:539:LEU:HD13	1:B:546:MET:HE1	1.93	0.51
1:A:436:THR:HG22	1:A:438:ALA:H	1.75	0.51
1:B:718:ARG:HG3	1:B:718:ARG:HH11	1.76	0.51
1:A:654:LEU:CD2	1:A:677:PHE:CE2	2.94	0.51
1:B:642:TYR:CE1	1:B:685:LEU:HA	2.42	0.51
1:B:325:LYS:O	1:B:741:ARG:NH1	2.43	0.51
1:B:233:LEU:HB2	1:B:289:HIS:HE1	1.73	0.51
1:B:371:THR:HG22	1:B:372:GLY:N	2.26	0.51
1:A:741:ARG:NH2	1:B:376:THR:HG22	2.21	0.51
1:A:411:MET:HG2	1:A:542:GLU:OE2	2.10	0.51
1:B:199:ARG:CB	1:B:200:PRO:CD	2.88	0.51
1:B:512:ARG:HG2	1:B:539:LEU:CD2	2.41	0.51
1:B:710:GLU:O	1:B:714:VAL:HG23	2.11	0.51
1:B:239:ALA:HA	1:B:242:ARG:NH1	2.25	0.51
1:B:718:ARG:CD	1:B:722:SER:HB3	2.39	0.51
1:A:327:ARG:HH21	1:A:755:GLU:HG2	1.76	0.51
1:B:344:GLU:O	1:B:345:ILE:C	2.48	0.51
1:A:522:LEU:O	1:A:525:ARG:HG3	2.11	0.51
1:A:278:LEU:HB3	1:A:283:HIS:CD2	2.41	0.51
1:A:255:LYS:HZ2	1:A:762:HIS:CE1	2.29	0.51
1:A:680:GLU:O	1:A:684:MET:SD	2.69	0.51
1:B:639:ILE:HG22	1:B:640:ALA:N	2.26	0.51
1:A:279:PHE:HD1	1:A:779:GLU:N	2.09	0.51
1:B:400:ARG:HD3	1:B:526:SER:O	2.10	0.51
1:B:250:TYR:CE1	1:B:261:LEU:HA	2.45	0.50
1:B:344:GLU:O	1:B:344:GLU:HG2	2.11	0.50
1:B:42:LYS:HE3	1:B:149:GLY:HA3	1.92	0.50
1:B:647:GLU:N	1:B:652:TRP:CZ2	2.78	0.50
1:A:562:GLY:HA2	1:A:569:ILE:CG1	2.39	0.50
1:A:247:GLU:O	1:A:249:ASP:N	2.44	0.50
1:B:610:ILE:HD12	1:B:723:LYS:NZ	2.26	0.50
1:A:251:THR:OG1	1:A:252:TYR:N	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:LYS:O	1:B:196:MET:HG3	2.11	0.50
1:B:101:LYS:O	1:B:104:GLU:HB2	2.10	0.50
1:B:69:VAL:O	1:B:73:SER:HB2	2.12	0.50
1:B:637:ARG:HB3	1:B:665:TYR:HH	1.74	0.50
1:B:549:PHE:CD2	1:B:549:PHE:N	2.79	0.50
1:B:666:LEU:HD21	1:B:692:ILE:HG13	1.94	0.50
1:A:100:MET:HG2	1:A:392:ILE:HB	1.92	0.50
1:A:548:ARG:NH1	1:B:735:ARG:HD3	2.26	0.50
1:B:215:ASP:OD1	1:B:517:ARG:NH2	2.45	0.50
1:B:190:VAL:CG2	1:B:195:GLN:HG3	2.38	0.50
1:A:689:MET:O	1:A:693:ILE:HG22	2.12	0.50
1:B:48:PHE:HE1	1:B:68:VAL:HG21	1.75	0.50
1:B:249:ASP:N	1:B:261:LEU:HB2	2.27	0.50
1:B:240:PHE:O	1:B:244:LEU:HD21	2.12	0.50
1:A:559:ASP:O	1:A:563:MET:HE2	2.11	0.50
1:B:380:GLU:CD	1:B:593:ARG:NH1	2.64	0.50
1:A:475:GLY:O	1:A:495:LEU:HA	2.11	0.50
1:A:588:ASN:OD1	1:B:588:ASN:HB3	2.12	0.50
1:B:642:TYR:HE1	1:B:685:LEU:CA	2.23	0.50
1:A:442:SER:HA	1:A:482:ILE:HD11	1.93	0.50
1:A:769:ASP:O	1:A:770:GLU:C	2.50	0.49
1:A:210:ASP:N	1:A:210:ASP:OD2	2.40	0.49
1:B:371:THR:HG22	1:B:373:THR:H	1.77	0.49
1:A:3:GLY:O	1:A:4:ILE:HG13	2.12	0.49
1:A:107:THR:HG22	1:A:141:MET:SD	2.52	0.49
1:A:486:MET:HG3	1:A:486:MET:O	2.12	0.49
1:B:432:VAL:HG13	1:B:506:ALA:HB3	1.93	0.49
1:B:261:LEU:HD13	1:B:261:LEU:O	2.13	0.49
1:B:484:THR:O	1:B:486:MET:N	2.45	0.49
1:A:232:LYS:CD	1:A:232:LYS:H	2.19	0.49
1:B:647:GLU:N	1:B:652:TRP:CZ3	2.76	0.49
1:A:190:VAL:HG13	1:A:195:GLN:HB2	1.94	0.49
1:B:248:LYS:O	1:B:248:LYS:HG3	2.13	0.49
1:A:243:THR:O	1:A:243:THR:CG2	2.55	0.49
1:B:233:LEU:CB	1:B:289:HIS:CE1	2.95	0.49
1:B:637:ARG:NE	1:B:769:ASP:CB	2.55	0.49
1:B:275:ILE:CD1	1:B:283:HIS:CD2	2.83	0.49
1:B:347:ASN:O	1:B:348:GLU:CD	2.51	0.49
1:B:637:ARG:NE	1:B:769:ASP:CA	2.70	0.49
1:A:301:GLN:HB2	1:A:306:TYR:CE1	2.48	0.49
1:A:279:PHE:C	1:A:778:ALA:HB1	2.33	0.49
1:A:647:GLU:CG	1:A:649:PRO:HD2	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:324:MET:CB	1:A:327:ARG:HD2	2.43	0.49
