



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:14 AM GMT

PDB ID : 2G67
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

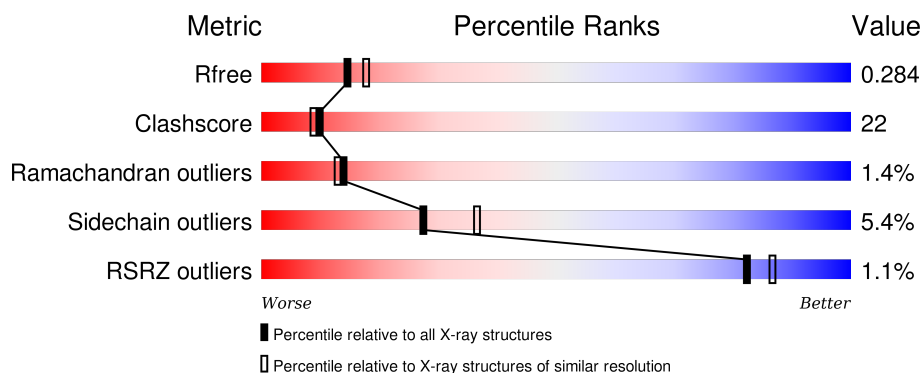
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	886	<div> <div></div> <div>52%</div> <div>34%</div> <div>•</div> <div>10%</div> </div>
1	B	886	<div> <div></div> <div>56%</div> <div>31%</div> <div>•</div> <div>10%</div> </div>

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			

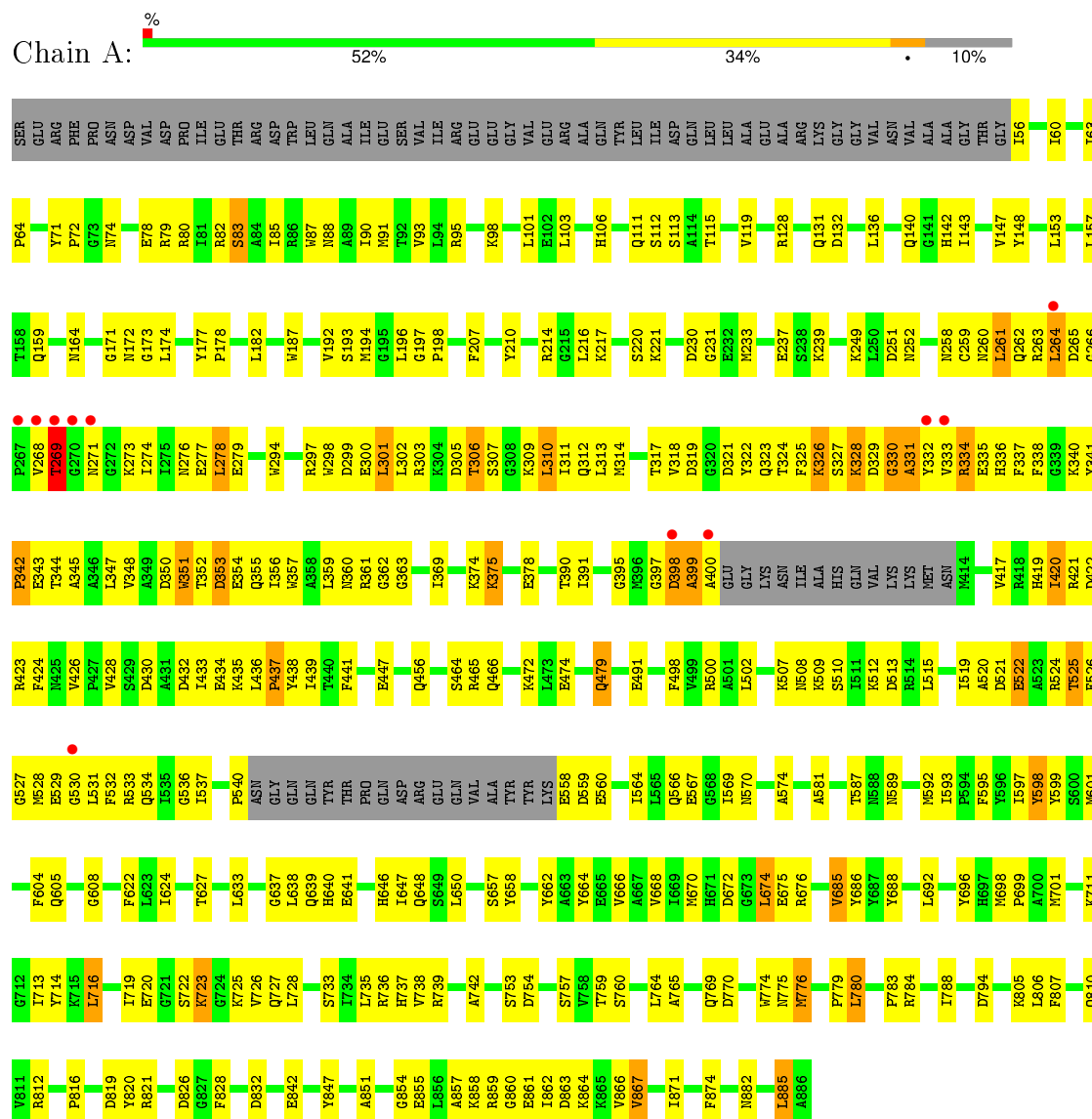
- Molecule 2 is water.

