



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:21 AM UTC

PDB ID : 1L8A / pdb_00001l8a
Title : E. COLI PYRUVATE DEHYDROGENASE
Authors : Furey, W.; Arjunan, P.
Deposited on : 2002-03-19
Resolution : 1.85 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

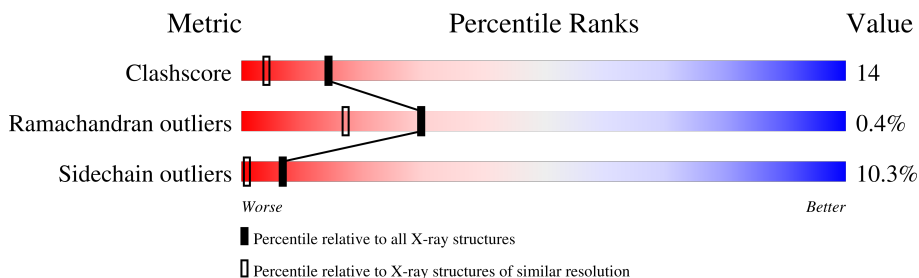
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13418 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.

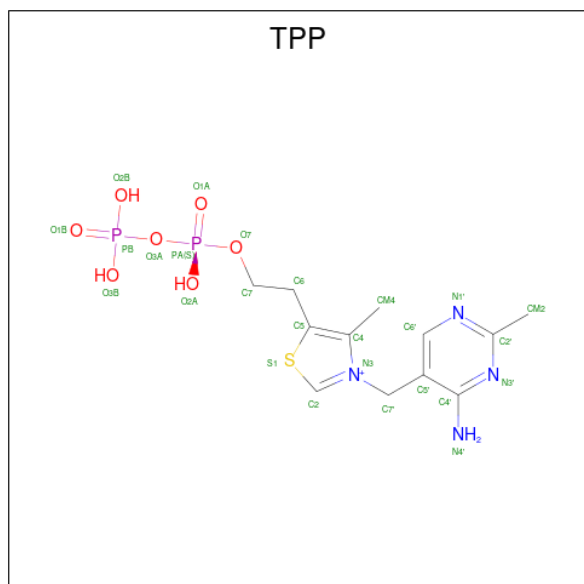
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			
1	B	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is water.

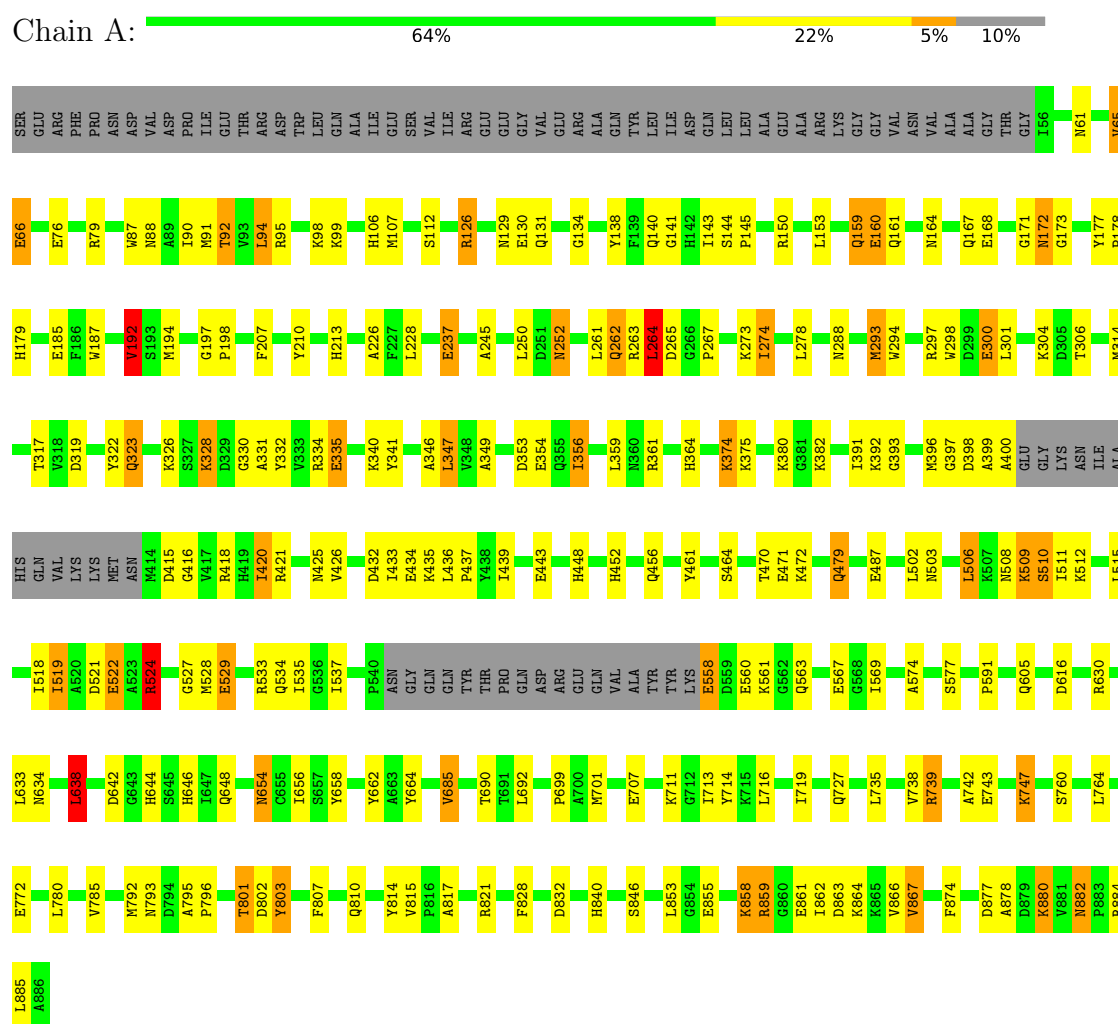
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	330	Total	O	0	0
			330	330		
4	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

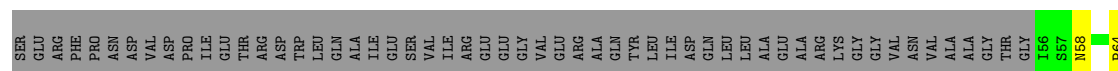
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Pyruvate dehydrogenase E1 component



- Molecule 1: Pyruvate dehydrogenase E1 component



L764	G635	D415	K326	V65	E66
D770	E636	G416	S327	H213	E67
M776	G637	V417	K328	K221	Q68
L777	L638	R418			P69
H778	Q639	H419	Y332	D234	E70
P779	A523	I420	V333		
L780	R524	R421	R334		
E781	E529	D422		E237	N74
M792	D642	R423	Y341	L75	
N793	G643	F424	P342	I244	E76
S800	H644	R424	E343	A245	L77
Y803	G645	N425	T344	T246	E78
M804	H646	V426		R247	
R812	N654	P427	T352		R79
D818	Y658	S429	L250		R80
D819	Y538	D430	D251		
Y820	S539	A431	N252		W87
R821	P540	D432	N360		I90
F828	ASN	I433	R361	N260	M91
D832	GLY	E434	G362	L261	
	GLN	K435	G363	Q262	L94
	TYR	L436	H364	R263	R95
	THR	P437		L264	
	PRO	Y438	K368	D265	K98
	GLN	I439	G266	G267	K99
	ASP	T440	K374	P267	
	ARG	F441	K375		H106
	GLU	P442	A376	I274	
	GLN		Q377		S112
V843	T690	S445		L278	H123
S846	T691	E446	G381	E279	F124
L853	L692	E447	K382	E283	
G854	M701	H452	V385		Q140
E855	I713	A453		G286	T143
A857	L716	Q454	T390	W287	
R858			I391	N288	L153
R859	L719	K457	K392	V289	
G860		K561	G393	I290	
E861			Y394	Q159	
I862	E567	H459	G395	W294	
D863	G568	G460	M396		Q167
R864	I569	Y461	K397	R297	E168
K865	K723	Q466	D398	W298	V169
	G724		A399	D299	
	K725	L572	A400	H170	G171
	V726	G573		E300	N172
	Q727	A574	GLU		G173
	L728		LYS	R303	
F874	L739	S577	GLY	K304	
			ASN		
K880	H737	P591	ILE	K309	P178
A886	V738		ALA		
	R739	N503	HIS	N315	W187
	D754	L610	GLN		
		R620	VAL	D319	V192
			LVS	G320	
		R630	LVS		L196
			MET	Q323	G197
			ASN	T324	P198
				F325	L199

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.69Å 141.60Å 82.46Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.85	Depositor
% Data completeness (in resolution range)	85.4 (8.00-1.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13418	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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: TPP, MG