1:B:199:ARG:CB	1:B:200:PRO:HD3	2.42	0.49
1:A:7:LYS:O	1:B:743:TYR:CD2	2.66	0.49
1:B:620:SER:OG	1:B:625:GLU:HG2	2.14	0.48
1:B:445:ILE:O	1:B:447:LYS:N	2.45	0.48
1:B:284:VAL:HG12	1:B:718:ARG:NH2	2.28	0.48
1:B:400:ARG:HD2	1:B:535:THR:CG2	2.42	0.48
1:B:673:LYS:HA	1:B:676:ILE:HG22	1.94	0.48
1:B:48:PHE:CE1	1:B:68:VAL:HG21	2.49	0.48
1:B:261:LEU:C	1:B:261:LEU:HD13	2.34	0.48
1:B:246:ALA:CB	1:B:268:LYS:NZ	2.75	0.48
1:A:379:GLU:O	1:A:383:ASN:HB3	2.13	0.48
1:A:177:ASN:N	1:A:177:ASN:OD1	2.46	0.48
1:A:89:GLY:HA2	1:A:92:LEU:HD12	1.95	0.48
1:B:185:LEU:HD22	1:B:353:ALA:CB	2.44	0.48
1:A:257:LYS:HZ3	1:A:660:LEU:HD12	1.78	0.48
1:A:624:ARG:HG2	1:A:627:VAL:HB	1.95	0.48
1:B:708:MET:HA	1:B:711:PHE:HB2	1.96	0.48
1:B:539:LEU:HD13	1:B:546:MET:CE	2.42	0.48
1:A:637:ARG:HG2	1:A:769:ASP:HA	1.94	0.48
1:A:513:HIS:CE1	1:A:518:ILE:HG22	2.49	0.48
1:A:82:PHE:CE1	2:A:781:ADP:N6	2.82	0.48
1:A:688:ILE:HG12	1:A:692:ILE:HD12	1.96	0.48
1:B:624:ARG:NH2	1:B:707:GLN:HB2	2.23	0.48
1:A:270:GLU:CD	1:A:278:LEU:HD21	2.33	0.48
1:A:645:ARG:O	1:A:646:GLU:CG	2.62	0.48
1:A:249:ASP:CB	1:A:260:GLN:O	2.62	0.48
1:B:616:GLU:OE1	1:B:616:GLU:HA	2.14	0.48
1:B:649:PRO:O	1:B:652:TRP:CZ3	2.67	0.48
1:B:340:LYS:N	1:B:340:LYS:CD	2.77	0.48
1:A:610:ILE:HD12	1:A:723:LYS:HZ1	1.78	0.48
1:B:637:ARG:O	1:B:638:ALA:C	2.52	0.48
1:A:284:VAL:HG11	1:A:717:LEU:HD11	1.95	0.48
1:B:626:ILE:HG23	1:B:715:ILE:HD11	1.93	0.48
1:A:576:ARG:HH22	1:B:346:GLN:NE2	2.11	0.48
1:A:414:LYS:HD3	1:A:540:SER:N	2.28	0.48
1:A:662:ASN:HB3	1:A:670:ALA:CB	2.42	0.47
1:A:322:ARG:NH1	1:A:743:TYR:CE1	2.81	0.47
1:B:572:LYS:O	1:B:575:SER:HB3	2.13	0.47
1:B:500:LYS:HE2	1:B:500:LYS:H	1.78	0.47
1:B:245:LYS:C	1:B:247:GLU:H	2.17	0.47
1:B:624:ARG:NH2	1:B:700:GLU:HG2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:PHE:HB2	1:A:779:GLU:N	2.30	0.47
1:B:617:VAL:HG11	1:B:716:VAL:CG2	2.45	0.47
1:A:380:GLU:OE1	1:A:593:ARG:NH1	2.46	0.47
1:A:10:ASP:HB3	1:A:11:PRO:HD2	0.68	0.47
1:A:203:PHE:CD2	1:A:204:ALA:N	2.82	0.47
1:A:549:PHE:CD2	1:A:561:PHE:HE2	2.32	0.47
1:A:324:MET:HG3	1:A:327:ARG:NH1	2.29	0.47
1:A:209:VAL:HG12	1:A:371:THR:HG22	1.95	0.47
1:B:248:LYS:HD2	1:B:265:GLY:CA	2.39	0.47
1:B:750:ARG:CG	1:B:750:ARG:NH1	2.56	0.47
1:B:627:VAL:HG13	1:B:696:TYR:CZ	2.49	0.47
1:A:382:ARG:HG3	1:A:382:ARG:O	2.14	0.47
1:B:484:THR:HG22	1:B:485:ASN:OD1	2.14	0.47
1:B:770:GLU:O	1:B:771:VAL:C	2.52	0.47
1:B:262:THR:O	1:B:264:GLU:N	2.48	0.47
1:B:548:ARG:HG3	1:B:549:PHE:H	1.80	0.47
1:B:679:LYS:HB3	1:B:683:GLU:HG3	1.97	0.47
1:A:738:ILE:HD11	1:A:743:TYR:HE2	1.80	0.47
1:A:194:GLU:HG3	1:A:195:GLN:H	1.77	0.47
1:B:248:LYS:HA	1:B:261:LEU:CB	2.45	0.47
1:B:262:THR:OG1	1:B:668:GLU:CD	2.53	0.47
1:A:554:THR:CG2	1:A:555:MET:N	2.78	0.47
1:A:360:TYR:O	1:A:363:MET:HG3	2.14	0.47
1:A:293:ALA:O	1:A:297:HIS:HD2	1.97	0.47
1:B:248:LYS:HZ3	1:B:268:LYS:HD2	1.79	0.47
1:A:226:GLN:NE2	1:A:228:ALA:HB2	2.30	0.47
1:A:647:GLU:CG	1:A:648:LEU:H	2.28	0.47
1:B:485:ASN:OD1	1:B:486:MET:HG2	2.14	0.47
1:A:662:ASN:O	1:A:777:LYS:NZ	2.47	0.46
1:B:708:MET:HA	1:B:711:PHE:CD1	2.50	0.46
1:B:74:ARG:NH1	1:B:74:ARG:HG3	2.29	0.46
1:B:88:GLY:HA3	1:B:109:THR:CG2	2.45	0.46
1:A:302:LYS:HG2	1:A:303:ASP:HB2	1.98	0.46
