



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 10:05 AM UTC

PDB ID : 2G67 / pdb_00002g67
Title : E. Coli Pyruvate Dehydrogenase E1 Component (Apoenzyme)
Authors : Furey, W.; Chandrasekhar, K.; Arjunan, P.
Deposited on : 2006-02-24
Resolution : 2.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

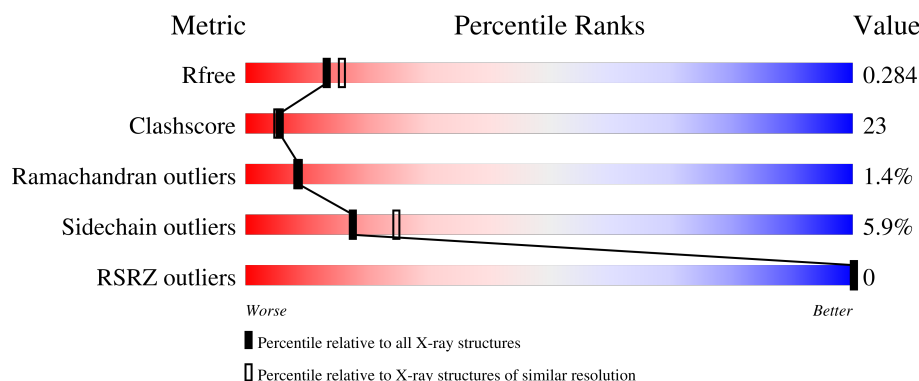
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	886	
1	B	886	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	1	0
			6351	4024	1096	1205	26			
1	B	801	Total	C	N	O	S	0	1	0
			6351	4024	1096	1205	26			

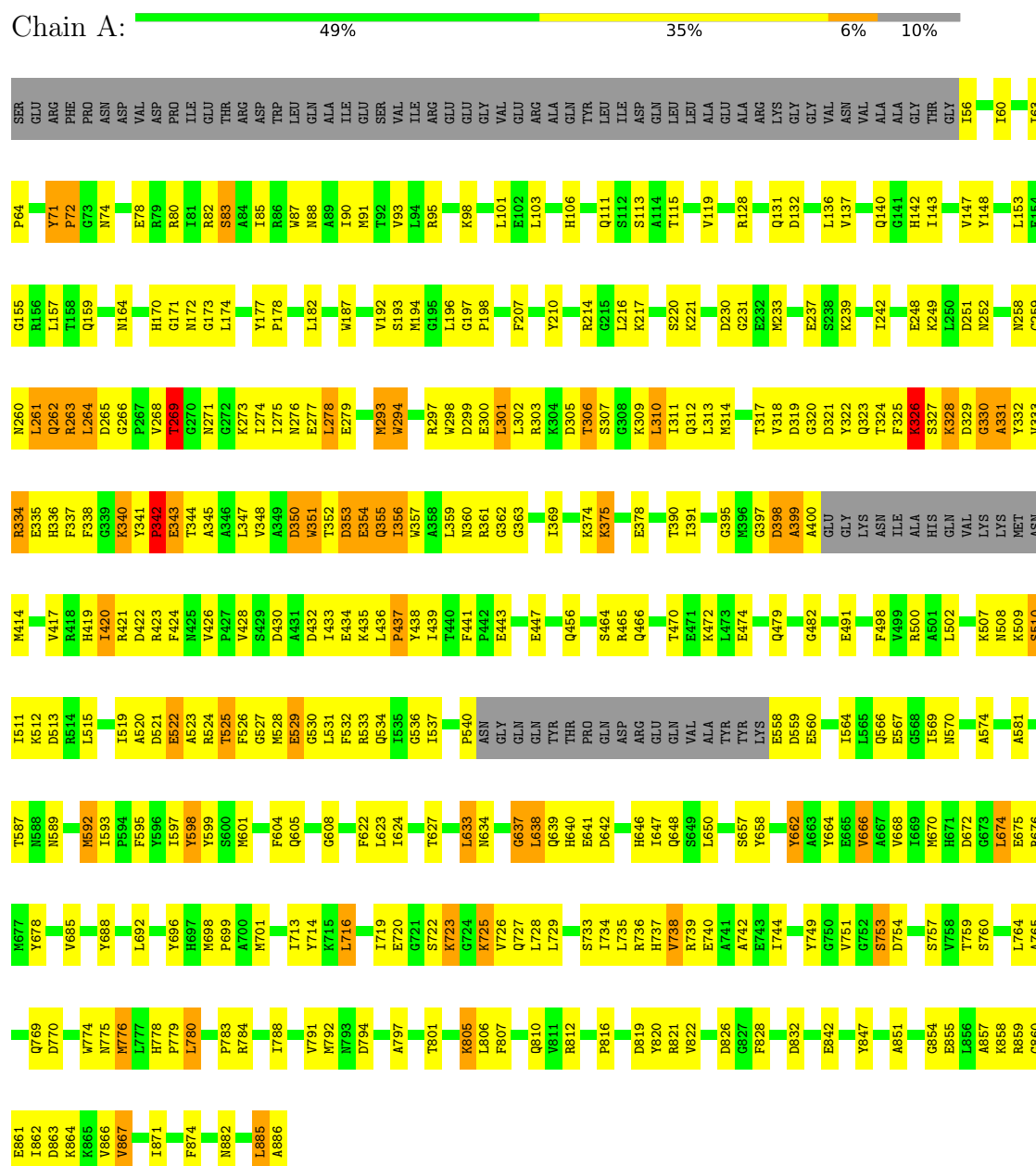
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	241	Total	O	0	0
			241	241		
2	B	207	Total	O	0	0
			207	207		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyruvate dehydrogenase E1 component



● Molecule 1: Pyruvate dehydrogenase E1 component

Chain B:  52% 34% 10%

SER	GLU	ARG	PHE	PRO	ASN	ASP	VAL	ASP	ASP	PRO	PRO	ILE	GLU	THR	ARG	ASP	TRP	LEU	GLN	ALA	ILE	SER	VAL	VAL	ILE	ARG	ALA	GLU	TYR	LEU	ILE	ASP	GLN	LEU	LEU	ALA	GLU	ALA	ARG	LYS	GLY	GLY	VAL	ASN	VAL	VAL	ALA	ALA	THR	GLY	GLY	N58	N58	N58	N61
T62	I63	P64	V65	E66	E67	Q68	Y71	N74	E76	L77	E78	R82	T85	R86	W87	I90	T91	T92	V93	L94	R95	A96	S97	K98	K99	L103	H106	M107	Q111	E130	Q131	Q140	G141	H142	I143	S144	P145	G146	V147	R150	A151	F152	L153	E154	G155	L157									
T158	Q159	E160	Q161	N164	F165	R166	Q167	E168	V169	H170	G171	N172	S175	S176	I177	P178	H179	P180	M183	P184	W187	Q188	F189	P190	T191	V192	S193	L196	G197	P198	T202	Y203	Q204	F207	L208	K209	Y210	L211	R214	A226	F227	L228	G229	D230	G231	E232	P236								
K239	I242	T243	I244	L250	D251	N252	F255	C259	N260	L261	Q262	R263	L264	D265	G266	V268	T269	K273	I274	L278	E279	F282	W287	N288	V289	I290	K291	D299	E300	L301	T306	K309	Q312	N315	E316	T317	V318	D319	G320	D321	Y322	Q323	T324	F325	K326										
S327	K328	Y332	H336	E343	A346	A349	D350	W351	T352	D353	E354	Q355	L356	W357	A358	L359	N360	R361	G362	G363	H364	D365	E378	T384	V385	H389	T390	I391	K392	M396	G397	D398	A399	A400	GLU	GLY	LYS	ASN	ILE	ALA	HIS	VAL	LYS	LYS	MET	ASN	P414	G416							
V417	R418	H419	I420	R421	D422	R423	V426	P427	V428	S429	D430	A431	D432	I433	E434	K435	L436	P437	Y438	I439	E446	E447	H452	A453	Q456	K457	L458	H459	G530	L462	P463	Q466	P467	N468	F469	T470	E471	L475	P476	S477	D480	A483	E486	Q487	Q488	S489	K490	S493	T494						
A497	F498	V499	R500	A501	L502	N503	V504	M505	L506	K509	S510	I511	K512	D513	R514	L515	V516	P517	I518	I519	A520	D521	E522	A523	R524	T525	F526	G527	M528	E529	L531	P540	ASN	GLY	GLN	GLN	TYR	THR	PRO	GLN	ASP	ARG	GLU	GLN	VAL	ALA	TYR	E558							
I564	L565	Q566	E567	G568	I569	N570	A574	T583	S584	T587	Y596	I597	R598	Y599	S600	M601	F604	Q605	R606	I607	G608	D609	L610	G615	D616	Q617	G626	T627	S628	G629	L633	N634	G635	E636	G637	L638	D642	G643	H644	T647	Q648	S649	L650	T651	I652	P653	I656								
S657	Y658	Y662	A663	I669	L674	Y678	G679	E680	K681	V685	Y686	L692	I713	T718	K723	G724	K725	L729	L734	L735	R736	H737	V738	R739	L745	A746	K747	G750	V751	G752	S753	D754	V755	Q769	D770	C771	P779	L780	F781	T782	P783	R784	V785												
P786	Y787	M792	A795	P796	A797	S800	T801	D802	Y803	L806	R821	F828	G829	D832	S833	R838	V843	D844	A845	S846	Y847	V848	V849	L853	G854	A857	K858	R859	I871	I876	N882	P883	R884	L885	A886																				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 140.63Å 81.91Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	34.62 – 2.32 34.62 – 2.32	Depositor EDS
% Data completeness (in resolution range)	91.7 (34.62-2.32) 91.7 (34.62-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.39 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.281 0.213 , 0.284	Depositor DCC
R_{free} test set	3618 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.057 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13150	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/6495	1.09	37/8781 (0.4%)
1	B	0.62	0/6495	1.10	38/8781 (0.4%)
All	All	0.62	0/12990	1.09	75/17562 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLY	N-CA-C	10.88	126.52	113.79
1	B	470	THR	N-CA-C	8.69	122.00	111.40
1	A	633	LEU	N-CA-C	-8.58	99.84	110.65
1	A	634	ASN	N-CA-C	8.14	121.18	111.33
1	B	459	HIS	N-CA-C	8.14	122.90	113.38
1	B	171	GLY	N-CA-C	8.04	126.60	115.27
1	B	634	ASN	N-CA-C	7.91	120.60	111.11
1	A	343	GLU	N-CA-C	-7.83	104.33	114.04
1	A	822	VAL	N-CA-C	7.79	119.07	108.17
1	B	183	MET	CA-C-N	7.78	129.57	119.84
1	B	183	MET	C-N-CA	7.78	129.57	119.84