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	0.42	0/6484	0.94	18/8766 (0.2%)
1	B	0.44	1/6484 (0.0%)	0.99	28/8766 (0.3%)
All	All	0.43	1/12968 (0.0%)	0.96	46/17532 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	LEU	N-CA	7.09	1.55	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	TYR	O-C-N	-16.68	100.41	122.59
1	A	634	ASN	N-CA-C	10.63	124.19	111.33
1	B	264	LEU	N-CA-C	9.90	131.89	110.80
1	B	634	ASN	N-CA-C	9.32	122.61	111.33
1	B	633	LEU	N-CA-C	-9.09	99.20	110.65
1	B	416	GLY	N-CA-C	-8.27	105.57	114.67
1	B	400	ALA	N-CA-CB	-8.05	98.32	110.40
1	A	633	LEU	N-CA-C	-7.96	99.62	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLY	N-CA-C	7.47	121.68	112.64
1	A	264	LEU	N-CA-C	6.36	124.35	110.80
1	A	638	LEU	N-CA-C	5.95	121.13	111.37
1	B	199	ILE	CB-CA-C	-5.88	104.11	112.22
1	A	415	ASP	N-CA-C	-5.86	104.48	111.69
1	B	510	SER	N-CA-C	5.85	117.33	111.07
1	A	785	VAL	N-CA-C	5.84	114.39	107.73
1	A	522	GLU	N-CA-C	5.84	118.18	109.59
1	A	524	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	B	124	PHE	N-CA-C	5.81	120.16	112.72
1	B	303	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	B	362	GLY	N-CA-C	5.74	119.83	112.83
1	B	395	GLY	N-CA-C	-5.68	99.71	113.18
1	A	662	TYR	N-CA-C	5.68	118.83	109.85
1	B	360	ASN	N-CA-C	5.64	118.89	110.14
1	B	880	LYS	N-CA-C	-5.48	102.90	110.35
1	A	263	ARG	N-CA-C	-5.47	101.31	109.96
1	B	638	LEU	N-CA-C	5.47	120.39	111.37
1	B	636	GLU	N-CA-C	5.46	117.99	111.71
1	A	293	MET	N-CA-C	5.45	119.89	112.04
1	B	394	TYR	CA-C-N	-5.36	110.91	121.41
1	B	394	TYR	C-N-CA	-5.36	110.91	121.41
1	A	577	SER	N-CA-C	-5.35	105.53	111.36
1	B	459	HIS	N-CA-C	5.29	119.69	113.23
1	B	533	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	577	SER	N-CA-C	-5.26	105.62	111.36
1	A	470	THR	N-CA-C	5.18	118.07	111.69
1	A	171	GLY	N-CA-C	5.17	125.43	113.18
1	B	778	HIS	CA-C-N	5.11	125.40	119.47
1	B	778	HIS	C-N-CA	5.11	125.40	119.47
1	B	630	ARG	N-CA-C	5.11	116.53	111.07
1	B	679	GLY	N-CA-C	-5.06	104.58	112.58
1	A	510	SER	N-CA-C	5.06	116.80	111.28
1	B	662	TYR	N-CA-C	5.04	117.78	109.72
1	B	637	GLY	N-CA-C	5.04	121.64	112.37
1	A	642	ASP	N-CA-C	5.02	116.82	107.99
1	B	642	ASP	N-CA-C	5.01	116.48	108.41
1	A	192	VAL	CB-CA-C	-5.01	104.39	112.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	803	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	6341	0	6179	181	0
1	B	6341	0	6179	186	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	3	0
4	A	330	0	0	11	0
4	B	352	0	0	9	0
All	All	13418	0	12390	354	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 14.

All (354) 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:A:801:THR:HG22	1:A:803:TYR:H	1.13	1.08
1:A:61:ASN:HD21	1:A:294:TRP:H	1.06	0.92