1:A:672:GLU:C	1:A:673:LYS:HG2	2.35	0.46
1:A:338:GLU:CG	1:A:345:ILE:HG13	2.35	0.46
1:B:229:LYS:HD3	1:B:289:HIS:CD2	2.50	0.46
1:B:307:VAL:CG1	1:B:308:VAL:H	2.28	0.46
1:B:302:LYS:HD3	1:B:341:GLU:CD	2.35	0.46
1:B:554:THR:HG21	1:B:574:VAL:HA	1.97	0.46
1:B:256:THR:CG2	1:B:295:LYS:HD2	2.42	0.46
1:A:706:GLU:O	1:A:709:ARG:N	2.49	0.46
1:B:39:ASP:OD2	1:B:42:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:611:TYR:O	1:B:614:ARG:HG2	2.16	0.46
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.25	0.46
1:A:600:ASP:O	1:A:604:ARG:N	2.36	0.46
1:A:9:PHE:HD2	1:A:10:ASP:N	2.09	0.46
1:B:238:ASN:HD21	1:B:340:LYS:HD2	1.79	0.46
1:B:403:ARG:HG2	1:B:404:PRO:HD2	1.96	0.46
1:A:123:GLY:HA2	1:A:171:ASP:O	2.16	0.46
1:A:84:VAL:HG21	1:A:395:ASN:HB2	1.97	0.46
1:B:279:PHE:HZ	1:B:773:LYS:HE2	1.80	0.46
1:A:463:ASN:O	1:A:467:GLU:HG3	2.15	0.46
1:A:439:VAL:HG23	1:B:411:MET:CE	2.46	0.46
1:A:513:HIS:ND1	1:A:519:ASP:OD2	2.49	0.46
1:A:739:HIS:HB3	1:B:583:LYS:HD2	1.98	0.46
1:A:160:SER:C	1:A:162:ASP:N	2.69	0.46
1:A:164:LYS:NZ	1:A:183:ASP:OD1	2.48	0.46
1:A:745:GLN:NE2	1:B:584:ARG:HA	2.31	0.46
1:B:414:LYS:NZ	1:B:510:THR:O	2.29	0.46
1:B:324:MET:HA	1:B:741:ARG:CD	2.37	0.46
1:B:376:THR:C	1:B:378:GLU:H	2.19	0.46
1:B:406:LEU:HD12	1:B:538:TYR:CE1	2.51	0.46
1:A:552:GLU:O	1:A:560:ARG:NH1	2.48	0.46
1:A:226:GLN:NE2	1:A:228:ALA:CB	2.79	0.46
1:B:711:PHE:O	1:B:715:ILE:HD12	2.15	0.46
1:A:244:LEU:HD22	1:A:248:LYS:HG3	1.98	0.46
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.98	0.46
1:B:686:GLU:CA	1:B:686:GLU:OE1	2.63	0.46
1:A:512:ARG:HH11	1:A:582:GLN:NE2	2.14	0.46
1:A:609:VAL:HG12	1:A:610:ILE:HD13	1.97	0.46
1:A:255:LYS:CE	1:A:762:HIS:HE1	2.29	0.46
1:B:155:ASN:HB3	1:B:175:SER:HB2	1.98	0.46
1:A:226:GLN:HE22	1:A:228:ALA:HB2	1.80	0.45
1:A:410:THR:HA	1:A:542:GLU:HB2	1.98	0.45
1:B:425:ARG:CD	1:B:430:GLN:OE1	2.61	0.45
1:B:611:TYR:O	1:B:615:PHE:HD1	2.00	0.45
1:A:740:LEU:H	1:A:740:LEU:CD2	2.24	0.45
1:B:602:VAL:O	1:B:606:GLN:HG3	2.16	0.45
1:B:248:LYS:HD3	1:B:265:GLY:HA2	1.94	0.45
1:B:218:ARG:HG2	1:B:218:ARG:O	2.16	0.45
1:B:617:VAL:O	1:B:617:VAL:CG1	2.65	0.45
1:B:231:THR:HB	1:B:348:GLU:CG	2.46	0.45
1:B:37:SER:N	1:B:40:ALA:HB3	2.30	0.45
1:B:426:TYR:CD2	1:B:454:ILE:HG23	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:528:ARG:NH1	1:A:528:ARG:HG3	2.27	0.45
1:A:442:SER:O	1:A:482:ILE:HD11	2.15	0.45
1:A:330:SER:C	1:A:331:GLU:HG3	2.36	0.45
1:A:283:HIS:O	1:A:285:ALA:N	2.50	0.45
1:A:659:ASP:O	1:A:660:LEU:C	2.55	0.45
1:A:5:LEU:HG	1:A:590:PHE:HZ	1.82	0.45
1:B:191:LEU:HD13	1:B:191:LEU:O	2.16	0.45
1:A:741:ARG:NH2	1:B:376:THR:O	2.50	0.45
1:B:376:THR:HB	1:B:377:GLU:OE2	2.16	0.45
1:B:252:TYR:CE2	1:B:254:ILE:HG22	2.50	0.45
1:A:88:GLY:HA2	1:A:392:ILE:CD1	2.46	0.45
1:A:682:ASP:HA	1:A:685:LEU:HG	1.99	0.45
1:A:45:THR:O	1:A:49:LYS:HG3	2.16	0.45
1:B:738:ILE:HD12	1:B:748:PRO:HB2	1.98	0.45
1:A:258:ALA:CB	1:A:295:LYS:HG2	2.45	0.45
1:A:642:TYR:CE1	1:A:684:MET:HB3	2.52	0.45
1:B:639:ILE:HG13	1:B:685:LEU:HD22	1.98	0.45
1:A:707:GLN:HB3	1:A:708:MET:HE1	1.98	0.45
1:B:89:GLY:HA2	1:B:113:PRO:HD3	1.98	0.45
1:A:203:PHE:HD2	1:A:204:ALA:N	2.14	0.45
1:B:248:LYS:HB3	1:B:265:GLY:HA2	1.89	0.45
1:A:279:PHE:O	1:A:778:ALA:CB	2.65	0.45
1:B:506:ALA:HA	1:B:534:ILE:HG23	1.99	0.45