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

• Molecule 1: Pyruvate dehydrogenase E1 component



• Molecule 1: Pyruvate dehydrogenase E1 component



K858	H737	Y596	D513	D430	E433	L250	H164	T62	SER
R859	V738	I597	R514	A431	E434	D251	F165	I63	GLU
I871	R739	Y598	I515	D432	A346	N252	F166	P64	ARG
I876	Y599	Y599	V516	I433	A346	F255	Q167	V65	PHE
	L745	F604	I517	E434	A349		E168	E66	PRO
	A746	R605	I518	K435	A349	C259	V169		ASN
	K747	R606	I519	L436	D350	N260	H170	N74	ASP
			A520	F437	R351	L261	G171	L75	VAL
	G750	L610	E522	I439	E354	Q262	N172	E76	ASP
	V751		A523		E354	R263		L77	PRO
	S753		R524	E446	E357	L264	S175	E78	ILE
	D754		T525	E447		D265	S176	R79	GLU
	V755		F526			G266	Y177		THR
			G527			P267	P178	R82	ARG
	Q769		M528	A453	R361	V268	H179	I85	ASP
	D770		E529		G362	T269		W87	TRP
	E771		G530	Q456	G363		P184		LEU
	E772		L531	K457	E378				GLN
			F532	L462	T384	K273	H187	I90	ALA
	P779		R533	P463	V385	I274	Q188		ILE
			I537				F189	V93	GLU
	T782		Y538	L466	H389	L278	P190		SER
	P783		S539	Q467	T390	E279	T191	L94	VAL
	R784		F540	K468	K392		V192	R95	ILE
	V785		ASN		K392	F282	S193	A96	ARG
	P786		GLY	E471		W287	H194	S97	GLU
			GLN	L475	D397	N288	G195	K99	GLU
	M792		GLN	P476	D398	V289	L196		GLY
	A795		TYR	S477	A399	K291	G197	L103	VAL
	P796		THR		A400		P198		GLU
			PRO	D480	GLU	D299	T202	H106	ARG
	S800		GLN		GLY	E300	K206		ALA
	T801		ASP	A483	LYS	L301	F207	Q111	GLN
	D802		ARG		ASN	E306	L208	E130	TYR
	Y803		GLU	E486	ILE	T306	K209	Q131	ILE
			GLN		ALA		Y210		ASP
	L806		VAL	E487	HIS	K309	L211	Q140	GLN
			ALA	Q488	GLN			G141	LEU
	R821		TYR	S489	VAL	Q312	R214	H142	LEU
			TYR	K490	LYS			I143	ALA
	F828		LYS			N315	A226	S144	GLU
	G829		E558	S493	ASN	E316	F227	P145	ARG
			I564	A497	D414	T317	L228	G146	LYS
	D832		I565	F498	D415	V318	G229	V147	GLY
	S833		Q566	V499	G416	D319	D230	R150	GLY
			E567	B500	V417	G320	E231	A151	VAL
	R838		G568	A501	R418	D321	E232	F152	ASN
			I569	I502	H419	Y322	D233	L153	VAL
	V843		N570	I503	I420	Q323	D234	L153	ALA
	D844		A574	V504	R421	F325	P236	G155	ALA
	A845			I506	D422	K326		R156	GLY
	S846				R423	S327	K239	L157	THR
	S846					K328		T158	GLY
	Y847							T156	LYS
	V848							S57	
	V849							N58	
								E160	
	L853							Q159	
	L735							E161	
	R736							N61	

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 34.72 – 2.31	Depositor EDS
% Data completeness (in resolution range)	91.7 (34.62-2.32) 90.3 (34.72-2.31)	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	3615 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.0	EDS
Estimated twinning fraction	0.057 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 71362 reflections	Xtriage
F_o, F_c correlation	0.89	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/6495	0.72	1/8781 (0.0%)
1	B	0.50	0/6495	0.72	2/8781 (0.0%)
All	All	0.51	0/12990	0.72	3/17562 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	171	GLY	N-CA-C	5.40	126.60	113.10
1	A	171	GLY	N-CA-C	5.37	126.52	113.10
1	B	637	GLY	N-CA-C	5.16	126.00	113.10

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	315	0
1	B	6351	0	6185	259	0
2	A	241	0	0	22	0
2	B	207	0	0	10	0
All	All	13150	0	12370	553	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 22.