1:A:364:HIS:HE1	1:A:391:ILE:H	1.16	0.88
1:B:620:ARG:HH12	1:B:682:GLN:HE21	1.18	0.88
1:B:644:HIS:HB3	1:B:804:MET:HE3	1.55	0.85
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.58	0.85
1:A:519:ILE:HD11	1:A:528:MET:HE2	1.57	0.84
1:B:364:HIS:HE1	1:B:391:ILE:H	1.24	0.84
1:A:261:LEU:HB2	1:A:323:GLN:HE22	1.42	0.83
1:A:522:GLU:HG2	1:B:264:LEU:HD12	1.61	0.83
1:A:882:ASN:HD22	1:A:884:ARG:H	1.26	0.83
1:B:288:ASN:HB2	1:B:382:LYS:HE3	1.62	0.81
1:A:727:GLN:HE22	1:A:793:ASN:H	1.29	0.78
1:A:801:THR:HG22	1:A:803:TYR:N	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TRP:CE3	1:B:385:VAL:HG22	2.19	0.77
1:A:508:ASN:HD22	1:A:511:ILE:H	1.33	0.77
1:A:79:ARG:HH12	1:A:425:ASN:HD22	1.31	0.76
1:A:252:ASN:HD22	1:A:252:ASN:H	1.34	0.76
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.66	0.76
1:B:418:ARG:HA	1:B:421:ARG:HG2	1.68	0.75
1:A:61:ASN:ND2	1:A:294:TRP:H	1.83	0.75
1:A:261:LEU:HB2	1:A:323:GLN:NE2	2.02	0.75
1:A:801:THR:CG2	1:A:803:TYR:H	1.97	0.74
1:B:856:LEU:HB2	1:B:862:ILE:CD1	2.17	0.74
1:B:853:LEU:O	1:B:862:ILE:HD11	1.89	0.73
1:A:61:ASN:HD21	1:A:294:TRP:N	1.86	0.73
1:A:364:HIS:CE1	1:A:391:ILE:H	2.03	0.73
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.71	0.73
1:B:252:ASN:H	1:B:252:ASN:HD22	1.36	0.72
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.71	0.71
1:B:396:MET:HB2	1:B:400:ALA:H	1.54	0.71
1:B:64:PRO:HG2	1:B:67:GLU:HB2	1.73	0.71
1:B:245:ALA:HA	1:B:250:LEU:HD22	1.71	0.71
1:A:326:LYS:HE2	1:A:391:ILE:HG23	1.72	0.70
1:A:506:LEU:HD13	1:A:515:LEU:HD12	1.73	0.70
1:A:524:ARG:HG3	1:A:529:GLU:HG2	1.73	0.70
1:B:421:ARG:HB2	1:B:426:VAL:HB	1.73	0.70
1:A:326:LYS:HE3	1:A:361:ARG:CZ	2.23	0.69
1:A:503:ASN:ND2	1:A:534:GLN:HE22	1.91	0.69
1:A:140:GLN:O	1:A:143:ILE:HG13	1.92	0.69
1:A:326:LYS:HE3	1:A:361:ARG:NH1	2.08	0.69
1:B:90:ILE:HG22	1:B:91:MET:HE2	1.75	0.68
1:B:452:HIS:HD2	1:B:461:TYR:OH	1.76	0.68
1:A:297:ARG:HB3	1:A:359:LEU:HD23	1.74	0.68
1:B:727:GLN:HE22	1:B:793:ASN:H	1.41	0.68
1:A:192:VAL:HG22	4:A:891:HOH:O	1.93	0.67
1:A:527:GLY:HA2	1:A:529:GLU:OE2	1.94	0.67
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.77	0.67
1:B:414:MET:SD	1:B:434:GLU:HB3	2.35	0.67
1:A:727:GLN:NE2	1:A:793:ASN:H	1.92	0.67
1:B:300:GLU:O	1:B:304:LYS:HG3	1.95	0.67
1:A:396:MET:HB3	1:A:399:ALA:HB3	1.77	0.66
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.77	0.66
1:A:192:VAL:HG23	1:B:639:GLN:NE2	2.11	0.66
1:A:393:GLY:HA3	1:A:400:ALA:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ASP:OD2	1:B:169:VAL:HB	1.96	0.66
1:A:61:ASN:HD22	1:A:293:MET:H	1.42	0.65
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.27	0.65
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.77	0.65
1:B:74:ASN:OD1	1:B:76:GLU:HG2	1.97	0.65