1:A:5:LEU:O	1:A:6:ASN:HB2	2.16	0.45
1:A:653:LYS:O	1:A:653:LYS:HE3	2.17	0.45
1:A:206:ILE:O	1:A:369:GLY:HA2	2.17	0.45
1:B:112:LEU:HB2	1:B:113:PRO:HD3	1.98	0.45
1:B:723:LYS:HG2	1:B:767:ILE:CG1	2.46	0.45
1:A:643:THR:N	1:A:644:PRO:HD2	2.32	0.45
1:A:645:ARG:C	1:A:646:GLU:HG3	2.37	0.45
1:A:66:PHE:HE2	1:A:112:LEU:C	2.20	0.45
1:A:436:THR:HG22	1:A:437:VAL:N	2.31	0.45
1:B:512:ARG:HD2	1:B:537:PHE:CD2	2.53	0.44
1:B:283:HIS:HB3	1:B:286:LEU:HB3	1.98	0.44
1:B:256:THR:O	1:B:257:LYS:HD3	2.16	0.44
1:A:2:LEU:O	1:A:3:GLY:C	2.55	0.44
1:B:596:LEU:HD12	1:B:596:LEU:HA	1.79	0.44
1:A:718:ARG:NH1	1:A:722:SER:HB3	2.32	0.44
1:B:13:LYS:O	1:B:16:LEU:HD23	2.18	0.44
1:B:222:ILE:HG12	1:B:354:THR:HG23	1.98	0.44
1:B:731:MET:O	1:B:735:ARG:HB2	2.17	0.44
1:A:210:ASP:OD2	1:A:371:THR:CB	2.64	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:737:GLY:C	1:A:739:HIS:H	2.21	0.44
1:A:718:ARG:HD3	1:A:770:GLU:HG2	1.98	0.44
1:B:354:THR:HG21	1:B:735:ARG:CZ	2.48	0.44
1:B:493:ILE:HD13	1:B:525:ARG:HB3	1.98	0.44
1:A:362:ARG:HH21	1:A:597:LEU:HD11	1.82	0.44
1:A:238:ASN:O	1:A:241:VAL:HG23	2.17	0.44
1:B:413:GLY:O	1:B:416:LYS:HB3	2.17	0.44
1:A:753:GLN:HG3	1:A:754:MET:H	1.83	0.44
1:B:516:ARG:N	1:B:516:ARG:HD2	2.33	0.44
1:B:238:ASN:CG	1:B:340:LYS:HD2	2.37	0.44
1:B:322:ARG:NH2	1:B:742:ALA:O	2.51	0.44
1:A:215:ASP:OD2	1:A:517:ARG:NH2	2.43	0.44
1:B:243:THR:CG2	1:B:243:THR:O	2.62	0.44
1:B:554:THR:CG2	1:B:574:VAL:HG22	2.48	0.44
1:B:755:GLU:O	1:B:759:MET:HG3	2.18	0.44
1:A:718:ARG:HD3	1:A:770:GLU:CG	2.48	0.44
1:A:637:ARG:HE	1:A:769:ASP:CA	2.31	0.44
1:A:558:LEU:HD12	1:A:558:LEU:HA	1.76	0.44
1:B:461:ALA:HA	1:B:467:GLU:OE2	2.18	0.44
1:B:379:GLU:HG2	1:B:383:ASN:ND2	2.29	0.44
1:B:102:THR:HA	1:B:106:LYS:NZ	2.32	0.44
1:A:641:ALA:HB1	1:A:660:LEU:CD1	2.48	0.44
1:B:614:ARG:NH1	1:B:720:VAL:CG2	2.67	0.44
1:B:337:ILE:HA	1:B:340:LYS:HG2	1.98	0.44
1:B:99:GLU:OE2	1:B:391:THR:HG23	2.18	0.44
1:B:262:THR:O	1:B:263:GLU:C	2.55	0.43
1:A:667:ASP:O	1:A:669:GLY:N	2.51	0.43
1:B:630:MET:HE2	1:B:630:MET:HB3	1.59	0.43
1:A:457:GLN:HE21	1:A:470:ILE:CD1	2.15	0.43
1:B:16:LEU:CD2	1:B:16:LEU:N	2.77	0.43
1:A:266:MET:HB3	1:A:277:ASN:OD1	2.18	0.43
1:B:457:GLN:HE21	1:B:470:ILE:HG23	1.82	0.43
1:A:723:LYS:HB2	1:A:763:MET:HG2	2.00	0.43
1:B:238:ASN:HD21	1:B:340:LYS:N	2.15	0.43
1:A:105:GLY:N	2:A:781:ADP:O3A	2.49	0.43
1:A:723:LYS:CD	1:A:763:MET:CE	2.82	0.43
1:B:760:PHE:O	1:B:763:MET:HB3	2.19	0.43
1:B:250:TYR:CD1	1:B:261:LEU:HA	2.52	0.43
1:B:270:GLU:HB3	1:B:275:ILE:O	2.18	0.43
1:B:716:VAL:O	1:B:720:VAL:HB	2.18	0.43
1:B:16:LEU:H	1:B:16:LEU:HD23	1.80	0.43
1:A:166:GLU:O	1:A:169:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LEU:H	1:A:278:LEU:CD2	2.20	0.43
1:A:657:LEU:O	1:A:660:LEU:HD23	2.18	0.43
1:B:422:VAL:HG13	1:B:432:VAL:HG11	2.00	0.43
1:A:647:GLU:CG	1:A:648:LEU:N	2.81	0.43
1:A:459:LEU:HB2	1:A:483:ALA:HA	1.99	0.43
1:A:745:GLN:NE2	1:B:587:GLY:HA3	2.34	0.43
1:A:610:ILE:CG2	1:A:723:LYS:HE2	2.47	0.43
1:A:425:ARG:HB2	1:A:432:VAL:HG21	2.00	0.43
1:B:509:GLY:O	1:B:538:TYR:N	2.45	0.43
1:B:204:ALA:HB3	1:B:367:LEU:HD12	2.01	0.43
1:B:639:ILE:CG2	1:B:640:ALA:N	2.82	0.43
1:B:643:THR:HA	1:B:646:GLU:OE2	2.18	0.43
1:B:741:ARG:O	1:B:742:ALA:C	2.56	0.43