1	B	637	GLY	N-CA-C	7.41	126.00	112.37
1	B	747	LYS	N-CA-C	7.35	119.37	111.36
1	A	71	TYR	CA-C-N	7.17	126.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	TYR	C-N-CA	7.17	126.80	119.56
1	A	638	LEU	N-CA-C	6.82	122.56	111.37
1	B	782	THR	CA-C-N	6.71	128.23	119.84
1	B	782	THR	C-N-CA	6.71	128.23	119.84
1	A	294	TRP	N-CA-C	6.67	120.05	109.50
1	A	753	SER	N-CA-C	6.67	118.69	108.42
1	B	681	LYS	N-CA-C	6.46	119.15	111.33
1	B	487	GLU	N-CA-C	-6.40	101.65	110.35
1	B	633	LEU	N-CA-C	-6.38	100.05	109.62
1	A	312	GLN	N-CA-C	-6.29	104.35	111.14
1	B	636	GLU	N-CA-C	6.25	118.10	111.28
1	A	523	ALA	N-CA-C	-6.19	104.70	112.93
1	B	523	ALA	N-CA-C	-6.13	105.65	113.01
1	B	511	ILE	N-CA-C	6.10	120.72	113.22
1	B	71	TYR	CA-C-N	6.08	125.70	119.56
1	B	71	TYR	C-N-CA	6.08	125.70	119.56
1	A	482	GLY	N-CA-C	5.95	119.83	112.64
1	A	137	VAL	N-CA-C	5.92	116.63	107.99
1	B	608	GLY	N-CA-C	5.90	120.03	112.83
1	B	652	ILE	CA-C-N	5.85	125.99	119.32
1	B	652	ILE	C-N-CA	5.85	125.99	119.32
1	B	430	ASP	N-CA-C	-5.83	106.25	113.19
1	A	778	HIS	CA-C-N	5.82	126.22	119.47
1	A	778	HIS	C-N-CA	5.82	126.22	119.47
1	B	754	ASP	N-CA-C	-5.76	99.01	108.41
1	A	170	HIS	N-CA-C	5.71	119.95	113.15
1	A	529	GLU	N-CA-C	5.70	117.17	111.07
1	A	791	VAL	N-CA-C	5.68	116.46	110.72
1	A	740	GLU	N-CA-C	-5.65	105.11	112.23
1	A	242	ILE	N-CA-C	5.65	120.02	111.89
1	A	293	MET	N-CA-C	5.65	118.29	111.40
1	B	635	GLY	N-CA-C	5.58	119.91	112.77
1	A	262	GLN	N-CA-C	5.54	117.77	108.73
1	A	805	LYS	N-CA-C	5.54	118.84	111.75
1	B	642	ASP	N-CA-C	5.49	117.66	107.99
1	A	355	GLN	N-CA-C	-5.48	105.47	111.82
1	A	678	TYR	N-CA-C	5.41	119.86	112.88
1	B	494	THR	N-CA-C	-5.41	106.18	112.89
1	B	192	VAL	CB-CA-C	-5.38	104.88	112.14
1	B	679	GLY	N-CA-C	-5.36	105.23	112.57
1	A	443	GLU	N-CA-C	-5.33	102.50	110.23
1	A	72	PRO	N-CA-C	5.33	120.52	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	GLY	N-CA-C	-5.31	106.36	112.73
1	A	592	MET	N-CA-C	-5.31	100.38	109.24
1	B	713	ILE	N-CA-C	5.31	114.17	107.70
1	A	662	TYR	N-CA-C	5.30	118.36	110.14
1	B	204	GLN	N-CA-C	-5.30	105.17	111.69
1	B	327	SER	N-CA-C	-5.27	106.53	113.17
1	B	169	VAL	N-CA-C	5.24	116.59	110.62
1	A	510	SER	N-CA-C	5.23	117.41	111.02
1	A	642	ASP	N-CA-C	5.20	117.09	108.20
1	B	662	TYR	N-CA-C	5.18	118.00	109.72
1	B	657	SER	N-CA-C	5.17	118.24	109.76
1	A	637	GLY	N-CA-C	5.13	121.82	112.37
1	A	470	THR	N-CA-C	5.13	119.62	112.90
1	A	797	ALA	N-CA-C	5.12	118.42	110.17
1	A	623	LEU	N-CA-C	-5.11	100.19	108.52
1	B	833	SER	N-CA-C	-5.10	103.80	110.53
1	A	511	ILE	N-CA-C	5.09	119.48	113.22
1	B	68	GLN	N-CA-C	5.05	116.26	109.24
1	B	797	ALA	N-CA-C	5.02	117.78	109.85

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	TYR	Sidechain
1	B	598	TYR	Sidechain
1	B	678	TYR	Sidechain
1	B	803	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6351	0	6185	330	0
1	B	6351	0	6185	280	0
2	A	241	0	0	22	0
2	B	207	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13150	0	12370	589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:HD21	1:B:531:LEU:HD11	1.19	1.14
1:B:490:LYS:HE2	1:B:500:ARG:HH22	1.15	1.07
1:B:638:LEU:HD21	1:B:828:PHE:HB3	1.41	1.02
1:A:177:TYR:CG	1:A:192:VAL:HG11	1.96	0.99
1:A:855:GLU:O	1:A:859:ARG:HG3	1.65	0.97
1:B:268:VAL:HB	1:B:274:ILE:HD13	1.45	0.95
1:A:821:ARG:NH1	1:A:851:ALA:HA	1.82	0.94
1:A:326:LYS:HD3	1:A:391:ILE:HG23	1.50	0.92
1:B:490:LYS:CE	1:B:500:ARG:HH22	1.83	0.92
1:A:519:ILE:HD11	1:A:528:MET:HG3	1.51	0.91
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.53	0.91
1:B:346:ALA:HA	1:B:349:ALA:HB2	1.51	0.91
1:B:309:LYS:HG3	1:B:343:GLU:HG3	1.53	0.91
1:B:502:LEU:HD21	1:B:531:LEU:CD1	2.02	0.88
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.40	0.86
1:B:502:LEU:CD2	1:B:531:LEU:HD11	2.03	0.86
1:B:638:LEU:CD2	1:B:828:PHE:HB3	2.06	0.85
1:B:533:ARG:HH11	1:B:533:ARG:HB2	1.42	0.85
1:B:282:PHE:CD2	1:B:385:VAL:HG21	2.12	0.84
1:A:862:ILE:HD12	1:A:866:VAL:HG21	1.60	0.84
1:A:98:LYS:NZ	1:A:436:LEU:HD12	1.92	0.84
1:B:421:ARG:HB2	1:B:426:VAL:HB	1.58	0.84
1:B:279:GLU:HG3	1:B:289:VAL:HG21	1.57	0.83
1:A:722:SER:O	1:A:723:LYS:HB2	1.77	0.83
1:B:354:GLU:CD	1:B:354:GLU:H	1.88	0.81
1:A:140:GLN:O	1:A:143:ILE:HG13	1.80	0.81
1:B:74:ASN:O	1:B:78:GLU:HG3	1.79	0.81
1:A:882:ASN:HB3	1:A:885:LEU:HD22	1.64	0.80
1:B:471:GLU:HG2	2:B:932:HOH:O	1.80	0.80
1:A:666:VAL:O	1:A:670:MET:HG3	1.82	0.80
1:A:98:LYS:HZ3	1:A:436:LEU:HD12	1.48	0.79
1:B:519:ILE:HD13	1:B:523:ALA:HB2	1.64	0.79
1:A:331:ALA:HA	1:A:334:ARG:HG2	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LYS:HE2	1:B:500:ARG:NH2	1.95	0.78