1:A:519:ILE:CD1	1:A:528:MET:HE2	2.26	0.65
1:A:735:LEU:O	1:A:738:VAL:HG22	1.97	0.64
1:A:330:GLY:HA3	1:A:353:ASP:O	1.98	0.64
1:A:364:HIS:HE1	1:A:391:ILE:N	1.94	0.64
1:A:65:VAL:HG22	4:A:1026:HOH:O	1.97	0.64
1:A:328:LYS:HG3	1:A:332:TYR:CD2	2.33	0.63
1:B:725:LYS:HE3	1:B:754:ASP:OD2	1.99	0.63
1:A:882:ASN:ND2	1:A:884:ARG:H	1.96	0.63
1:B:76:GLU:CD	1:B:76:GLU:H	2.06	0.62
1:A:801:THR:HG21	1:A:807:PHE:HD2	1.64	0.62
1:A:262:GLN:HA	1:A:267:PRO:HA	1.80	0.62
1:B:274:ILE:HG13	1:B:319:ASP:OD2	2.00	0.62
1:B:171:GLY:O	1:B:173:GLY:N	2.32	0.61
1:A:61:ASN:ND2	1:A:293:MET:H	1.97	0.61
1:A:508:ASN:O	1:A:512:LYS:HB3	2.00	0.61
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.36	0.61
1:B:469:PHE:H	1:B:682:GLN:HE22	1.48	0.61
1:A:177:TYR:CD1	1:A:192:VAL:HG11	2.36	0.61
1:B:620:ARG:HH12	1:B:682:GLN:NE2	1.96	0.61
1:B:856:LEU:HB2	1:B:862:ILE:HD11	1.82	0.61
1:A:522:GLU:CG	1:B:264:LEU:HD12	2.31	0.61
1:B:262:GLN:HG3	1:B:266:GLY:O	2.01	0.61
1:B:395:GLY:HA3	1:B:424:PHE:CE1	2.36	0.60
1:A:99:LYS:NZ	1:A:167:GLN:HE21	1.99	0.60
1:A:858:LYS:HD3	1:A:858:LYS:N	2.16	0.60
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.84	0.60
1:A:331:ALA:HA	1:A:334:ARG:HG2	1.83	0.59
1:A:160:GLU:HG2	1:A:161:GLN:N	2.18	0.59
1:B:727:GLN:NE2	1:B:793:ASN:H	2.01	0.58
1:A:129:ASN:HD22	1:A:131:GLN:H	1.51	0.58
1:A:106:HIS:HD2	4:A:958:HOH:O	1.86	0.58
1:A:179:HIS:HD2	1:A:616:ASP:OD2	1.87	0.58
1:B:423:ARG:CZ	1:B:423:ARG:HB2	2.34	0.58
1:A:793:ASN:HD22	1:A:795:ALA:H	1.52	0.57
1:B:263:ARG:NH1	4:B:1056:HOH:O	2.36	0.57
1:B:244:ILE:HD13	1:B:247:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:CE1	1:B:391:ILE:H	2.14	0.57
1:A:264:LEU:HD12	1:B:522:GLU:HG3	1.86	0.57
1:A:878:ALA:HA	1:B:777:LEU:HG	1.86	0.57
1:B:65:VAL:HA	1:B:68:GLN:HG2	1.85	0.57
1:B:646:HIS:HE1	1:B:690:THR:OG1	1.86	0.57
1:B:654:ASN:H	1:B:654:ASN:HD22	1.52	0.57
1:A:864:LYS:HD3	1:B:779:PRO:O	2.04	0.57
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.34	0.57
1:B:859:ARG:HG3	1:B:859:ARG:HH11	1.69	0.56
1:B:140:GLN:O	1:B:143:ILE:HG13	2.04	0.56
1:A:508:ASN:HD21	1:A:510:SER:HB3	1.69	0.56
1:A:304:LYS:HE2	1:A:347:LEU:HG	1.88	0.56
1:A:245:ALA:HA	1:A:250:LEU:HD12	1.87	0.56
1:A:107:MET:HE3	1:A:396:MET:HE1	1.86	0.56
1:A:274:ILE:HG13	1:A:319:ASP:OD2	2.06	0.56
1:A:323:GLN:O	1:A:326:LYS:HB2	2.06	0.56
3:B:887:TPP:H2	4:B:1240:HOH:O	2.05	0.55
1:A:79:ARG:NH1	1:A:425:ASN:HD22	2.03	0.55
1:A:317:THR:HB	1:A:322:TYR:CE1	2.41	0.55
1:B:213:HIS:O	1:B:561:LYS:HD3	2.06	0.55
1:B:320:GLY:O	1:B:324:THR:HG23	2.06	0.54
1:B:381:GLY:C	1:B:382:LYS:HG3	2.33	0.54
1:B:423:ARG:HG3	1:B:424:PHE:CD1	2.41	0.54
1:A:518:ILE:O	1:A:519:ILE:HD12	2.08	0.54
1:A:420:ILE:HG13	1:A:421:ARG:N	2.22	0.54
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.37	0.54
1:B:863:ASP:OD1	1:B:865:LYS:HB2	2.07	0.54