1:B:603:LEU:HD12	1:B:603:LEU:HA	1.82	0.43
1:B:354:THR:HG22	1:B:735:ARG:HH22	1.80	0.43
1:A:244:LEU:O	1:A:244:LEU:HD13	2.18	0.43
1:B:227:ALA:HB3	1:B:348:GLU:OE1	2.19	0.43
1:A:218:ARG:HB3	1:B:549:PHE:CD2	2.54	0.43
1:B:160:SER:O	1:B:164:LYS:HG3	2.19	0.43
1:B:262:THR:HG23	1:B:263:GLU:N	2.34	0.43
1:A:666:LEU:HD23	1:A:670:ALA:HB2	2.00	0.43
1:B:11:PRO:O	1:B:13:LYS:N	2.51	0.43
1:A:313:VAL:CG2	1:A:337:ILE:CD1	2.96	0.43
1:B:627:VAL:HG22	1:B:711:PHE:CE1	2.53	0.43
1:B:716:VAL:O	1:B:716:VAL:HG12	2.18	0.43
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.76	0.43
1:B:201:LEU:HD12	1:B:363:MET:HE2	2.01	0.43
1:B:642:TYR:O	1:B:645:ARG:N	2.52	0.43
1:A:228:ALA:C	1:A:230:SER:N	2.69	0.43
1:B:209:VAL:CG1	1:B:210:ASP:N	2.81	0.43
1:B:199:ARG:HB3	1:B:200:PRO:HD2	1.97	0.43
1:B:36:LEU:HD13	1:B:40:ALA:O	2.19	0.43
1:A:604:ARG:HA	1:A:607:ARG:CZ	2.49	0.43
1:B:363:MET:HE3	1:B:363:MET:HB3	1.49	0.43
1:B:127:VAL:HG13	1:B:180:LEU:HD12	2.01	0.43
1:B:718:ARG:CG	1:B:770:GLU:CD	2.71	0.42
1:A:576:ARG:HH12	1:B:346:GLN:NE2	2.14	0.42
1:A:160:SER:O	1:A:162:ASP:N	2.52	0.42
1:A:182:PHE:CB	1:A:186:ARG:NH2	2.75	0.42
1:A:322:ARG:NE	1:A:324:MET:HE1	2.34	0.42
1:B:475:GLY:HA3	1:B:494:LYS:O	2.19	0.42
1:B:724:TRP:CZ2	1:B:728:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147:PHE:C	1:B:149:GLY:N	2.73	0.42
1:B:445:ILE:C	1:B:447:LYS:H	2.22	0.42
1:B:256:THR:OG1	1:B:295:LYS:HE3	2.19	0.42
1:A:334:HIS:HA	1:A:337:ILE:HG13	2.00	0.42
1:B:476:GLN:NE2	1:B:494:LYS:HZ1	2.16	0.42
1:A:685:LEU:O	1:A:689:MET:HB2	2.19	0.42
1:B:29:ILE:HD12	1:B:33:TYR:HE1	1.83	0.42
1:B:70:ARG:O	1:B:70:ARG:HG2	2.19	0.42
1:A:637:ARG:HE	1:A:769:ASP:CB	2.28	0.42
1:A:564:ASP:OD2	1:A:566:SER:HB2	2.20	0.42
1:A:708:MET:CE	1:A:711:PHE:CE1	3.03	0.42
1:A:484:THR:O	1:A:485:ASN:C	2.57	0.42
1:A:426:TYR:CD2	1:A:426:TYR:O	2.71	0.42
1:B:107:THR:O	1:B:110:SER:OG	2.29	0.42
1:B:754:MET:HB3	1:B:754:MET:HE3	1.72	0.42
1:B:61:LEU:O	1:B:62:LEU:C	2.58	0.42
1:B:241:VAL:HG21	1:B:293:ALA:HB3	2.01	0.42
1:A:338:GLU:O	1:A:343:LEU:HA	2.19	0.42
1:A:252:TYR:HB2	1:A:253:ASP:H	1.51	0.42
1:A:642:TYR:CD1	1:A:684:MET:HB3	2.55	0.42
1:B:539:LEU:HB3	1:B:546:MET:HE2	2.02	0.42
1:A:224:SER:HA	1:A:350:MET:O	2.19	0.42
1:B:617:VAL:HG11	1:B:716:VAL:HG23	2.02	0.42
1:A:103:GLY:HA3	1:A:528:ARG:HB2	2.02	0.42
1:A:699:LYS:HD2	1:A:707:GLN:HE22	1.85	0.42
1:B:322:ARG:HG3	1:B:742:ALA:CB	2.50	0.42
1:A:648:LEU:N	1:A:649:PRO:CD	2.82	0.42
1:A:553:ARG:HE	1:A:560:ARG:NH2	2.18	0.42
1:B:302:LYS:HD3	1:B:341:GLU:OE2	2.19	0.42
1:A:425:ARG:NH1	1:A:534:ILE:HD11	2.34	0.42
1:A:288:HIS:HE2	1:A:331:GLU:HB2	1.85	0.42
1:A:331:GLU:OE2	1:A:766:SER:OG	2.31	0.42
1:B:315:ILE:HD13	1:B:329:TYR:CZ	2.55	0.42
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.68	0.42
1:A:252:TYR:CE1	1:A:256:THR:HA	2.55	0.41
1:B:630:MET:O	1:B:630:MET:HE3	2.20	0.41
1:B:39:ASP:CG	1:B:42:LYS:HB3	2.40	0.41
1:A:689:MET:SD	1:A:693:ILE:HB	2.60	0.41
1:A:699:LYS:HE3	1:A:779:GLU:OE1	2.20	0.41
1:B:460:ASN:O	1:B:461:ALA:HB3	2.19	0.41
1:B:254:ILE:CG2	1:B:255:LYS:N	2.83	0.41
1:B:211:SER:O	1:B:216:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:331:GLU:OE2	1:B:722:SER:CB	2.55	0.41
1:B:301:GLN:H	1:B:305:ASP:HB2	1.84	0.41
1:A:109:THR:O	1:A:113:PRO:HD2	2.20	0.41