All (553) 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:B:490:LYS:CE	1:B:500:ARG:HH22	1.83	0.92
1:A:326:LYS:HD3	1:A:391:ILE:HG23	1.50	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:A:98:LYS:HZ3	1:A:436:LEU:HD12	1.35	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:ASN:O	1:B:78:GLU:HG3	1.79	0.81
1:A:140:GLN:O	1:A:143:ILE:HG13	1.80	0.81
1:B:471:GLU:HG2	2:B:932:HOH:O	1.80	0.80
1:A:882:ASN:HB3	1:A:885:LEU:HD22	1.64	0.80
1:A:666:VAL:O	1:A:670:MET:HG3	1.82	0.80
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
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:HD2	1:B:509:LYS:H	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:512:LYS:HG3	1:A:513:ASP:N	2.01	0.76
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.65	0.76
1:B:354:GLU:H	1:B:354:GLU:CD	1.88	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: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:B:274:ILE:O	1:B:278:LEU:HD23	1.90	0.72
1:A:352:THR:H	1:A:355:GLN:HB2	1.53	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: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:B:421:ARG:NH1	1:B:421:ARG:HG3	2.07	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:533:ARG:NH1	1:B:533:ARG:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ILE:CD1	1:A:528:MET:HG3	2.23	0.69
1:A:301:LEU:HD12	1:A:310:LEU:HD12	1.74	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:502:LEU:HD23	1:B:502:LEU:C	2.13	0.69
1:B:287:TRP:CE3	1:B:385:VAL:HG23	2.29	0.68
1:B:859:ARG:HB2	1:B:859:ARG:HH11	1.58	0.68
1:A:512:LYS:HG3	1:A:513:ASP:H	1.56	0.68
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: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:A:348:VAL:HB	1:A:356:ILE:HD11	1.74	0.68
1:B:522:GLU:HG2	1:B:599:TYR:OH	1.94	0.68
1:B:361:ARG:HD3	1:B:389:HIS:CD2	2.29	0.68
1:B:859:ARG:NH1	1:B:859:ARG:HB2	2.09	0.67
1:A:338:PHE:O	1:A:345:ALA:HB2	1.95	0.67
1:B:558:GLU:O	1:B:558:GLU:HG2	1.95	0.67
1:A:249:LYS:HE3	2:A:1100:HOH:O	1.93	0.67
1:B:529:GLU:OE1	1:B:529:GLU:N	2.28	0.67
1:A:309:LYS:HB3	1:A:344:THR:HG23	1.77	0.67
1:A:74:ASN:O	1:A:78:GLU:HG3	1.94	0.67
1:B:434:GLU:CD	1:B:434:GLU:H	1.98	0.66
1:B:130:GLU:CD	1:B:131:GLN:HE22	2.00	0.66
1:B:512:LYS:HG3	1:B:513:ASP:N	2.10	0.66
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:509:LYS:HD2	1:B:509:LYS:N	2.13	0.64
1:A:433:ILE:HG23	1:A:434:GLU:HG3	1.79	0.64
1:B:207:PHE:O	1:B:210:TYR:HB3	1.98	0.64
1:B:85:ILE:HG12	1:B:153:LEU:HD22	1.80	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:A:207:PHE:CZ	1:A:581:ALA:HA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLN:HG2	2:B:1068:HOH:O	1.98	0.62
1:A:132:ASP:HA	1:A:217:LYS:HE3	1.82	0.62
1:A:466:GLN:HE22	1:A:589:ASN:CG	2.04	0.61
1:A:177:TYR:CB	1:A:192:VAL:HG11	2.30	0.61
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: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:812:ARG:HD2	1:A:820:TYR:HD2	1.63	0.61
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.36	0.61
1:A:305:ASP:C	1:A:307:SER:H	2.04	0.61
1:A:857:ALA:HB1	1:A:864:LYS:HG2	1.82	0.60
1:A:627:THR:HB	1:A:633:LEU:HD13	1.83	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: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:B:509:LYS:H	1:B:509:LYS:CD	2.14	0.59
1:B:178:PRO:HA	1:B:187:TRP:CG	2.37	0.59
1:A:605:GLN:HB2	1:A:648:GLN:HE22	1.66	0.59
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.35	0.59
1:B:95:ARG:HD2	1:B:438:TYR:OH	2.02	0.59
1:A:164:ASN:HB2	1:A:173:GLY:HA2	1.85	0.59
1:A:500:ARG:NH1	2:A:1057:HOH:O	2.33	0.59
1:A:324:THR:O	1:A:328:LYS:HG2	2.02	0.59
1:A:326:LYS:CB	1:A:326:LYS:HZ2	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:HH11	1:B:418:ARG:HG2	1.68	0.58