3:A:887:TPP:H2	4:A:1041:HOH:O	2.06	0.53
1:A:177:TYR:CG	1:A:192:VAL:HG11	2.43	0.53
1:B:287:TRP:HE3	1:B:385:VAL:HG22	1.69	0.53
1:A:273:LYS:HG2	4:A:1067:HOH:O	2.08	0.53
1:B:856:LEU:HB2	1:B:862:ILE:HD13	1.87	0.53
1:B:192:VAL:CG2	4:B:921:HOH:O	2.57	0.53
1:A:99:LYS:HZ2	1:A:167:GLN:HE21	1.56	0.53
1:B:87:TRP:HZ3	1:B:421:ARG:HB3	1.74	0.53
1:A:87:TRP:HE3	1:A:420:ILE:HD11	1.74	0.53
1:A:654:ASN:HD22	1:A:654:ASN:H	1.56	0.53
1:A:340:LYS:HG2	1:A:341:TYR:CE1	2.44	0.53
1:B:262:GLN:HA	1:B:267:PRO:HA	1.89	0.53
1:A:452:HIS:HD2	1:A:461:TYR:OH	1.92	0.52
1:B:540:PRO:HA	1:B:560:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLU:HG3	1:A:814:TYR:HE2	1.75	0.52
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.91	0.52
1:A:452:HIS:HE1	4:A:1202:HOH:O	1.93	0.52
1:B:415:ASP:O	1:B:418:ARG:HB3	2.09	0.52
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.10	0.52
1:B:723:LYS:HD3	1:B:723:LYS:N	2.23	0.52
1:A:91:MET:O	1:A:95:ARG:HG3	2.09	0.52
1:A:646:HIS:HE1	1:A:690:THR:OG1	1.92	0.52
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.39	0.52
1:B:778:HIS:HB3	1:B:781:GLU:OE1	2.10	0.51
1:A:537:ILE:HB	1:A:558:GLU:HG2	1.90	0.51
1:B:861:GLU:C	1:B:862:ILE:HG23	2.35	0.51
1:A:61:ASN:ND2	1:A:293:MET:N	2.58	0.51
1:A:853:LEU:O	1:A:862:ILE:HD11	2.10	0.51
1:A:884:ARG:NH1	4:A:1046:HOH:O	2.44	0.51
1:A:328:LYS:HG3	1:A:332:TYR:CE2	2.46	0.51
1:A:518:ILE:C	1:A:519:ILE:HD12	2.36	0.51
1:A:846:SER:HB2	1:A:874:PHE:HB3	1.92	0.51
1:A:864:LYS:HB3	1:B:780:LEU:HD23	1.92	0.51
1:B:58:ASN:ND2	1:B:315:ASN:HD21	2.08	0.51
1:A:509:LYS:HA	1:A:512:LYS:HE2	1.92	0.51
1:B:861:GLU:O	1:B:862:ILE:CG2	2.59	0.51
1:A:66:GLU:H	1:A:66:GLU:CD	2.18	0.51
1:A:727:GLN:HE22	1:A:792:MET:HB3	1.76	0.50
1:B:423:ARG:HB2	1:B:423:ARG:NH1	2.27	0.50
1:A:521:ASP:CG	1:B:263:ARG:HD2	2.37	0.50
1:B:192:VAL:HG23	4:B:921:HOH:O	2.10	0.50
1:B:426:VAL:HG13	1:B:439:ILE:HD11	1.92	0.50
1:B:334:ARG:HG2	4:B:1110:HOH:O	2.11	0.50
1:B:396:MET:HA	1:B:420:ILE:HD12	1.93	0.50
1:B:454:GLN:HE22	1:B:457:LYS:NZ	2.09	0.50
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.41	0.50
1:A:664:TYR:CG	1:A:701:MET:HB2	2.47	0.50
1:B:421:ARG:CD	1:B:433:ILE:HD11	2.42	0.50
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.42	0.49
1:A:323:GLN:OE1	1:A:326:LYS:HD2	2.12	0.49
1:A:508:ASN:ND2	1:A:511:ILE:H	2.05	0.49
1:B:396:MET:HB2	1:B:399:ALA:HB3	1.94	0.49
1:B:654:ASN:H	1:B:654:ASN:ND2	2.09	0.49
1:A:524:ARG:HG3	1:A:529:GLU:CG	2.42	0.49
1:A:654:ASN:H	1:A:654:ASN:ND2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:VAL:HG12	1:A:817:ALA:H	1.77	0.49
1:B:861:GLU:O	1:B:862:ILE:HG23	2.13	0.49
1:B:417:VAL:HA	1:B:420:ILE:HG12	1.93	0.49
1:B:442:PRO:HG2	1:B:445:SER:HB3	1.93	0.49
1:B:569:ILE:HD11	3:B:887:TPP:H61	1.93	0.49