1:A:625:GLU:HA	1:A:628:GLU:HB3	2.02	0.41
1:A:405:ASP:HB3	1:A:539:LEU:HD12	2.02	0.41
1:B:780:ILE:HG22	1:B:780:ILE:OXT	2.20	0.41
1:A:258:ALA:H	1:A:295:LYS:HE2	1.85	0.41
1:A:226:GLN:HA	1:A:350:MET:HE3	2.01	0.41
1:B:708:MET:CA	1:B:711:PHE:HB2	2.50	0.41
1:B:190:VAL:HG13	1:B:192:TYR:H	1.85	0.41
1:B:754:MET:HE2	1:B:754:MET:HB2	1.73	0.41
1:B:261:LEU:HD12	1:B:261:LEU:C	2.39	0.41
1:A:257:LYS:HZ1	1:A:660:LEU:HD12	1.86	0.41
1:B:282:LYS:NZ	1:B:283:HIS:NE2	2.69	0.41
1:B:461:ALA:HB2	1:B:487:ALA:HA	2.02	0.41
1:A:728:ILE:HA	1:A:728:ILE:HD13	1.82	0.41
1:B:42:LYS:O	1:B:45:THR:HB	2.20	0.41
1:A:628:GLU:HG3	1:A:632:LYS:HZ2	1.86	0.41
1:B:424:GLN:C	1:B:426:TYR:H	2.24	0.41
1:A:261:LEU:HD13	1:A:294:LEU:HD22	2.03	0.41
1:A:741:ARG:HH22	1:B:376:THR:CG2	2.22	0.41
1:B:19:TYR:C	1:B:87:MET:HE3	2.40	0.41
1:B:112:LEU:HB2	1:B:113:PRO:CD	2.51	0.41
1:B:484:THR:O	1:B:485:ASN:C	2.58	0.41
1:B:458:VAL:O	1:B:458:VAL:HG12	2.20	0.41
1:B:516:ARG:H	1:B:516:ARG:HD2	1.86	0.41
1:B:217:ALA:HB3	1:B:593:ARG:CD	2.51	0.41
1:B:302:LYS:O	1:B:302:LYS:HG2	2.20	0.41
1:A:686:GLU:CG	1:A:687:LEU:N	2.83	0.41
1:A:374:ALA:HB1	1:A:381:PHE:CE1	2.56	0.41
1:B:168:TYR:HD1	1:B:197:VAL:HG12	1.86	0.41
1:B:744:ALA:HB1	1:B:748:PRO:HG3	2.03	0.41
1:B:551:ALA:C	1:B:553:ARG:H	2.23	0.41
1:A:637:ARG:HA	1:A:637:ARG:HD3	1.58	0.41
1:B:708:MET:C	1:B:711:PHE:HB2	2.41	0.41
1:B:263:GLU:N	1:B:263:GLU:OE2	2.50	0.41
1:A:659:ASP:HA	1:A:662:ASN:OD1	2.21	0.41
1:B:218:ARG:HH11	1:B:592:SER:CB	2.33	0.41
1:A:652:TRP:O	1:A:653:LYS:HG3	2.21	0.41
1:A:576:ARG:O	1:A:579:GLU:HB2	2.20	0.41
1:B:339:ALA:HB2	1:B:345:ILE:HG12	2.03	0.41
1:A:247:GLU:HB2	1:A:261:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:THR:O	1:A:177:ASN:C	2.59	0.41
1:A:72:ALA:HB2	1:A:148:LEU:HD21	2.03	0.41
1:B:599:TYR:N	1:B:599:TYR:HD1	2.18	0.41
1:A:624:ARG:O	1:A:624:ARG:HG2	2.21	0.41
1:A:332:GLY:HA2	1:A:334:HIS:NE2	2.36	0.41
1:B:637:ARG:NH2	1:B:765:GLU:O	2.54	0.40
1:A:685:LEU:O	1:A:689:MET:CB	2.69	0.40
1:B:607:ARG:O	1:B:608:GLU:C	2.58	0.40
1:B:642:TYR:OH	1:B:688:ILE:HD12	2.22	0.40
1:A:279:PHE:CZ	1:A:780:ILE:HG23	2.56	0.40
1:B:358:GLN:HB3	1:B:597:LEU:HD13	2.03	0.40
1:A:206:ILE:CD1	1:A:206:ILE:H	2.33	0.40
1:A:613:GLN:O	1:A:617:VAL:HG23	2.20	0.40
1:A:747:ASN:HD22	1:A:747:ASN:HA	1.57	0.40
1:B:515:SER:C	1:B:516:ARG:HH11	2.25	0.40
1:B:377:GLU:HB2	1:B:381:PHE:HE1	1.86	0.40
1:A:442:SER:O	1:A:482:ILE:CD1	2.69	0.40
1:A:763:MET:HE2	1:A:763:MET:HB3	1.88	0.40
1:B:741:ARG:CG	1:B:742:ALA:N	2.83	0.40
1:A:317:ASP:O	1:A:319:PHE:N	2.55	0.40
1:B:593:ARG:O	1:B:594:LYS:C	2.59	0.40
1:B:400:ARG:HB2	1:B:527:GLY:HA3	2.04	0.40
1:A:442:SER:CA	1:A:482:ILE:HD11	2.51	0.40
1:B:512:ARG:CG	1:B:539:LEU:HD21	2.51	0.40
1:A:374:ALA:HB1	1:A:381:PHE:HE1	1.87	0.40
1:A:671:LEU:CD1	1:A:674:SER:HA	2.52	0.40
1:A:100:MET:O	1:A:372:GLY:HA2	2.22	0.40
1:B:599:TYR:N	1:B:599:TYR:CD1	2.89	0.40
1:A:665:TYR:O	1:A:776:MET:HB3	2.21	0.40
1:A:747:ASN:C	1:A:749:LEU:N	2.74	0.40
1:A:641:ALA:CB	1:A:660:LEU:HD11	2.52	0.40
1:A:679:LYS:O	1:A:680:GLU:HG2	2.21	0.40
1:A:541:MET:HA	1:A:546:MET:HG2	2.04	0.40
1:A:458:VAL:CG1	1:A:459:LEU:N	2.84	0.40
1:B:302:LYS:HA	1:B:306:TYR:CZ	2.56	0.40
1:A:203:PHE:HD2	1:A:204:ALA:H	1.69	0.40