1:A:857:ALA:O	1:A:860:GLY:N	2.37	0.58
1:B:354:GLU:CD	1:B:354:GLU:N	2.57	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:O	1:A:264:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:CD	1:B:66:GLU:H	2.07	0.58
1:B:638:LEU:HD23	1:B:829:GLY:O	2.03	0.57
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:420:ILE:HG13	1:B:421:ARG:N	2.19	0.57
1:B:533:ARG:HH11	1:B:533:ARG:CB	2.14	0.57
1:A:330:GLY:O	1:A:331:ALA:C	2.43	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:B:521:ASP:HB2	1:B:568:GLY:HA2	1.87	0.57
1:A:720:GLU:HA	2:A:1117:HOH:O	2.05	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:472:LYS:NZ	1:A:474:GLU:OE2	2.32	0.57
1:B:537:ILE:HD13	1:B:538:TYR:O	2.05	0.56
1:A:479:GLN:HG3	2:A:983:HOH:O	2.05	0.56
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.41	0.56
1:A:360:ASN:OD1	1:A:361:ARG:N	2.33	0.56
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.35	0.56
1:A:333:VAL:C	1:A:335:GLU:H	2.09	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:B:76:GLU:H	1:B:76:GLU:CD	2.09	0.56
1:B:64:PRO:HB2	1:B:66:GLU:OE2	2.06	0.56
1:A:260:ASN:O	1:A:262:GLN:N	2.38	0.56
1:A:530:GLY:HA2	1:A:533:ARG:NH1	2.20	0.56
1:A:142[O]:HIS:ND1	1:A:142[O]:HIS:N	2.51	0.56
1:A:863:ASP:O	1:A:866:VAL:HG22	2.05	0.56
1:A:214:ARG:HB3	1:A:216:LEU:HD13	1.87	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:B:198:PRO:HG3	1:B:228:LEU:CD2	2.32	0.55
1:A:207:PHE:O	1:A:210:TYR:HB3	2.06	0.55
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.88	0.55
1:A:220:SER:HA	2:A:1038:HOH:O	2.05	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:A:329:ASP:O	1:A:330:GLY:C	2.45	0.55
1:A:153:LEU:HD21	1:A:441:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ALA:HA	1:B:486:GLU:OE2	2.06	0.54
1:A:776:MET:HB2	1:B:821:ARG:NH1	2.22	0.54
1:A:328:LYS:HG3	1:A:332:TYR:CZ	2.43	0.54
1:A:271:ASN:O	1:A:318:VAL:HG21	2.07	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:859:ARG:NH1	1:A:861:GLU:OE1	2.41	0.54
1:A:115:THR:O	1:A:119:VAL:HG23	2.08	0.54
1:A:522:GLU:CG	1:A:599:TYR:HE1	2.20	0.54
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.89	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: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:417:VAL:CG1	1:A:433:ILE:HD11	2.37	0.53
1:A:131:GLN:OE1	1:A:221:LYS:HD2	2.08	0.53
1:A:770:ASP:OD1	1:B:882:ASN:ND2	2.40	0.53
1:B:729:LEU:HD11	1:B:792:MET:CE	2.38	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:584:SER:HA	1:B:587:THR:CG2	2.38	0.52
1:B:518:ILE:HG12	1:B:565:LEU:HB2	1.91	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:B:143:ILE:O	1:B:143:ILE:HD12	2.10	0.52
1:A:722:SER:O	1:A:723:LYS:CB	2.53	0.52
1:A:90:ILE:HG22	1:A:91:MET:HE2	1.91	0.52
1:B:429:SER:C	1:B:431:ALA:H	2.12	0.52
1:A:650:LEU:HD12	1:A:650:LEU:C	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:SER:HB3	1:A:258:ASN:ND2	2.25	0.51
1:B:421:ARG:HA	1:B:426:VAL:HG23	1.92	0.51
1:A:515:LEU:HD23	1:A:593:ILE:HB	1.93	0.51
1:A:862:ILE:CD1	1:A:866:VAL:HG21	2.37	0.51
1:A:570:ASN:OD1	1:B:236:PRO:HD3	2.11	0.51
1:A:309:LYS:HB3	1:A:344:THR:CG2	2.40	0.51
1:B:884:ARG:CB	1:B:884:ARG:HH11	2.23	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: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:B:537:ILE:HD13	1:B:537:ILE:C	2.32	0.51
1:A:664:TYR:O	1:A:668:VAL:HG23	2.11	0.51
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:828:PHE:CE2	1:B:653:PRO:HB2	2.46	0.50
1:A:350:ASP:O	1:A:351:TRP:O	2.28	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:140:GLN:O	1:B:143:ILE:HG13	2.12	0.50
1:B:195:GLY:C	1:B:198:PRO:HD2	2.32	0.50
1:B:844:ASP:O	1:B:848:VAL:HG23	2.12	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: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:B:433:ILE:C	1:B:435:LYS:N	2.65	0.49