1:B:261:LEU:O	1:B:267:PRO:HA	1.84	0.78
1:A:821:ARG:HH11	1:A:851:ALA:HA	1.47	0.78
1:B:509:LYS:H	1:B:509:LYS:HD2	1.47	0.78
1:A:638:LEU:HD21	1:A:828:PHE:CD1	2.19	0.77
1:A:268:VAL:O	1:A:269:THR:HG23	1.85	0.76
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.65	0.76
1:A:512:LYS:HG3	1:A:513:ASP:N	2.01	0.75
1:A:522:GLU:HG3	1:A:599:TYR:HE1	1.51	0.74
1:A:532:PHE:CD2	1:A:537:ILE:HD11	2.22	0.74
1:A:90:ILE:HD12	1:A:420:ILE:HD12	1.69	0.73
1:B:352:THR:HB	1:B:354:GLU:OE1	1.87	0.73
1:B:502:LEU:C	1:B:502:LEU:HD23	2.13	0.73
1:B:502:LEU:HD23	1:B:503:ASN:N	2.04	0.73
1:A:842:GLU:HG2	1:A:847:TYR:CE2	2.23	0.73
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.72	0.72
1:B:844:ASP:OD1	1:B:846:SER:HB3	1.90	0.72
1:B:309:LYS:CG	1:B:343:GLU:HG3	2.19	0.72
1:A:352:THR:H	1:A:355:GLN:HB2	1.53	0.72
1:B:274:ILE:O	1:B:278:LEU:HD23	1.90	0.72
1:B:417:VAL:O	1:B:420:ILE:HG12	1.90	0.72
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.88	0.71
1:B:434:GLU:CD	1:B:434:GLU:H	1.98	0.71
1:A:527:GLY:HA2	1:A:529:GLU:OE1	1.91	0.70
1:A:214:ARG:CB	1:A:216:LEU:HD13	2.21	0.70
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.21	0.70
1:B:98:LYS:HE3	1:B:436:LEU:HD11	1.71	0.70
1:B:421:ARG:HG3	1:B:421:ARG:NH1	2.07	0.70
1:B:533:ARG:HB2	1:B:533:ARG:NH1	2.07	0.70
1:A:269:THR:HG21	2:A:954:HOH:O	1.91	0.70
1:A:301:LEU:CD1	1:A:347:LEU:HD13	2.21	0.70
1:A:83:SER:OG	1:A:424:PHE:HB3	1.92	0.69
1:A:56:ILE:HG23	1:A:279:GLU:OE1	1.92	0.69
1:A:301:LEU:HD12	1:A:310:LEU:HD12	1.74	0.69
1:A:519:ILE:CD1	1:A:528:MET:HG3	2.23	0.69
1:B:421:ARG:HD2	1:B:421:ARG:O	1.93	0.69
1:A:417:VAL:HG12	1:A:433:ILE:HD11	1.74	0.69
1:B:130:GLU:CD	1:B:131:GLN:HE22	2.00	0.69
1:B:287:TRP:CE3	1:B:385:VAL:HG23	2.29	0.68
1:B:859:ARG:HH11	1:B:859:ARG:HB2	1.58	0.68
1:A:512:LYS:HG3	1:A:513:ASP:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ASP:OD2	1:B:169:VAL:HB	1.94	0.68
1:A:340:LYS:HB2	1:A:340:LYS:NZ	2.09	0.68
1:A:348:VAL:HB	1:A:356:ILE:HD11	1.74	0.68
1:B:361:ARG:HD3	1:B:389:HIS:CD2	2.29	0.68
1:B:522:GLU:HG2	1:B:599:TYR:OH	1.94	0.68
1:B:638:LEU:HD21	1:B:828:PHE:CB	2.21	0.68
1:B:844:ASP:HB2	2:B:1069:HOH:O	1.94	0.68
1:B:859:ARG:HB2	1:B:859:ARG:NH1	2.09	0.67
1:A:338:PHE:O	1:A:345:ALA:HB2	1.95	0.67
1:A:249:LYS:HE3	2:A:1100:HOH:O	1.93	0.67
1:B:558:GLU:O	1:B:558:GLU:HG2	1.95	0.67
1:B:529:GLU:N	1:B:529:GLU:OE1	2.28	0.67
1:A:74:ASN:O	1:A:78:GLU:HG3	1.94	0.67
1:A:309:LYS:HB3	1:A:344:THR:HG23	1.77	0.67
1:A:466:GLN:HE22	1:A:589:ASN:CG	2.04	0.66
1:B:512:LYS:HG3	1:B:513:ASP:N	2.10	0.66
1:A:414:MET:HE1	1:A:436:LEU:HD21	1.77	0.65
1:A:305:ASP:C	1:A:307:SER:H	2.04	0.65
1:A:325:PHE:O	1:A:327:SER:N	2.30	0.65
1:A:432:ASP:HA	1:A:435:LYS:HD3	1.78	0.65
1:A:536:GLY:O	1:A:564:ILE:HD12	1.96	0.65
1:B:273:LYS:HD2	2:B:992:HOH:O	1.97	0.64
1:B:729:LEU:HD11	1:B:792:MET:HE3	1.78	0.64
1:A:433:ILE:HG23	1:A:434:GLU:HG3	1.79	0.64
1:B:509:LYS:HD2	1:B:509:LYS:N	2.13	0.64
1:B:85:ILE:HG12	1:B:153:LEU:HD22	1.80	0.64
1:B:207:PHE:O	1:B:210:TYR:HB3	1.98	0.64
1:A:456:GLN:HA	1:A:456:GLN:NE2	2.11	0.64
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.78	0.64
1:A:214:ARG:HB2	1:A:216:LEU:HD13	1.80	0.63
1:A:297:ARG:HD2	1:A:359:LEU:HA	1.79	0.63
1:A:318:VAL:HG12	1:A:321:ASP:OD2	1.99	0.63
1:A:805:LYS:HG3	1:A:826:ASP:OD1	1.99	0.63
1:B:854:GLY:O	1:B:858:LYS:HG3	1.98	0.63
1:B:354:GLU:CD	1:B:354:GLU:N	2.57	0.62
1:B:66:GLU:CD	1:B:66:GLU:H	2.07	0.62
1:A:207:PHE:CZ	1:A:581:ALA:HA	2.34	0.62
1:B:566:GLN:HG2	2:B:1068:HOH:O	1.98	0.62
1:A:330:GLY:O	1:A:331:ALA:C	2.43	0.62
1:A:132:ASP:HA	1:A:217:LYS:HE3	1.82	0.62
1:A:177:TYR:CB	1:A:192:VAL:HG11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:NE	1:A:422:ASP:OD1	2.31	0.61
1:B:537:ILE:HG23	1:B:558:GLU:HA	1.82	0.61
1:A:90:ILE:HG22	1:A:91:MET:HE2	1.82	0.61
1:B:363:GLY:HA3	1:B:390:THR:HG22	1.83	0.61
1:B:567:GLU:HG3	1:B:574:ALA:HA	1.81	0.61
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.82	0.61
1:A:330:GLY:O	1:A:333:VAL:N	2.30	0.61
1:A:333:VAL:C	1:A:335:GLU:H	2.09	0.61
1:A:812:ARG:HD2	1:A:820:TYR:HD2	1.63	0.61
1:B:76:GLU:CD	1:B:76:GLU:H	2.09	0.61
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.36	0.61
1:A:627:THR:HB	1:A:633:LEU:HD13	1.83	0.60
1:A:857:ALA:HB1	1:A:864:LYS:HG2	1.82	0.60
1:B:103:LEU:O	1:B:166:ARG:HD3	2.01	0.60
1:A:87:TRP:CD2	1:A:426:VAL:HG11	2.36	0.60
1:A:90:ILE:CD1	1:A:420:ILE:HD12	2.30	0.60
1:A:305:ASP:HB2	1:A:347:LEU:HD11	1.84	0.60
1:B:505:MET:HE2	1:B:674:LEU:HD13	1.83	0.60
1:B:519:ILE:CD1	1:B:523:ALA:HB2	2.32	0.60