1:A:262:GLN:HG3	1:A:323:GLN:HE21	1.77	0.49
1:B:288:ASN:CB	1:B:382:LYS:HE3	2.38	0.49
1:B:421:ARG:NE	1:B:433:ILE:HD11	2.28	0.48
1:A:654:ASN:HD22	1:A:654:ASN:N	2.11	0.48
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.48	0.48
1:A:801:THR:HB	4:A:895:HOH:O	2.14	0.48
1:A:264:LEU:HD13	1:A:265:ASP:OD2	2.13	0.48
1:A:314:MET:HA	1:A:322:TYR:OH	2.14	0.48
1:B:429:SER:OG	1:B:431:ALA:HB3	2.14	0.48
1:B:654:ASN:HD22	1:B:654:ASN:N	2.09	0.48
1:A:471:GLU:OE2	1:A:591:PRO:HD2	2.14	0.48
1:A:864:LYS:O	1:A:867:VAL:HG13	2.14	0.48
1:B:91:MET:O	1:B:95:ARG:HG2	2.13	0.48
1:A:840:HIS:HE1	4:A:1022:HOH:O	1.97	0.47
1:B:196:LEU:HA	1:B:199:ILE:HD11	1.95	0.47
1:B:395:GLY:HA3	1:B:424:PHE:HE1	1.79	0.47
1:A:262:GLN:OE1	1:A:326:LYS:NZ	2.47	0.47
1:B:396:MET:H	1:B:396:MET:HG2	1.55	0.47
1:B:426:VAL:HG13	1:B:439:ILE:CD1	2.44	0.47
1:B:309:LYS:HG2	1:B:343:GLU:CG	2.45	0.47
1:A:197:GLY:N	1:A:198:PRO:HD2	2.29	0.47
1:B:716:LEU:HD13	1:B:739:ARG:CZ	2.44	0.47
1:A:503:ASN:HD21	1:A:534:GLN:HE22	1.62	0.47
1:B:199:ILE:HG12	1:B:237:GLU:HB3	1.97	0.47
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.50	0.47
3:A:887:TPP:H62	1:B:264:LEU:H	1.80	0.47
1:B:244:ILE:CD1	1:B:247:ARG:HD2	2.45	0.47
1:B:364:HIS:HD2	4:B:1224:HOH:O	1.97	0.47
1:B:423:ARG:CZ	1:B:423:ARG:CB	2.92	0.47
1:B:537:ILE:O	1:B:558:GLU:HA	2.15	0.47
1:A:261:LEU:HD23	1:A:274:ILE:HD11	1.96	0.46
1:A:300:GLU:O	1:A:304:LYS:HG2	2.15	0.46
1:A:796:PRO:HG3	1:A:859:ARG:NE	2.30	0.46
1:B:99:LYS:NZ	1:B:167:GLN:HE21	2.12	0.46
1:B:288:ASN:HB2	1:B:382:LYS:CE	2.41	0.46
1:B:395:GLY:HA3	1:B:423:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TRP:CE3	1:A:420:ILE:HD11	2.51	0.46
1:A:213:HIS:HB3	1:A:560:GLU:O	2.15	0.46
1:B:393:GLY:HA3	1:B:400:ALA:CB	2.45	0.46
1:B:432:ASP:O	1:B:437:PRO:HD3	2.15	0.46
1:A:821:ARG:HD2	1:A:855:GLU:CG	2.46	0.46
1:A:863:ASP:O	1:A:866:VAL:HB	2.15	0.46
1:B:78:GLU:OE2	1:B:123:HIS:HE1	1.99	0.46
1:A:138:TYR:HB2	1:A:226:ALA:HA	1.98	0.46
1:A:328:LYS:HB3	1:A:332:TYR:HB3	1.98	0.46
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.98	0.46
1:A:262:GLN:HG3	1:A:323:GLN:NE2	2.31	0.46
1:B:159:GLN:HG2	1:B:438:TYR:CE1	2.51	0.46
1:A:237:GLU:H	1:A:237:GLU:CD	2.23	0.46
1:A:743:GLU:O	1:A:747:LYS:HB2	2.15	0.46
1:B:737:HIS:HE1	4:B:906:HOH:O	1.98	0.46
1:B:567:GLU:HG3	1:B:574:ALA:HA	1.98	0.45
1:B:178:PRO:HA	1:B:187:TRP:CG	2.52	0.45
1:B:855:GLU:O	1:B:859:ARG:HG2	2.15	0.45
1:A:143:ILE:C	1:A:143:ILE:HD12	2.41	0.45
1:A:416:GLY:O	1:A:420:ILE:HG23	2.16	0.45
1:A:801:THR:CG2	1:A:802:ASP:N	2.78	0.45
1:A:880:LYS:HD3	4:A:1080:HOH:O	2.15	0.45
1:B:328:LYS:HG3	1:B:332:TYR:CD2	2.51	0.45
1:A:192:VAL:HG23	1:B:639:GLN:HE21	1.80	0.45
1:A:334:ARG:HG3	1:A:335:GLU:N	2.32	0.45
1:A:522:GLU:CD	1:B:264:LEU:HD12	2.41	0.45
1:B:309:LYS:HB2	1:B:343:GLU:HG3	1.98	0.45