1:B:255:PHE:HB2	1:B:385:VAL:HG22	1.94	0.49
1:A:417:VAL:O	1:A:420:ILE:HG22	2.12	0.49
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.42	0.49
1:A:794:ASP:HA	1:A:816:PRO:O	2.11	0.49
1:B:260:ASN:ND2	1:B:392:LYS:HE3	2.27	0.49
1:B:143:ILE:HD12	1:B:143:ILE:C	2.33	0.49
1:A:268:VAL:HG13	2:A:978:HOH:O	2.12	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:B:99:LYS:HE2	1:B:167:GLN:OE1	2.13	0.49
1:A:569:ILE:HG21	1:B:194:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASP:O	1:A:332:TYR:HB3	2.12	0.49
1:B:421:ARG:HD3	1:B:428:VAL:HG12	1.94	0.49
1:B:90:ILE:O	1:B:94:LEU:HG	2.13	0.49
1:A:98:LYS:CE	1:A:436:LEU:HD12	2.43	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:B:638:LEU:HD21	1:B:828:PHE:CD1	2.47	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:322:TYR:O	1:B:326:LYS:HG2	2.13	0.49
1:B:177:TYR:CD2	1:B:192:VAL:HG11	2.48	0.49
1:A:237:GLU:CD	1:B:606:ARG:HH21	2.16	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: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:B:65:VAL:HG21	1:B:299:ASP:CG	2.33	0.48
1:B:423:ARG:HD3	1:B:423:ARG:O	2.13	0.48
1:A:157:LEU:HD13	1:A:174:LEU:HD21	1.94	0.48
1:B:239:LYS:HA	1:B:242:ILE:HG23	1.94	0.48
1:A:638:LEU:HD21	1:A:828:PHE:HD1	1.77	0.48
1:B:261:LEU:HA	1:B:274:ILE:HD12	1.94	0.48
1:A:302:LEU:HD23	1:A:310:LEU:HD13	1.95	0.48
1:B:262:GLN:OE1	1:B:392:LYS:HB3	2.14	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:326:LYS:HB3	1:A:326:LYS:HZ2	1.76	0.48
1:A:330:GLY:O	1:A:332:TYR:N	2.47	0.48
1:A:524:ARG:NH1	1:A:529:GLU:OE2	2.47	0.48
1:A:60:ILE:HG21	1:A:311:ILE:CD1	2.44	0.48
1:A:433:ILE:HG23	1:A:434:GLU:N	2.29	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:B:524:ARG:HH11	1:B:524:ARG:CG	2.26	0.48
1:A:342:PRO:HD3	2:A:960:HOH:O	2.14	0.48
1:A:331:ALA:HB2	1:A:353:ASP:OD2	2.13	0.47
1:B:729:LEU:HD11	1:B:792:MET:HE3	1.95	0.47
1:B:106:HIS:CD2	1:B:106:HIS:N	2.81	0.47
1:B:421:ARG:HA	1:B:426:VAL:CG2	2.44	0.47
2:A:890:HOH:O	1:B:192:VAL:HG22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:MET:CE	1:B:674:LEU:HD13	2.44	0.47
1:B:178:PRO:HA	1:B:187:TRP:CD1	2.49	0.47
1:A:559:ASP:C	1:A:559:ASP:OD1	2.52	0.47
1:A:508:ASN:OD1	1:A:510:SER:HB3	2.14	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:177:TYR:HB3	1:A:192:VAL:HG13	1.96	0.47
1:B:274:ILE:HG12	1:B:319:ASP:OD2	2.13	0.47
1:A:857:ALA:O	1:A:858:LYS:C	2.53	0.47
1:A:351:TRP:CH2	1:A:359:LEU:HD21	2.50	0.47
1:B:85:ILE:CG1	1:B:153:LEU:HD22	2.44	0.47
1:A:728:LEU:HD12	1:A:742:ALA:HB2	1.96	0.47
1:B:145:PRO:HG3	1:B:165:PHE:CZ	2.50	0.47
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.95	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:B:650:LEU:HD12	1:B:650:LEU:C	2.35	0.47
1:A:859:ARG:CZ	1:A:861:GLU:OE1	2.63	0.47
1:A:526:PHE:HB3	1:A:597:ILE:HD13	1.97	0.47
1:A:302:LEU:CD2	1:A:310:LEU:HD13	2.45	0.47
1:B:583:THR:HG21	1:B:617:GLN:HG2	1.96	0.47
1:A:775:ASN:OD1	1:A:784:ARG:N	2.43	0.47
1:B:433:ILE:C	1:B:435:LYS:H	2.18	0.46
1:A:111:GLN:HA	1:A:111:GLN:OE1	2.15	0.46
1:B:282:PHE:CE2	1:B:385:VAL:HG21	2.50	0.46
1:A:194:MET:HE2	1:A:194:MET:N	2.31	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:429:SER:C	1:B:431:ALA:N	2.69	0.46
1:B:627:THR:HB	1:B:633:LEU:HD22	1.96	0.46
1:B:488:GLN:OE1	1:B:500:ARG:NH1	2.47	0.46
1:A:819:ASP:OD1	1:A:855:GLU:HG2	2.16	0.46
1:A:333:VAL:O	1:A:335:GLU:N	2.49	0.46
1:B:725:LYS:HE3	1:B:754:ASP:OD2	2.16	0.46
1:A:197:GLY:N	1:A:198:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LEU:HA	1:B:463:PRO:C	2.36	0.46
1:A:421:ARG:HD2	1:A:421:ARG:C	2.36	0.46
1:B:361:ARG:HD3	1:B:389:HIS:NE2	2.31	0.46
1:A:264:LEU:C	1:A:264:LEU:HD13	2.36	0.46