1:B:86:ARG:HB3	1:B:111:GLN:OE1	2.02	0.59
1:A:329:ASP:O	1:A:330:GLY:C	2.45	0.59
1:A:605:GLN:HB2	1:A:648:GLN:HE22	1.66	0.59
1:B:178:PRO:HA	1:B:187:TRP:CG	2.37	0.59
1:B:509:LYS:H	1:B:509:LYS:CD	2.14	0.59
1:A:164:ASN:HB2	1:A:173:GLY:HA2	1.85	0.59
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.35	0.59
1:A:500:ARG:NH1	2:A:1057:HOH:O	2.33	0.59
1:B:95:ARG:HD2	1:B:438:TYR:OH	2.02	0.59
1:A:324:THR:O	1:A:328:LYS:HG2	2.02	0.59
1:A:326:LYS:HZ2	1:A:326:LYS:CB	2.16	0.59
1:B:884:ARG:HB3	1:B:884:ARG:NH1	2.18	0.59
1:A:221:LYS:HE2	2:A:1089:HOH:O	2.03	0.59
1:A:558:GLU:N	2:A:1058:HOH:O	2.35	0.58
1:A:301:LEU:HD11	1:A:347:LEU:HD13	1.85	0.58
1:A:638:LEU:HB3	1:B:179:HIS:CE1	2.37	0.58
1:B:418:ARG:HG2	1:B:418:ARG:HH11	1.68	0.58
1:A:857:ALA:O	1:A:860:GLY:N	2.37	0.58
1:B:328:LYS:HE3	1:B:332:TYR:CE2	2.39	0.58
1:A:263:ARG:N	1:A:266:GLY:O	2.36	0.58
1:A:264:LEU:HD13	1:A:264:LEU:O	2.03	0.58
1:B:638:LEU:HD23	1:B:829:GLY:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HA	1:A:338:PHE:HB2	1.85	0.57
1:A:397:GLY:HA3	1:A:419:HIS:CE1	2.40	0.57
1:B:512:LYS:HG3	1:B:513:ASP:H	1.68	0.57
1:B:429:SER:C	1:B:431:ALA:H	2.12	0.57
1:B:533:ARG:HH11	1:B:533:ARG:CB	2.14	0.57
1:B:884:ARG:HB3	1:B:884:ARG:HH11	1.68	0.57
1:A:638:LEU:CD2	1:A:828:PHE:HB3	2.35	0.57
1:A:95:ARG:HA	1:A:98:LYS:CE	2.35	0.57
1:A:720:GLU:HA	2:A:1117:HOH:O	2.05	0.57
1:B:521:ASP:HB2	1:B:568:GLY:HA2	1.87	0.57
1:A:326:LYS:HB3	1:A:326:LYS:NZ	2.20	0.57
1:B:520:ALA:O	1:B:521:ASP:HB3	2.04	0.57
1:A:479:GLN:HG3	2:A:983:HOH:O	2.05	0.56
1:B:537:ILE:HD13	1:B:538:TYR:O	2.05	0.56
1:A:360:ASN:OD1	1:A:361:ARG:N	2.33	0.56
1:A:650:LEU:C	1:A:650:LEU:HD12	2.31	0.56
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.41	0.56
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.35	0.56
1:A:882:ASN:HB3	1:A:885:LEU:CD2	2.33	0.56
1:A:95:ARG:HA	1:A:98:LYS:HE2	1.88	0.56
1:A:260:ASN:O	1:A:262:GLN:N	2.38	0.56
1:B:64:PRO:HB2	1:B:66:GLU:OE2	2.06	0.56
1:B:420:ILE:HG13	1:B:421:ARG:N	2.19	0.56
1:A:142[O]:HIS:ND1	1:A:142[O]:HIS:N	2.51	0.56
1:A:530:GLY:HA2	1:A:533:ARG:NH1	2.20	0.56
1:A:214:ARG:HB3	1:A:216:LEU:HD13	1.87	0.56
1:A:863:ASP:O	1:A:866:VAL:HG22	2.05	0.56
1:B:537:ILE:CG2	1:B:558:GLU:HA	2.35	0.55
1:B:435:LYS:HB3	2:B:966:HOH:O	2.06	0.55
1:A:207:PHE:O	1:A:210:TYR:HB3	2.06	0.55
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.32	0.55
1:A:220:SER:HA	2:A:1038:HOH:O	2.05	0.55
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.88	0.55
1:B:87:TRP:HZ3	1:B:421:ARG:HB3	1.72	0.55
1:A:420:ILE:HG23	1:A:421:ARG:N	2.22	0.55
1:B:537:ILE:HD13	1:B:537:ILE:C	2.32	0.55
1:A:153:LEU:HD21	1:A:441:PHE:CE2	2.42	0.55
1:B:195:GLY:C	1:B:198:PRO:HD2	2.32	0.55
1:A:776:MET:HB2	1:B:821:ARG:NH1	2.22	0.54
1:B:483:ALA:HA	1:B:486:GLU:OE2	2.06	0.54
1:A:271:ASN:O	1:A:318:VAL:HG21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HG3	1:A:332:TYR:CZ	2.43	0.54
1:B:65:VAL:HG21	1:B:299:ASP:CG	2.33	0.54
1:B:433:ILE:C	1:B:435:LYS:N	2.65	0.54
1:A:854:GLY:O	1:A:858:LYS:HD3	2.08	0.54
1:A:177:TYR:HB3	1:A:192:VAL:CG1	2.37	0.54
1:A:321:ASP:HA	2:A:1045:HOH:O	2.07	0.54
1:A:115:THR:O	1:A:119:VAL:HG23	2.08	0.54
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.41	0.54
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.89	0.54
1:A:522:GLU:CG	1:A:599:TYR:HE1	2.20	0.54
1:B:266:GLY:N	2:B:1026:HOH:O	2.40	0.54
1:A:646:HIS:CE1	1:A:657:SER:HB3	2.43	0.54
1:B:143:ILE:HD12	1:B:143:ILE:C	2.33	0.54
1:A:237:GLU:CD	1:B:606:ARG:HH21	2.16	0.53
1:A:522:GLU:HG3	1:A:599:TYR:CE1	2.39	0.53
1:B:210:TYR:CZ	1:B:214:ARG:HD2	2.43	0.53
1:B:849:VAL:O	1:B:853:LEU:HG	2.08	0.53
1:B:499:VAL:O	1:B:502:LEU:HD22	2.08	0.53
1:B:584:SER:HA	1:B:587:THR:HG22	1.90	0.53
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.44	0.53
1:A:423:ARG:HD2	1:A:423:ARG:O	2.09	0.53
1:A:131:GLN:OE1	1:A:221:LYS:HD2	2.08	0.53
1:A:417:VAL:CG1	1:A:433:ILE:HD11	2.37	0.53
1:A:770:ASP:OD1	1:B:882:ASN:ND2	2.40	0.53
1:A:192:VAL:O	1:A:194:MET:HE3	2.09	0.53
1:A:658:TYR:CD1	1:A:760:SER:HB2	2.43	0.53
1:A:662:TYR:CD1	1:A:699:PRO:HD2	2.44	0.52
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.92	0.52
1:B:729:LEU:HD11	1:B:792:MET:CE	2.38	0.52
1:B:518:ILE:HG12	1:B:565:LEU:HB2	1.91	0.52
1:B:584:SER:HA	1:B:587:THR:CG2	2.38	0.52
1:A:430:ASP:O	1:A:433:ILE:HG22	2.10	0.52
1:A:80:ARG:HD2	1:A:447:GLU:OE2	2.10	0.52
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.45	0.52
1:B:517:PRO:HB2	1:B:564:ILE:HG12	1.92	0.52
1:A:322:TYR:HA	1:A:325:PHE:HD2	1.74	0.52