1:A:168:TYR:OH	1:A:180:LEU:HD23	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	778/780 (100%)	647 (83%)	99 (13%)	32 (4%)	4	32
1	B	768/780 (98%)	626 (82%)	118 (15%)	24 (3%)	7	41
All	All	1546/1560 (99%)	1273 (82%)	217 (14%)	56 (4%)	5	36

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	259	VAL
1	A	275	ILE
1	A	280	ASP
1	A	304	VAL
1	A	544	GLU
1	A	563	MET
1	A	668	GLU
1	B	12	THR
1	B	120	THR
1	B	122	LYS
1	B	245	LYS
1	B	345	ILE
1	B	485	ASN
1	A	161	LYS
1	A	284	VAL
1	A	299	ALA
1	A	342	GLY
1	A	548	ARG
1	A	690	ASP
1	A	737	GLY
1	B	133	LEU
1	B	446	SER
1	B	655	ASP
1	A	248	LYS
1	A	254	ILE
1	A	257	LYS

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Mol	Chain	Res	Type
1	A	311	GLY
1	A	318	SER
1	B	253	ASP
1	B	318	SER
1	B	625	GLU
1	B	743	TYR
1	A	310	ASP
1	A	679	LYS
1	B	263	GLU
1	B	544	GLU
1	A	3	GLY
1	A	376	THR
1	A	461	ALA
1	A	485	ASN
1	A	674	SER
1	B	251	THR
1	B	575	SER
1	B	627	VAL
1	A	562	GLY
1	A	660	LEU
1	A	681	PRO
1	B	132	TYR
1	B	547	ARG
1	B	565	ASP
1	A	738	ILE
1	B	254	ILE
1	A	274	GLY
1	B	212	ILE
1	B	644	PRO

### 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	670/670 (100%)	576 (86%)	94 (14%)	5	23
1	B	661/670 (99%)	558 (84%)	103 (16%)	4	17
All	All	1331/1340 (99%)	1134 (85%)	197 (15%)	4	20

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	13	LYS
1	A	16	LEU
1	A	21	LYS
1	A	30	ARG
1	A	35	ASN
1	A	61	LEU
1	A	62	LEU
1	A	120	THR
1	A	158	SER
1	A	194	GLU
1	A	200	PRO
1	A	207	ASP
1	A	210	ASP
1	A	221	LEU
1	A	224	SER
1	A	232	LYS
1	A	238	ASN
1	A	244	LEU
1	A	250	TYR
1	A	251	THR
1	A	260	GLN
1	A	278	LEU
1	A	279	PHE
1	A	284	VAL
1	A	287	ASN
1	A	301	GLN
1	A	309	GLU
1	A	316	VAL
1	A	323	LEU
1	A	328	ARG
1	A	331	GLU
1	A	337	ILE
1	A	343	LEU
1	A	344	GLU
1	A	345	ILE
1	A	346	GLN
1	A	348	GLU
1	A	354	THR
1	A	363	MET
1	A	371	THR
1	A	376	THR

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Mol	Chain	Res	Type
1	A	377	GLU
1	A	382	ARG
1	A	426	TYR
1	A	428	THR
1	A	439	VAL
1	A	442	SER
1	A	443	GLU
1	A	448	LEU
1	A	471	ILE
1	A	481	THR
1	A	482	ILE
1	A	492	ASP
1	A	500	LYS
1	A	501	GLU
1	A	517	ARG
1	A	534	ILE
1	A	535	THR
1	A	559	ASP
1	A	569	ILE
1	A	601	ASP
1	A	630	MET
1	A	634	SER
1	A	636	GLU
1	A	637	ARG
1	A	653	LYS
1	A	655	ASP
1	A	660	LEU
1	A	663	THR
1	A	666	LEU
1	A	673	LYS
1	A	675	ASP
1	A	684	MET
1	A	686	GLU
1	A	691	ARG
1	A	695	LYS
1	A	696	TYR
1	A	700	GLU
1	A	707	GLN
1	A	708	MET
1	A	709	ARG
1	A	717	LEU
1	A	718	ARG

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Mol	Chain	Res	Type
1	A	722	SER
1	A	723	LYS
1	A	724	TRP
1	A	731	MET
1	A	740	LEU
1	A	741	ARG
1	A	747	ASN
1	A	751	GLU
1	A	763	MET
1	A	766	SER
1	B	14	ARG
1	B	16	LEU
1	B	30	ARG
1	B	53	GLU
1	B	61	LEU
1	B	73	SER
1	B	83	LYS
1	B	146	GLU
1	B	187	ASP
1	B	191	LEU
1	B	195	GLN
1	B	219	THR
1	B	226	GLN
1	B	231	THR
1	B	233	LEU
1	B	244	LEU
1	B	255	LYS
1	B	260	GLN
1	B	261	LEU
1	B	262	THR
1	B	263	GLU
1	B	266	MET
1	B	275	ILE
1	B	276	ASP
1	B	278	LEU
1	B	280	ASP
1	B	281	VAL
1	B	289	HIS
1	B	294	LEU
1	B	305	ASP
1	B	320	THR
1	B	328	ARG

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Mol	Chain	Res	Type
1	B	330	SER
1	B	340	LYS
1	B	347	ASN
1	B	354	THR
1	B	363	MET
1	B	376	THR
1	B	382	ARG
1	B	388	GLN
1	B	391	THR
1	B	399	VAL
1	B	405	ASP
1	B	422	VAL
1	B	442	SER