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.46	0.46
1:A:83:SER:HG	1:A:424:PHE:HB3	1.80	0.46
1:B:164:ASN:ND2	1:B:172:ASN:ND2	2.64	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:287:TRP:CE3	1:B:385:VAL:CG2	2.98	0.45
1:B:260:ASN:HA	1:B:390:THR:O	2.15	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:B:147:VAL:HG11	1:B:187:TRP:CH2	2.51	0.45
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.96	0.45
1:A:456:GLN:HA	1:A:456:GLN:HE21	1.81	0.45
1:A:233:MET:O	1:A:239:LYS:NZ	2.49	0.45
1:B:428:VAL:HG22	1:B:433:ILE:HG13	1.98	0.45
1:A:298:TRP:O	1:A:299:ASP:C	2.54	0.45
1:A:725:LYS:HD3	1:A:726:VAL:N	2.31	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:60:ILE:HG22	1:A:314:MET:SD	2.56	0.45
1:B:583:THR:O	1:B:587:THR:HG22	2.17	0.45
1:B:518:ILE:O	1:B:596:TYR:HA	2.17	0.45
1:B:250:LEU:C	1:B:252:ASN:H	2.20	0.45
1:A:805:LYS:HB2	1:B:769:GLN:NE2	2.32	0.45
1:A:664:TYR:CG	1:A:701:MET:HB2	2.52	0.45
1:A:595:PHE:CE2	1:A:622:PHE:CD1	3.04	0.45
1:A:779:PRO:HG2	1:A:780:LEU:HD13	1.99	0.45
1:A:765:ALA:O	1:A:769:GLN:HG3	2.16	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:B:318:VAL:HA	2:B:992:HOH:O	2.16	0.45
1:A:775:ASN:OD1	1:A:783:PRO:HA	2.17	0.45
1:A:273:LYS:HA	1:A:319:ASP:CG	2.38	0.45
1:A:491:GLU:OE1	1:A:696:TYR:HA	2.17	0.45
1:A:325:PHE:C	1:A:327:SER:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:HD3	1:B:428:VAL:CG1	2.47	0.44
1:B:263:ARG:NH1	1:B:266:GLY:O	2.51	0.44
1:A:507:LYS:HE2	1:A:507:LYS:HB3	1.73	0.44
1:A:333:VAL:C	1:A:335:GLU:N	2.71	0.44
1:B:198:PRO:O	1:B:202:ILE:HG13	2.17	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:A:261:LEU:HD12	1:A:323:GLN:OE1	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:A:672:ASP:O	1:A:676:ARG:HG3	2.17	0.44
1:A:231:GLY:C	1:B:569:ILE:HD12	2.38	0.44
1:B:843:VAL:CG1	1:B:843:VAL:O	2.66	0.44
1:A:537:ILE:O	1:A:558:GLU:HA	2.17	0.44
1:A:352:THR:O	1:A:355:GLN:N	2.50	0.44
1:A:601:MET:HE1	1:A:641:GLU:O	2.18	0.44
1:B:656:ILE:HD11	1:B:685:VAL:HG21	1.99	0.44
1:B:288:ASN:O	1:B:384:THR:HG23	2.18	0.44
1:B:871:ILE:HG23	1:B:876:ILE:CG2	2.48	0.44
1:B:493:SER:HB2	1:B:692:LEU:O	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:B:521:ASP:HA	1:B:566:GLN:OE1	2.17	0.44
1:A:498:PHE:CE1	1:A:624:ILE:HG13	2.52	0.44
1:A:103:LEU:O	1:B:635:GLY:HA3	2.18	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:745:LEU:HB3	1:B:751:VAL:HB	2.00	0.44
1:B:497:ALA:HB2	1:B:663:ALA:HB2	2.00	0.44
1:B:415:ASP:OD1	1:B:418:ARG:HD3	2.17	0.44
1:B:287:TRP:HE3	1:B:385:VAL:HG23	1.78	0.44
1:A:237:GLU:H	1:A:237:GLU:CD	2.20	0.44
1:B:782:THR:HA	1:B:783:PRO:HD3	1.86	0.44
1:A:821:ARG:HH22	1:A:854:GLY:HA3	1.82	0.43
1:A:520:ALA:O	1:A:522:GLU:N	2.49	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:356:ILE:HG22	1:A:357:TRP:N	2.33	0.43
1:A:263:ARG:HD2	1:B:521:ASP:OD1	2.18	0.43
1:A:774:TRP:CZ3	1:A:784:ARG:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:341:TYR:C	1:A:343:GLU:H	2.22	0.43
1:A:567:GLU:HA	1:A:567:GLU:OE1	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:261:LEU:HA	1:B:274:ILE:CD1	2.49	0.43
1:A:305:ASP:C	1:A:307:SER:N	2.70	0.43
1:B:871:ILE:HG23	1:B:876:ILE:HG22	2.01	0.43
1:B:658:TYR:CG	1:B:669:ILE:HD13	2.53	0.43
1:A:521:ASP:OD1	1:B:264:LEU:HD23	2.17	0.43
1:A:332:TYR:O	1:A:336:HIS:ND1	2.51	0.43
1:A:526:PHE:O	1:A:527:GLY:C	2.56	0.43
1:B:158:THR:OG1	1:B:161:GLN:HG3	2.18	0.43
1:B:157:LEU:HA	1:B:161:GLN:OE1	2.19	0.43
1:B:800:SER:OG	1:B:843:VAL:HG13	2.18	0.43
1:A:230:ASP:OD2	1:A:259:CYS:HA	2.19	0.43
1:B:739:ARG:HG2	1:B:755:VAL:HG11	2.01	0.43
1:B:415:ASP:C	1:B:417:VAL:H	2.22	0.43
1:A:310:LEU:O	1:A:314:MET:HG3	2.18	0.43
1:A:305:ASP:CB	1:A:347:LEU:HD11	2.48	0.43