1:A:842:GLU:HG2	1:A:847:TYR:CZ	2.43	0.52
1:A:522:GLU:HB3	1:A:525:THR:OG1	2.10	0.52
1:A:559:ASP:C	1:A:559:ASP:OD1	2.52	0.52
1:B:143:ILE:HD12	1:B:143:ILE:O	2.10	0.52
1:A:722:SER:O	1:A:723:LYS:CB	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ALA:O	1:A:858:LYS:C	2.53	0.52
1:A:113:SER:HB3	1:A:258:ASN:ND2	2.25	0.51
1:A:334:ARG:NH2	1:A:353:ASP:OD1	2.42	0.51
1:A:352:THR:HG23	1:A:355:GLN:NE2	2.25	0.51
1:A:515:LEU:HD23	1:A:593:ILE:HB	1.93	0.51
1:B:421:ARG:HA	1:B:426:VAL:HG23	1.92	0.51
1:B:650:LEU:HD12	1:B:650:LEU:C	2.35	0.51
1:A:570:ASN:OD1	1:B:236:PRO:HD3	2.11	0.51
1:A:862:ILE:CD1	1:A:866:VAL:HG21	2.37	0.51
1:B:433:ILE:C	1:B:435:LYS:H	2.18	0.51
1:A:309:LYS:HB3	1:A:344:THR:CG2	2.40	0.51
1:A:657:SER:HA	1:A:688:TYR:O	2.11	0.51
1:B:323:GLN:OE1	1:B:326:LYS:HD3	2.11	0.51
1:B:884:ARG:HH11	1:B:884:ARG:CB	2.23	0.51
1:A:326:LYS:CD	1:A:391:ILE:HG23	2.31	0.51
1:A:417:VAL:HG12	1:A:433:ILE:CD1	2.41	0.51
1:A:664:TYR:O	1:A:668:VAL:HG23	2.11	0.51
1:B:107:MET:HB2	1:B:396:MET:HE1	1.93	0.51
1:B:90:ILE:HG22	1:B:91:MET:HE2	1.93	0.50
1:A:264:LEU:HD13	1:A:264:LEU:C	2.36	0.50
1:A:421:ARG:HD2	1:A:421:ARG:C	2.36	0.50
1:B:462:LEU:HA	1:B:463:PRO:C	2.36	0.50
1:B:509:LYS:HG2	1:B:510:SER:N	2.26	0.50
1:A:328:LYS:HG3	1:A:332:TYR:CE1	2.46	0.50
1:A:350:ASP:O	1:A:351:TRP:O	2.28	0.50
1:A:828:PHE:CE2	1:B:653:PRO:HB2	2.46	0.50
1:B:324:THR:O	1:B:328:LYS:HG2	2.12	0.50
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.93	0.50
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.40	0.50
1:B:429:SER:C	1:B:431:ALA:N	2.69	0.50
1:B:140:GLN:O	1:B:143:ILE:HG13	2.12	0.50
1:B:250:LEU:C	1:B:252:ASN:H	2.20	0.50
1:A:298:TRP:O	1:A:299:ASP:C	2.54	0.50
1:B:288:ASN:HD22	1:B:384:THR:HG23	1.77	0.50
1:B:312:GLN:O	1:B:316:GLU:HG2	2.12	0.50
1:B:844:ASP:O	1:B:848:VAL:HG23	2.12	0.50
1:A:252:ASN:HA	2:A:1107:HOH:O	2.11	0.50
1:A:637:GLY:O	1:A:641:GLU:HG3	2.12	0.50
1:A:417:VAL:O	1:A:420:ILE:HG22	2.12	0.49
1:A:794:ASP:HA	1:A:816:PRO:O	2.11	0.49
1:B:255:PHE:HB2	1:B:385:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.42	0.49
1:A:273:LYS:HA	1:A:319:ASP:CG	2.38	0.49
1:B:260:ASN:ND2	1:B:392:LYS:HE3	2.27	0.49
1:A:56:ILE:HA	2:A:1053:HOH:O	2.11	0.49
1:A:265:ASP:HB2	1:B:521:ASP:O	2.12	0.49
1:A:268:VAL:HG13	2:A:978:HOH:O	2.12	0.49
1:B:99:LYS:HE2	1:B:167:GLN:OE1	2.13	0.49
1:A:325:PHE:C	1:A:327:SER:N	2.70	0.49
1:A:569:ILE:HG21	1:B:194:MET:HG3	1.93	0.49
1:A:329:ASP:O	1:A:332:TYR:HB3	2.12	0.49
1:B:90:ILE:O	1:B:94:LEU:HG	2.13	0.49
1:B:421:ARG:HD3	1:B:428:VAL:HG12	1.94	0.49
1:A:98:LYS:CE	1:A:436:LEU:HD12	2.43	0.49
1:A:231:GLY:C	1:B:569:ILE:HD12	2.38	0.49
1:B:747:LYS:HD2	1:B:747:LYS:N	2.27	0.49
1:A:714:TYR:HA	2:A:970:HOH:O	2.13	0.49
1:B:58:ASN:OD1	1:B:315:ASN:ND2	2.34	0.49
1:A:298:TRP:O	1:A:301:LEU:N	2.45	0.49
1:B:477:SER:O	1:B:480:ASP:HB2	2.13	0.49
1:B:638:LEU:HD21	1:B:828:PHE:CD1	2.47	0.49
1:B:177:TYR:CD2	1:B:192:VAL:HG11	2.48	0.49
1:B:322:TYR:O	1:B:326:LYS:HG2	2.13	0.49
1:B:452:HIS:O	1:B:456:GLN:HG2	2.13	0.49
1:A:128:ARG:NH2	2:A:1071:HOH:O	2.45	0.48
1:A:237:GLU:CD	1:A:237:GLU:H	2.20	0.48
1:B:431:ALA:O	1:B:434:GLU:OE1	2.31	0.48
1:B:476:PRO:HB3	2:B:950:HOH:O	2.13	0.48
1:A:157:LEU:HD13	1:A:174:LEU:HD21	1.94	0.48
1:A:601:MET:HE2	1:A:641:GLU:C	2.37	0.48
1:A:729:LEU:HD11	1:A:792:MET:HE3	1.95	0.48
1:B:239:LYS:HA	1:B:242:ILE:HG23	1.94	0.48
1:B:423:ARG:O	1:B:423:ARG:HD3	2.13	0.48
1:A:638:LEU:HD21	1:A:828:PHE:HD1	1.77	0.48
1:A:302:LEU:HD23	1:A:310:LEU:HD13	1.95	0.48
1:B:261:LEU:HA	1:B:274:ILE:HD12	1.94	0.48
1:B:262:GLN:OE1	1:B:392:LYS:HB3	2.14	0.48
1:B:415:ASP:C	1:B:417:VAL:H	2.22	0.48
1:B:629:GLY:HA3	1:B:802:ASP:OD2	2.13	0.48
1:A:274:ILE:HG13	1:A:278:LEU:CD2	2.44	0.48
1:A:60:ILE:HG21	1:A:311:ILE:CD1	2.44	0.48
1:A:326:LYS:HZ2	1:A:326:LYS:HB3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:O	1:A:332:TYR:N	2.47	0.48
1:A:341:TYR:C	1:A:343:GLU:H	2.22	0.48
1:A:524:ARG:NH1	1:A:529:GLU:OE2	2.47	0.48
1:A:526:PHE:O	1:A:527:GLY:C	2.56	0.48
1:A:214:ARG:HB3	1:A:216:LEU:CD1	2.44	0.48
1:A:340:LYS:HB2	1:A:340:LYS:HZ3	1.79	0.48
1:A:342:PRO:HD3	2:A:960:HOH:O	2.14	0.48
1:A:351:TRP:CD1	1:A:351:TRP:H	2.32	0.48
1:A:433:ILE:HG23	1:A:434:GLU:N	2.29	0.48
1:B:524:ARG:CG	1:B:524:ARG:HH11	2.26	0.48
1:A:331:ALA:HB2	1:A:353:ASP:OD2	2.13	0.47
1:B:106:HIS:N	1:B:106:HIS:CD2	2.81	0.47
1:A:325:PHE:O	1:A:326:LYS:C	2.56	0.47
2:A:890:HOH:O	1:B:192:VAL:HG22	2.12	0.47
1:B:421:ARG:HA	1:B:426:VAL:CG2	2.44	0.47
1:A:508:ASN:OD1	1:A:510:SER:HB3	2.14	0.47
1:B:97:SER:O	1:B:98:LYS:C	2.57	0.47