1:B:532:PHE:CG	1:B:537:ILE:HD11	2.52	0.45
1:B:664:TYR:CG	1:B:701:MET:HB2	2.51	0.45
1:B:859:ARG:HG3	1:B:859:ARG:NH1	2.32	0.45
1:A:252:ASN:HD22	1:A:252:ASN:N	2.03	0.45
1:B:106:HIS:CD2	1:B:106:HIS:N	2.85	0.45
1:B:846:SER:HB2	1:B:874:PHE:HB3	1.99	0.45
1:A:288:ASN:HD21	1:A:375:LYS:HE2	1.82	0.45
1:B:91:MET:O	1:B:95:ARG:CG	2.65	0.45
1:A:90:ILE:HG23	1:A:94:LEU:HD23	1.99	0.45
1:B:471:GLU:OE2	1:B:591:PRO:HD2	2.17	0.45
1:B:532:PHE:CD1	1:B:537:ILE:HD11	2.52	0.45
1:A:867:VAL:CG2	1:B:779:PRO:HG3	2.38	0.45
1:B:112:SER:HB3	1:B:392:LYS:HA	1.98	0.45
1:B:508:ASN:OD1	1:B:510:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:HG3	1:B:422:ASP:N	2.31	0.44
1:B:297:ARG:HG3	1:B:360:ASN:OD1	2.17	0.44
1:B:279:GLU:O	1:B:283:GLU:HB2	2.17	0.44
1:A:300:GLU:HG3	1:A:301:LEU:N	2.31	0.44
1:B:274:ILE:HG13	1:B:274:ILE:H	1.48	0.44
1:A:630:ARG:HH12	1:A:644:HIS:HD1	1.65	0.44
1:A:160:GLU:CD	1:A:172:ASN:OD1	2.60	0.44
1:B:68:GLN:HE22	1:B:368:LYS:NZ	2.16	0.44
1:B:524:ARG:HA	1:B:529:GLU:OE1	2.18	0.44
1:A:569:ILE:HD11	3:A:887:TPP:H61	2.00	0.44
1:A:374:LYS:HD3	1:A:374:LYS:HA	1.66	0.44
1:A:432:ASP:OD2	1:A:435:LYS:HE2	2.18	0.44
1:A:877:ASP:HB3	1:A:880:LYS:HD2	1.99	0.44
1:B:419:HIS:O	1:B:423:ARG:HG2	2.18	0.44
1:B:633:LEU:HG	1:B:636:GLU:HB2	2.00	0.43
1:B:821:ARG:HD2	1:B:855:GLU:HG3	1.99	0.43
1:A:144:SER:OG	1:A:145:PRO:HD3	2.18	0.43
1:A:656:ILE:HG12	1:A:685:VAL:HG13	2.00	0.43
1:A:713:ILE:HG12	1:A:714:TYR:N	2.32	0.43
1:B:426:VAL:CG1	1:B:439:ILE:HD11	2.48	0.43
1:B:729:LEU:HD11	1:B:792:MET:HE3	2.01	0.43
1:B:800:SER:OG	1:B:843:VAL:HG22	2.18	0.43
1:A:107:MET:HE3	1:A:396:MET:CE	2.47	0.43
1:A:323:GLN:OE1	1:A:323:GLN:HA	2.19	0.43
1:B:396:MET:HE2	1:B:396:MET:HB3	1.73	0.43
1:B:676:ARG:HD3	1:B:687:TYR:OH	2.18	0.43
1:B:260:ASN:HA	1:B:390:THR:O	2.18	0.43
1:B:261:LEU:HA	1:B:274:ILE:HD11	2.01	0.43
1:B:286:GLY:O	1:B:382:LYS:NZ	2.51	0.43
1:A:178:PRO:HA	1:A:187:TRP:CG	2.52	0.43
1:A:194:MET:HE1	3:B:887:TPP:S1	2.59	0.43
1:B:237:GLU:HG2	1:B:572:LEU:HD11	2.00	0.43
1:A:487:GLU:HG3	1:A:699:PRO:HA	2.01	0.43
1:B:77:LEU:CD2	1:B:447:GLU:HG3	2.47	0.43
1:B:341:TYR:HB2	1:B:344:THR:OG1	2.18	0.43
1:B:309:LYS:HG2	1:B:343:GLU:HG3	2.01	0.43
1:B:430:ASP:HA	1:B:433:ILE:HB	2.00	0.43
1:A:207:PHE:O	1:A:210:TYR:HB3	2.19	0.43
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.54	0.43
1:B:429:SER:C	1:B:431:ALA:H	2.27	0.43
1:A:436:LEU:N	1:A:437:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:HG3	1:A:574:ALA:HA	2.01	0.42
1:B:452:HIS:HE1	4:B:1014:HOH:O	2.01	0.42
1:B:153:LEU:HD21	1:B:441:PHE:HE1	1.85	0.42
1:B:323:GLN:HE21	1:B:361:ARG:HH22	1.66	0.42
1:B:221:LYS:HB2	4:B:1072:HOH:O	2.19	0.42
1:A:159:GLN:HE21	1:A:159:GLN:HB2	1.65	0.42
1:A:535:ILE:HB	1:A:563:GLN:HB3	2.00	0.42