1:B:427:PRO:HG2	1:B:439:ILE:HD13	2.01	0.43
1:A:159:GLN:HG3	1:A:438:TYR:CD2	2.53	0.43
1:A:325:PHE:O	1:A:326:LYS:C	2.56	0.43
1:B:97:SER:O	1:B:98:LYS:C	2.57	0.43
1:A:874:PHE:HZ	2:A:1068:HOH:O	2.01	0.43
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:A:128:ARG:NH2	1:A:464:SER:OG	2.51	0.42
1:A:714:TYR:CE1	1:A:757:SER:HB3	2.54	0.42
1:B:397:GLY:O	1:B:398:ASP:C	2.57	0.42
1:A:698:MET:HB3	2:A:1120:HOH:O	2.19	0.42
1:A:598:TYR:HB2	2:A:927:HOH:O	2.20	0.42
1:A:525:THR:HG21	1:A:599:TYR:OH	2.19	0.42
1:B:729:LEU:HD12	1:B:729:LEU:N	2.35	0.42
1:A:509:LYS:CG	1:A:510:SER:N	2.83	0.42
1:A:531:LEU:HA	1:A:534:GLN:HB3	2.02	0.42
1:A:375:LYS:O	1:A:375:LYS:HD3	2.19	0.42
1:A:807:PHE:O	1:A:810:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PRO:HA	1:A:560:GLU:HB3	2.00	0.42
1:A:193:SER:HB3	1:A:196:LEU:HD12	2.01	0.42
1:A:63:ILE:HA	1:A:64:PRO:HD2	1.88	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:HH11	1:A:297:ARG:HG2	1.84	0.42
1:A:633:LEU:HD23	1:A:640:HIS:HB3	2.01	0.42
1:A:601:MET:HG2	1:A:639:GLN:O	2.19	0.42
1:B:723:LYS:HB2	1:B:750:GLY:O	2.19	0.42
1:B:453:ALA:O	1:B:457:LYS:HG3	2.20	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:101:LEU:HD13	1:B:833:SER:HB3	2.01	0.42
1:B:268:VAL:HG12	1:B:269:THR:HG23	2.02	0.42
1:A:398:ASP:CG	1:A:399:ALA:H	2.23	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:421:ARG:NH1	1:B:421:ARG:CG	2.74	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:A:93:VAL:HG21	1:A:106:HIS:O	2.20	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:764:LEU:HD13	1:A:788:ILE:HD12	2.02	0.41
1:A:726:VAL:O	1:A:753:SER:HA	2.20	0.41
1:A:273:LYS:NZ	1:A:317:THR:O	2.40	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:A:260:ASN:HB3	1:A:390:THR:OG1	2.20	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:B:197:GLY:N	1:B:198:PRO:CD	2.83	0.41
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.34	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:527:GLY:C	1:B:529:GLU:OE1	2.59	0.41
1:B:729:LEU:HD11	1:B:792:MET:HE1	2.03	0.41
1:B:93:VAL:O	1:B:96:ALA:HB3	2.20	0.41
1:B:651:THR:O	1:B:653:PRO:HD3	2.20	0.41
1:B:529:GLU:HG2	1:B:530:GLY:N	2.35	0.41
1:A:274:ILE:HG13	1:A:278:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:HB	1:B:290:ILE:HG23	2.02	0.41
1:A:164:ASN:CB	1:A:173:GLY:HA2	2.51	0.41
1:A:294:TRP:HA	1:A:362:GLY:H	1.86	0.41
1:B:350:ASP:OD1	1:B:350:ASP:N	2.53	0.41
1:A:604:PHE:O	1:A:608:GLY:N	2.52	0.41
1:B:785:VAL:HA	1:B:786:PRO:HD3	1.96	0.41
1:A:327:SER:O	1:A:328:LYS:HG2	2.20	0.41
1:B:417:VAL:C	1:B:419:HIS:N	2.73	0.41
1:A:866:VAL:HG23	1:A:867:VAL:N	2.35	0.41
1:A:269:THR:HA	2:A:964:HOH:O	2.21	0.41
1:B:525:THR:O	1:B:525:THR:HG22	2.19	0.41
1:B:522:GLU:HB3	1:B:525:THR:HB	2.02	0.41
1:B:734:ILE:HG12	1:B:802:ASP:HB2	2.03	0.41
1:B:106:HIS:CE1	1:B:142[A]:HIS:ND1	2.89	0.41
1:A:88:ASN:OD1	1:A:438:TYR:HA	2.21	0.41
1:B:736:ARG:HD3	2:B:910:HOH:O	2.21	0.41
1:A:674:LEU:HA	1:A:674:LEU:HD23	1.84	0.41
1:A:685:VAL:CG1	1:A:686:TYR:N	2.83	0.40
1:B:317:THR:CG2	1:B:321:ASP:HB2	2.51	0.40
2:A:1031:HOH:O	1:B:885:LEU:HD23	2.20	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:216:LEU:HD23	1:A:592:MET:SD	2.62	0.40
1:A:132:ASP:HA	1:A:217:LYS:CE	2.50	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:A:313:LEU:HD21	1:A:337:PHE:O	2.21	0.40
1:B:354:GLU:O	1:B:357:TRP:N	2.54	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:B:274:ILE:CG1	1:B:319:ASP:OD2	2.70	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:A:638:LEU:HD23	1:A:828:PHE:HB3	2.02	0.40
1:B:325:PHE:O	1:B:328:LYS:HB2	2.21	0.40
1:A:71:TYR:HA	1:A:72:PRO:HD2	1.96	0.40
1:A:727:GLN:HG2	1:A:754:ASP:HB2	2.04	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