1:B:178:PRO:HA	1:B:187:TRP:CD1	2.49	0.47
1:A:325:PHE:HE1	1:A:336:HIS:HB2	1.79	0.47
1:A:300:GLU:OE2	1:A:303:ARG:NH1	2.48	0.47
1:A:519:ILE:HD11	1:A:528:MET:HE2	1.95	0.47
1:B:397:GLY:O	1:B:398:ASP:C	2.57	0.47
1:A:177:TYR:HB3	1:A:192:VAL:HG13	1.96	0.47
1:A:351:TRP:CH2	1:A:359:LEU:HD21	2.50	0.47
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.95	0.47
1:A:728:LEU:HD12	1:A:742:ALA:HB2	1.96	0.47
1:B:85:ILE:CG1	1:B:153:LEU:HD22	2.44	0.47
1:B:145:PRO:HG3	1:B:165:PHE:CZ	2.50	0.47
1:B:274:ILE:HG12	1:B:319:ASP:OD2	2.13	0.47
1:B:505:MET:CE	1:B:674:LEU:HD13	2.44	0.47
1:A:305:ASP:C	1:A:307:SER:N	2.70	0.47
1:A:519:ILE:CG2	1:A:520:ALA:N	2.77	0.47
1:A:638:LEU:HB3	1:B:179:HIS:ND1	2.30	0.47
1:B:150:ARG:O	1:B:154:GLU:HG3	2.15	0.47
1:B:168:GLU:OE1	1:B:175:SER:OG	2.26	0.47
1:A:395:GLY:O	1:A:419:HIS:HE1	1.98	0.47
1:B:151:ALA:HB3	1:B:157:LEU:HD12	1.96	0.47
1:A:302:LEU:CD2	1:A:310:LEU:HD13	2.45	0.47
1:A:526:PHE:HB3	1:A:597:ILE:HD13	1.97	0.47
1:A:775:ASN:OD1	1:A:784:ARG:N	2.43	0.47
1:A:859:ARG:CZ	1:A:861:GLU:OE1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:THR:HG21	1:B:617:GLN:HG2	1.96	0.47
1:A:111:GLN:HA	1:A:111:GLN:OE1	2.15	0.46
1:A:398:ASP:CG	1:A:399:ALA:H	2.23	0.46
1:B:282:PHE:CE2	1:B:385:VAL:HG21	2.50	0.46
1:B:725:LYS:HD2	1:B:795:ALA:CB	2.45	0.46
1:B:418:ARG:HD3	1:B:430:ASP:OD1	2.16	0.46
1:B:433:ILE:O	1:B:435:LYS:N	2.49	0.46
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.80	0.46
1:B:627:THR:HB	1:B:633:LEU:HD22	1.96	0.46
1:A:197:GLY:N	1:A:198:PRO:HD2	2.31	0.46
1:A:333:VAL:O	1:A:335:GLU:N	2.49	0.46
1:A:819:ASP:OD1	1:A:855:GLU:HG2	2.16	0.46
1:B:192:VAL:O	1:B:194:MET:HE2	2.16	0.46
1:B:488:GLN:OE1	1:B:500:ARG:NH1	2.47	0.46
1:B:527:GLY:C	1:B:529:GLU:OE1	2.59	0.46
1:B:725:LYS:HE3	1:B:754:ASP:OD2	2.16	0.46
1:A:302:LEU:HD21	1:A:314:MET:HE1	1.98	0.46
1:B:361:ARG:HD3	1:B:389:HIS:NE2	2.31	0.46
1:B:164:ASN:ND2	1:B:172:ASN:ND2	2.64	0.46
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.46	0.46
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.84	0.45
1:A:821:ARG:HD2	1:A:851:ALA:HB1	1.98	0.45
1:B:76:GLU:CD	1:B:76:GLU:N	2.74	0.45
1:B:260:ASN:HA	1:B:390:THR:O	2.15	0.45
1:B:287:TRP:CE3	1:B:385:VAL:CG2	2.98	0.45
1:B:417:VAL:C	1:B:419:HIS:N	2.73	0.45
1:B:466:GLN:NE2	1:B:468:ASN:O	2.49	0.45
1:B:652:ILE:HD13	1:B:686:TYR:OH	2.16	0.45
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.96	0.45
1:B:147:VAL:HG11	1:B:187:TRP:CH2	2.51	0.45
1:A:233:MET:O	1:A:239:LYS:NZ	2.49	0.45
1:A:456:GLN:HA	1:A:456:GLN:HE21	1.81	0.45
1:A:82:ARG:O	1:A:85:ILE:HB	2.16	0.45
1:A:136:LEU:HD13	1:A:587:THR:HG21	1.98	0.45
1:A:725:LYS:HD3	1:A:726:VAL:N	2.31	0.45
1:B:428:VAL:HG22	1:B:433:ILE:HG13	1.98	0.45
1:A:60:ILE:HG22	1:A:314:MET:SD	2.56	0.45
1:B:518:ILE:O	1:B:596:TYR:HA	2.17	0.45
1:B:583:THR:O	1:B:587:THR:HG22	2.17	0.45
1:A:595:PHE:CE2	1:A:622:PHE:CD1	3.04	0.45
1:A:664:TYR:CG	1:A:701:MET:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ALA:O	1:A:769:GLN:HG3	2.16	0.45
1:A:779:PRO:HG2	1:A:780:LEU:HD13	1.99	0.45
1:A:805:LYS:HB2	1:B:769:GLN:NE2	2.32	0.45
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.17	0.45
1:A:374:LYS:HG3	1:A:378:GLU:OE2	2.17	0.45
1:A:491:GLU:OE1	1:A:696:TYR:HA	2.17	0.45
1:A:775:ASN:OD1	1:A:783:PRO:HA	2.17	0.45
1:B:318:VAL:HA	2:B:992:HOH:O	2.16	0.45
1:A:318:VAL:O	1:A:319:ASP:C	2.59	0.45
1:B:288:ASN:ND2	1:B:384:THR:HG23	2.30	0.45
1:B:796:PRO:HA	2:B:1073:HOH:O	2.16	0.45
1:B:604:PHE:CE1	1:B:649:SER:HB3	2.53	0.44
1:A:507:LYS:HB3	1:A:507:LYS:HE2	1.73	0.44
1:B:263:ARG:NH1	1:B:266:GLY:O	2.51	0.44
1:B:421:ARG:HD3	1:B:428:VAL:CG1	2.47	0.44
1:A:261:LEU:HD12	1:A:323:GLN:OE1	2.17	0.44
1:A:319:ASP:O	1:A:320:GLY:C	2.61	0.44
1:A:340:LYS:HB2	1:A:340:LYS:HZ2	1.81	0.44
1:A:736:ARG:NH1	1:A:737:HIS:HE1	2.15	0.44
1:B:198:PRO:O	1:B:202:ILE:HG13	2.17	0.44
1:A:672:ASP:O	1:A:676:ARG:HG3	2.17	0.44
1:A:867:VAL:O	1:A:871:ILE:HG13	2.17	0.44
1:B:82:ARG:HE	1:B:86:ARG:NH2	2.15	0.44
1:B:634:ASN:HB2	1:B:832:ASP:O	2.16	0.44
1:B:843:VAL:O	1:B:843:VAL:CG1	2.66	0.44
1:A:352:THR:O	1:A:355:GLN:N	2.50	0.44
1:A:537:ILE:O	1:A:558:GLU:HA	2.17	0.44
1:B:288:ASN:O	1:B:384:THR:HG23	2.18	0.44
1:B:493:SER:HB2	1:B:692:LEU:O	2.18	0.44
1:B:656:ILE:HD11	1:B:685:VAL:HG21	1.99	0.44
1:B:871:ILE:HG23	1:B:876:ILE:CG2	2.48	0.44
1:A:103:LEU:O	1:B:635:GLY:HA3	2.18	0.44
1:A:207:PHE:CE1	1:A:581:ALA:HB2	2.53	0.44
1:A:305:ASP:O	1:A:307:SER:N	2.50	0.44
1:A:498:PHE:CE1	1:A:624:ILE:HG13	2.52	0.44
1:B:521:ASP:HA	1:B:566:GLN:OE1	2.17	0.44