1	B	444	LEU
1	B	446	SER
1	B	459	LEU
1	B	463	ASN
1	B	473	GLU
1	B	476	GLN
1	B	477	LYS
1	B	481	THR
1	B	494	LYS
1	B	495	LEU
1	B	500	LYS
1	B	514	GLU
1	B	516	ARG
1	B	526	SER
1	B	528	ARG
1	B	544	GLU
1	B	545	LEU
1	B	546	MET
1	B	547	ARG
1	B	549	PHE
1	B	555	MET
1	B	557	MET
1	B	569	ILE
1	B	571	SER
1	B	579	GLU
1	B	580	SER
1	B	603	LEU
1	B	613	GLN
1	B	618	ILE

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Mol	Chain	Res	Type
1	B	624	ARG
1	B	630	MET
1	B	636	GLU
1	B	639	ILE
1	B	646	GLU
1	B	647	GLU
1	B	648	LEU
1	B	650	GLU
1	B	659	ASP
1	B	663	THR
1	B	667	ASP
1	B	673	LYS
1	B	680	GLU
1	B	686	GLU
1	B	693	ILE
1	B	707	GLN
1	B	711	PHE
1	B	712	GLU
1	B	720	VAL
1	B	722	SER
1	B	723	LYS
1	B	734	LEU
1	B	738	ILE
1	B	743	TYR
1	B	746	THR
1	B	747	ASN
1	B	750	ARG
1	B	766	SER
1	B	780	ILE

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	35	ASN
1	A	93	HIS
1	A	125	HIS
1	A	226	GLN
1	A	238	ASN
1	A	297	HIS
1	A	312	GLN
1	A	457	GLN
1	A	570	GLN

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Mol	Chain	Res	Type
1	A	598	GLN
1	A	629	ASN
1	A	697	ASN
1	A	727	HIS
1	A	745	GLN
1	A	747	ASN
1	A	762	HIS
1	B	17	ASN
1	B	202	HIS
1	B	226	GLN
1	B	288	HIS
1	B	292	GLN
1	B	297	HIS
1	B	312	GLN
1	B	346	GLN
1	B	358	GLN
1	B	383	ASN
1	B	424	GLN
1	B	457	GLN
1	B	460	ASN
1	B	463	ASN
1	B	476	GLN
1	B	582	GLN
1	B	739	HIS
1	B	747	ASN
1	B	753	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	ADP	A	781	-	29,29,29	1.29	2 (6%)	45,45,45	1.95	9 (20%)

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	ADP	A	781	-	-	0/16/32/32	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	781	ADP	C5-C4	3.70	1.48	1.40
2	A	781	ADP	O3'-C3'	3.01	1.50	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	781	ADP	N3-C2-N1	-6.86	122.97	128.71
2	A	781	ADP	N3-C4-N9	5.46	135.30	125.43
2	A	781	ADP	C3'-C2'-C1'	4.09	107.31	100.91
2	A	781	ADP	C4-C5-N7	-3.78	106.28	109.52
2	A	781	ADP	C5-C4-N3	-3.30	118.51	125.70
2	A	781	ADP	C2-N3-C4	2.67	121.62	114.01
2	A	781	ADP	O4'-C1'-N9	2.42	110.69	108.44
2	A	781	ADP	PA-O3A-PB	-2.38	124.70	131.68
2	A	781	ADP	O4'-C4'-C3'	2.26	109.76	105.17

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 ⓘ

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	780/780 (100%)	0.24	19 (2%)	56 13	20, 45, 80, 187	0
1	B	770/780 (98%)	0.23	16 (2%)	60 15	18, 46, 61, 187	0
All	All	1550/1560 (99%)	0.23	35 (2%)	57 13	18, 46, 73, 187	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	623	LEU	4.8
1	A	651	GLU	4.3
1	B	622	ASN	4.2
1	B	261	LEU	4.0
1	A	646	GLU	3.9
1	A	654	LEU	3.7
1	B	621	GLU	3.4
1	A	699	LYS	3.2
1	A	622	ASN	3.1
1	A	676	ILE	3.0
1	A	675	ASP	2.9
1	B	250	TYR	2.8
1	A	655	ASP	2.7
1	A	743	TYR	2.7
1	A	706	GLU	2.7
1	A	701	GLU	2.7
1	A	642	TYR	2.6
1	A	338	GLU	2.5
1	B	557	MET	2.5
1	B	549	PHE	2.5
1	A	650	GLU	2.4
1	B	248	LYS	2.4
1	A	702	GLN	2.4
1	B	553	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	558	LEU	2.3
1	B	563	MET	2.3
1	B	52	LEU	2.3
1	A	344	GLU	2.2
1	A	671	LEU	2.2
1	B	701	GLU	2.2
1	A	247	GLU	2.2
1	B	705	LYS	2.2
1	B	262	THR	2.2
1	A	250	TYR	2.1
1	B	554	THR	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	ADP	A	781	27/27	0.68	9.29	47,108,108,108	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.