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	796/886 (90%)	712 (89%)	68 (8%)	16 (2%)	9	7
1	B	796/886 (90%)	722 (91%)	67 (8%)	7 (1%)	21	23
All	All	1592/1772 (90%)	1434 (90%)	135 (8%)	23 (1%)	14	13

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%)	637 (96%)	29 (4%)	35	47
1	B	666/735 (91%)	623 (94%)	43 (6%)	21	27
All	All	1332/1470 (91%)	1260 (95%)	72 (5%)	27	36

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	83	SER
1	A	112	SER
1	A	172	ASN
1	A	182	LEU
1	A	251	ASP
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	312	GLN
1	A	375	LYS
1	A	420	ILE
1	A	437	PRO
1	A	479	GLN
1	A	502	LEU
1	A	525	THR
1	A	674	LEU
1	A	675	GLU
1	A	685	VAL
1	A	711	LYS
1	A	716	LEU
1	A	759	THR
1	A	776	MET
1	A	780	LEU

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Mol	Chain	Res	Type
1	A	867	VAL
1	A	885	LEU
1	B	77	LEU
1	B	79	ARG
1	B	156	ARG
1	B	192	VAL
1	B	196	LEU
1	B	206	LYS
1	B	209	LYS
1	B	211	LEU
1	B	228	LEU
1	B	230	ASP
1	B	232	GLU
1	B	234	ASP
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	378	GLU
1	B	398	ASP
1	B	421	ARG
1	B	422	ASP
1	B	423	ARG
1	B	432	ASP
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	537	ILE
1	B	539	SER
1	B	566	GLN
1	B	610	LEU
1	B	638	LEU
1	B	718	THR
1	B	725	LYS

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Mol	Chain	Res	Type
1	B	747	LYS
1	B	772	GLU
1	B	832	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	355	GLN
1	A	419	HIS
1	A	456	GLN
1	A	466	GLN
1	A	737	HIS
1	B	106	HIS
1	B	131	GLN
1	B	164	ASN
1	B	288	ASN
1	B	377	GLN
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 carbohydrates 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%)	-0.16	11 (1%) 78 83	2, 13, 35, 44	0
1	B	801/886 (90%)	-0.23	6 (0%) 89 92	3, 14, 31, 45	0
All	All	1602/1772 (90%)	-0.19	17 (1%) 82 87	2, 13, 34, 45	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	PRO	4.9
1	B	400	ALA	4.4
1	A	268	VAL	4.2
1	B	399	ALA	3.3
1	A	269	THR	3.3
1	A	271	ASN	3.2
1	B	397	GLY	3.2
1	A	332	TYR	3.1
1	B	414	MET	3.0
1	A	270	GLY	2.6
1	A	333	VAL	2.6
1	A	400	ALA	2.6
1	B	417	VAL	2.3
1	B	415	ASP	2.3
1	A	530	GLY	2.2
1	A	264	LEU	2.1
1	A	398	ASP	2.0

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 carbohydrates 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.