1:B:718:THR:HA	1:B:753:SER:O	2.17	0.44
1:A:318:VAL:O	1:A:321:ASP:HB2	2.18	0.44
1:B:497:ALA:HB2	1:B:663:ALA:HB2	2.00	0.44
1:B:745:LEU:HB3	1:B:751:VAL:HB	2.00	0.44
1:B:287:TRP:HE3	1:B:385:VAL:HG23	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:OD1	1:B:418:ARG:HD3	2.17	0.44
1:B:782:THR:HA	1:B:783:PRO:HD3	1.86	0.44
1:A:263:ARG:HD2	1:B:521:ASP:OD1	2.18	0.43
1:A:356:ILE:HG22	1:A:357:TRP:N	2.33	0.43
1:A:520:ALA:O	1:A:522:GLU:N	2.49	0.43
1:A:774:TRP:CZ3	1:A:784:ARG:HG3	2.53	0.43
1:A:821:ARG:HH22	1:A:854:GLY:HA3	1.82	0.43
1:B:87:TRP:CE2	1:B:91:MET:HE3	2.53	0.43
1:B:195:GLY:O	1:B:198:PRO:HD2	2.18	0.43
1:B:226:ALA:HB3	1:B:255:PHE:CD1	2.53	0.43
1:A:143:ILE:HD12	1:A:147:VAL:HG23	1.99	0.43
1:A:601:MET:CE	1:A:641:GLU:O	2.66	0.43
1:B:230:ASP:OD2	1:B:259:CYS:HA	2.18	0.43
1:B:358:ALA:O	1:B:359:LEU:C	2.59	0.43
1:A:567:GLU:OE1	1:A:567:GLU:HA	2.18	0.43
1:A:90:ILE:HD12	1:A:420:ILE:CD1	2.44	0.43
1:A:363:GLY:O	1:A:369:ILE:HD11	2.18	0.43
1:A:399:ALA:O	1:A:400:ALA:HB2	2.19	0.43
1:B:522:GLU:C	1:B:524:ARG:N	2.76	0.43
1:A:521:ASP:OD1	1:B:264:LEU:HD23	2.17	0.43
1:B:74:ASN:CG	1:B:77:LEU:HB2	2.43	0.43
1:B:261:LEU:HA	1:B:274:ILE:CD1	2.49	0.43
1:B:658:TYR:CG	1:B:669:ILE:HD13	2.53	0.43
1:B:871:ILE:HG23	1:B:876:ILE:HG22	2.01	0.43
1:A:332:TYR:O	1:A:336:HIS:ND1	2.51	0.43
1:B:158:THR:OG1	1:B:161:GLN:HG3	2.18	0.43
1:A:230:ASP:OD2	1:A:259:CYS:HA	2.19	0.43
1:B:157:LEU:HA	1:B:161:GLN:OE1	2.19	0.43
1:B:601:MET:HE1	1:B:644:HIS:HE1	1.84	0.43
1:B:800:SER:OG	1:B:843:VAL:HG13	2.18	0.43
1:A:260:ASN:C	1:A:262:GLN:H	2.26	0.43
1:B:739:ARG:HG2	1:B:755:VAL:HG11	2.01	0.43
1:A:159:GLN:HG3	1:A:438:TYR:CD2	2.53	0.43
1:A:305:ASP:CB	1:A:347:LEU:HD11	2.48	0.43
1:A:310:LEU:O	1:A:314:MET:HG3	2.18	0.43
1:B:427:PRO:HG2	1:B:439:ILE:HD13	2.01	0.43
1:A:874:PHE:HZ	2:A:1068:HOH:O	2.01	0.43
1:A:128:ARG:NH2	1:A:464:SER:OG	2.51	0.42
1:A:426:VAL:O	1:A:428:VAL:N	2.49	0.42
1:A:832:ASP:OD2	1:B:169:VAL:CB	2.65	0.42
1:B:398:ASP:C	1:B:400:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:C	1:A:155:GLY:H	2.27	0.42
1:B:420:ILE:C	1:B:422:ASP:H	2.28	0.42
1:A:248:GLU:O	1:A:249:LYS:C	2.61	0.42
1:A:352:THR:C	1:A:354:GLU:N	2.77	0.42
1:A:698:MET:HB3	2:A:1120:HOH:O	2.19	0.42
1:A:714:TYR:CE1	1:A:757:SER:HB3	2.54	0.42
1:A:395:GLY:C	1:A:397:GLY:H	2.28	0.42
1:A:598:TYR:HB2	2:A:927:HOH:O	2.20	0.42
1:A:375:LYS:O	1:A:375:LYS:HD3	2.19	0.42
1:A:525:THR:HG21	1:A:599:TYR:OH	2.19	0.42
1:A:531:LEU:HA	1:A:534:GLN:HB3	2.02	0.42
1:B:529:GLU:C	1:B:531:LEU:N	2.76	0.42
1:B:729:LEU:N	1:B:729:LEU:HD12	2.35	0.42
1:A:63:ILE:HA	1:A:64:PRO:HD2	1.88	0.42
1:A:193:SER:HB3	1:A:196:LEU:HD12	2.01	0.42
1:A:540:PRO:HA	1:A:560:GLU:HB3	2.00	0.42
1:A:807:PHE:O	1:A:810:GLN:HG2	2.19	0.42
1:B:447:GLU:OE1	1:B:447:GLU:N	2.46	0.42
1:B:771:CYS:HB3	1:B:784:ARG:O	2.18	0.42
1:A:297:ARG:HG2	1:A:297:ARG:HH11	1.84	0.42
1:A:601:MET:HG2	1:A:639:GLN:O	2.19	0.42
1:A:633:LEU:HD23	1:A:640:HIS:HB3	2.01	0.42
1:B:453:ALA:O	1:B:457:LYS:HG3	2.20	0.42
1:B:723:LYS:HB2	1:B:750:GLY:O	2.19	0.42
1:A:101:LEU:HD13	1:B:833:SER:HB3	2.01	0.42
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.55	0.42
1:B:140:GLN:HG3	1:B:227:PHE:HB3	2.01	0.42
1:A:187:TRP:O	1:A:465:ARG:HD2	2.20	0.42
1:B:61:ASN:HA	1:B:291:LYS:O	2.20	0.42
1:B:130:GLU:CD	1:B:131:GLN:NE2	2.73	0.42
1:B:268:VAL:HG12	1:B:269:THR:HG23	2.02	0.42
1:A:93:VAL:HG21	1:A:106:HIS:O	2.20	0.42
1:A:341:TYR:O	1:A:343:GLU:N	2.52	0.42
1:B:77:LEU:HD21	1:B:446:GLU:HG2	2.01	0.42
1:B:421:ARG:NH1	1:B:421:ARG:CG	2.74	0.42
1:B:786:PRO:O	1:B:787:TYR:C	2.63	0.42
1:A:332:TYR:CZ	1:A:336:HIS:NE2	2.88	0.41
1:A:432:ASP:O	1:A:437:PRO:HD3	2.20	0.41
1:A:734:ILE:HG13	1:A:801:THR:C	2.44	0.41
1:B:260:ASN:C	1:B:261:LEU:HG	2.45	0.41
1:B:626:GLY:O	1:B:627:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:NZ	1:A:317:THR:O	2.40	0.41
1:A:726:VAL:O	1:A:753:SER:HA	2.20	0.41
1:A:764:LEU:HD13	1:A:788:ILE:HD12	2.02	0.41
1:A:885:LEU:C	1:A:886:ALA:OXT	2.62	0.41
1:A:260:ASN:HB3	1:A:390:THR:OG1	2.20	0.41
1:A:329:ASP:O	1:A:330:GLY:O	2.37	0.41
1:B:332:TYR:CE1	1:B:336:HIS:CG	3.08	0.41
1:B:417:VAL:C	1:B:419:HIS:H	2.28	0.41
1:A:326:LYS:CB	1:A:326:LYS:NZ	2.78	0.41
1:A:329:ASP:O	1:A:332:TYR:CB	2.68	0.41
1:A:749:TYR:C	1:A:751:VAL:H	2.27	0.41
1:B:318:VAL:C	1:B:320:GLY:N	2.77	0.41
1:A:529:GLU:HG2	1:A:530:GLY:H	1.86	0.41
1:A:716:LEU:HD23	1:A:716:LEU:HA	1.87	0.41
1:B:197:GLY:N	1:B:198:PRO:CD	2.83	0.41
1:B:418:ARG:HG2	1:B:418:ARG:NH1	2.34	0.41
1:B:93:VAL:O	1:B:96:ALA:HB3	2.20	0.41
1:A:274:ILE:HG13	1:A:278:LEU:HD22	2.02	0.41
1:B:62:THR:HB	1:B:290:ILE:HG23	2.02	0.41
1:B:529:GLU:HG2	1:B:530:GLY:N	2.35	0.41
1:B:651:THR:O	1:B:653:PRO:HD3	2.20	0.41
1:A:164:ASN:CB	1:A:173:GLY:HA2	2.51	0.41
1:A:263:ARG:O	1:A:264:LEU:C	2.63	0.41
1:A:294:TRP:HA	1:A:362:GLY:H	1.86	0.41
1:A:604:PHE:O	1:A:608:GLY:N	2.52	0.41
1:B:350:ASP:OD1	1:B:350:ASP:N	2.53	0.41
1:B:785:VAL:HA	1:B:786:PRO:HD3	1.96	0.41
1:A:88:ASN:OD1	1:A:438:TYR:HA	2.21	0.41
1:A:269:THR:HA	2:A:964:HOH:O	2.21	0.41
1:A:327:SER:O	1:A:328:LYS:HG2	2.20	0.41
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.84	0.41
1:B:106:HIS:CE1	1:B:142[A]:HIS:ND1	2.89	0.41
1:B:522:GLU:HB3	1:B:525:THR:HB	2.02	0.41
1:B:525:THR:O	1:B:525:THR:HG22	2.19	0.41
1:B:734:ILE:HG12	1:B:802:ASP:HB2	2.03	0.41
1:B:736:ARG:HD3	2:B:910:HOH:O	2.21	0.41
1:B:857:ALA:C	1:B:859:ARG:H	2.29	0.41
1:A:333:VAL:C	1:A:335:GLU:N	2.71	0.41
1:A:509:LYS:CG	1:A:510:SER:N	2.83	0.41
2:A:1031:HOH:O	1:B:885:LEU:HD23	2.20	0.40
1:B:317:THR:CG2	1:B:321:ASP:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:HA	1:A:217:LYS:CE	2.50	0.40
1:A:216:LEU:HD23	1:A:592:MET:SD	2.62	0.40
1:A:313:LEU:HD21	1:A:337:PHE:O	2.21	0.40
1:A:328:LYS:HD3	1:A:328:LYS:HA	1.87	0.40
1:A:352:THR:O	1:A:354:GLU:N	2.54	0.40
1:A:472:LYS:NZ	1:A:474:GLU:OE2	2.32	0.40
1:A:521:ASP:HA	1:A:566:GLN:OE1	2.22	0.40
1:A:647:ILE:HG22	1:B:647:ILE:HG22	2.03	0.40
1:B:365:ASP:OD1	1:B:365:ASP:C	2.64	0.40
1:A:148:TYR:CD2	1:A:174:LEU:HD13	2.56	0.40
1:A:274:ILE:O	1:A:278:LEU:HD22	2.21	0.40
1:A:275:ILE:HD13	1:A:293:MET:HE1	2.02	0.40
1:B:354:GLU:O	1:B:357:TRP:N	2.54	0.40
1:A:214:ARG:NH2	2:A:928:HOH:O	2.48	0.40
1:A:735:LEU:O	1:A:738:VAL:HG22	2.21	0.40
1:B:274:ILE:CG1	1:B:319:ASP:OD2	2.70	0.40
1:A:71:TYR:HA	1:A:72:PRO:HD2	1.96	0.40
1:A:638:LEU:HD23	1:A:828:PHE:HB3	2.02	0.40
1:A:727:GLN:HG2	1:A:754:ASP:HB2	2.04	0.40
1:A:866:VAL:HG23	1:A:867:VAL:N	2.35	0.40
1:B:325:PHE:O	1:B:328:LYS:HB2	2.21	0.40
1:B:354:GLU:O	1:B:355:GLN:C	2.64	0.40
1:B:737:HIS:CE1	1:B:838:ARG:NH1	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	796/886 (90%)	712 (89%)	68 (8%)	16 (2%)	6 4
1	B	796/886 (90%)	722 (91%)	67 (8%)	7 (1%)	14 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1592/1772 (90%)	1434 (90%)	135 (8%)	23 (1%)	9 8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	LEU
1	A	326	LYS
1	A	330	GLY
1	A	351	TRP
1	A	398	ASP
1	B	398	ASP
1	A	306	THR
1	A	331	ALA
1	A	334	ARG
1	A	399	ALA
1	A	269	THR
1	A	522	GLU
1	A	723	LYS
1	B	432	ASP
1	B	489	SER
1	A	328	LYS
1	A	342	PRO
1	A	353	ASP
1	B	434	GLU
1	B	570	ASN
1	A	178	PRO
1	B	416	GLY
1	B	184	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	666/735 (91%)	631 (95%)	35 (5%)	20 29
1	B	666/735 (91%)	623 (94%)	43 (6%)	15 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1332/1470 (91%)	1254 (94%)	78 (6%)	18	25

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	A	172	ASN
1	A	182	LEU
1	A	251	ASP
1	A	263	ARG
1	A	264	LEU
1	A	269	THR
1	A	278	LEU
1	A	301	LEU
1	A	306	THR
1	A	310	LEU
1	A	326	LYS
1	A	340	LYS
1	A	342	PRO
1	A	350	ASP
1	A	354	GLU
1	A	356	ILE
1	A	375	LYS
1	A	420	ILE
1	A	437	PRO
1	A	502	LEU
1	A	525	THR
1	A	666	VAL
1	A	674	LEU
1	A	675	GLU
1	A	685	VAL
1	A	716	LEU
1	A	725	LYS
1	A	738	VAL
1	A	744	ILE
1	A	759	THR
1	A	776	MET
1	A	780	LEU
1	A	867	VAL
1	A	885	LEU
1	B	65	VAL
1	B	66	GLU

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Mol	Chain	Res	Type
1	B	77	LEU
1	B	106	HIS
1	B	153	LEU
1	B	156	ARG
1	B	180	PRO
1	B	192	VAL
1	B	196	LEU
1	B	209	LYS
1	B	211	LEU
1	B	228	LEU
1	B	230	ASP
1	B	232	GLU
1	B	243	THR
1	B	244	ILE
1	B	274	ILE
1	B	289	VAL
1	B	301	LEU
1	B	306	THR
1	B	343	GLU
1	B	378	GLU
1	B	398	ASP
1	B	421	ARG
1	B	433	ILE
1	B	435	LYS
1	B	475	LEU
1	B	490	LYS
1	B	502	LEU
1	B	509	LYS
1	B	522	GLU
1	B	524	ARG
1	B	529	GLU
1	B	533	ARG
1	B	537	ILE
1	B	539	SER
1	B	610	LEU
1	B	638	LEU
1	B	718	THR
1	B	725	LYS
1	B	772	GLU
1	B	780	LEU
1	B	858	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	271	ASN
1	A	323	GLN
1	A	355	GLN
1	A	389	HIS
1	A	419	HIS
1	A	456	GLN
1	A	466	GLN
1	A	479	GLN
1	A	588	ASN
1	A	695	ASN
1	A	697	HIS
1	A	737	HIS
1	A	839	HIS
1	B	106	HIS
1	B	131	GLN
1	B	164	ASN
1	B	170	HIS
1	B	288	ASN
1	B	377	GLN
1	B	454	GLN
1	B	534	GLN
1	B	695	ASN
1	B	697	HIS
1	B	737	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	801/886 (90%)	-1.51	0 100 100	2, 13, 35, 44	1 (0%)
1	B	801/886 (90%)	-1.53	0 100 100	3, 14, 31, 45	1 (0%)
All	All	1602/1772 (90%)	-1.52	0 100 100	2, 13, 34, 45	2 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.