1:B:324:THR:O	1:B:328:LYS:HG2	2.20	0.42
1:B:414:MET:HE2	1:B:415:ASP:HB2	2.02	0.42
1:A:261:LEU:HA	1:A:274:ILE:HD11	2.00	0.42
1:B:197:GLY:N	1:B:198:PRO:HD2	2.35	0.42
1:B:812:ARG:HD2	1:B:820:TYR:HD2	1.85	0.42
1:A:864:LYS:CB	1:B:780:LEU:HD23	2.49	0.42
1:B:64:PRO:HB2	1:B:66:GLU:CD	2.45	0.42
1:A:443:GLU:HG3	1:A:448:HIS:CE1	2.55	0.41
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.54	0.41
1:B:392:LYS:C	1:B:394:TYR:H	2.28	0.41
1:A:707:GLU:O	1:A:711:LYS:HG2	2.20	0.41
1:A:436:LEU:N	1:A:437:PRO:CD	2.83	0.41
1:A:658:TYR:CD2	1:A:760:SER:HB2	2.56	0.41
1:A:772:GLU:OE1	1:A:772:GLU:HA	2.20	0.41
1:B:529:GLU:O	1:B:532:PHE:HB2	2.20	0.41
1:A:112:SER:HB3	1:A:392:LYS:HA	2.02	0.41
1:A:807:PHE:O	1:A:810:GLN:HG2	2.21	0.41
1:A:150:ARG:NH2	4:A:1071:HOH:O	2.37	0.41
1:B:199:ILE:HD13	1:B:572:LEU:HD13	2.02	0.41
1:B:213:HIS:HB3	1:B:560:GLU:O	2.20	0.41
1:A:126:ARG:HG2	1:A:134:GLY:HA2	2.02	0.41
1:B:658:TYR:CD2	1:B:760:SER:HB2	2.55	0.41
1:A:605:GLN:HE21	1:A:648:GLN:HE22	1.69	0.41
1:A:328:LYS:HD2	1:A:332:TYR:CD1	2.56	0.41
1:B:374:LYS:NZ	1:B:377:GLN:HE22	2.19	0.41
1:B:395:GLY:CA	1:B:423:ARG:HD3	2.50	0.41
1:B:634:ASN:HB2	1:B:832:ASP:O	2.21	0.41
1:B:758:VAL:O	1:B:758:VAL:HG22	2.20	0.41
1:B:856:LEU:C	1:B:862:ILE:HG12	2.46	0.41
1:B:396:MET:HB2	1:B:400:ALA:N	2.29	0.41
1:A:346:ALA:HA	1:A:349:ALA:HB2	2.01	0.40
1:B:435:LYS:HG2	1:B:435:LYS:O	2.21	0.40
1:A:88:ASN:O	1:A:92:THR:HG23	2.19	0.40
1:B:654:ASN:ND2	1:B:654:ASN:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:HA	1:A:353:ASP:OD2	2.22	0.40
1:B:857:ALA:N	1:B:862:ILE:HG12	2.37	0.40
1:A:164:ASN:HB3	1:A:173:GLY:HA2	2.03	0.40
1:A:479:GLN:NE2	1:A:479:GLN:HA	2.34	0.40
1:A:716:LEU:HD13	1:A:739:ARG:NE	2.37	0.40
1:A:884:ARG:NH2	1:B:770:ASP:OD2	2.55	0.40
1:B:79:ARG:HG3	1:B:80:ARG:N	2.37	0.40
1:B:244:ILE:CD1	1:B:247:ARG:NH1	2.84	0.40
1:B:415:ASP:C	1:B:417:VAL:N	2.80	0.40
1:B:421:ARG:HD3	1:B:428:VAL:HG13	2.02	0.40
1:B:812:ARG:NE	1:B:820:TYR:HB3	2.37	0.40
1:B:290:ILE:CD1	1:B:375:LYS:HD3	2.51	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	795/886 (90%)	756 (95%)	38 (5%)	1 (0%)	48	35
1	B	795/886 (90%)	754 (95%)	36 (4%)	5 (1%)	21	10
All	All	1590/1772 (90%)	1510 (95%)	74 (5%)	6 (0%)	30	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ASN
1	B	397	GLY
1	A	397	GLY
1	B	394	TYR
1	B	521	ASP
1	B	428	VAL

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	665/735 (90%)	600 (90%)	65 (10%)	7	1
1	B	665/735 (90%)	593 (89%)	72 (11%)	6	1
All	All	1330/1470 (90%)	1193 (90%)	137 (10%)	7	1

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	66	GLU
1	A	76	GLU
1	A	92	THR
1	A	94	LEU
1	A	126	ARG
1	A	130	GLU
1	A	153	LEU
1	A	159	GLN
1	A	160	GLU
1	A	168	GLU
1	A	172	ASN
1	A	185	GLU
1	A	192	VAL
1	A	228	LEU
1	A	237	GLU
1	A	252	ASN
1	A	262	GLN
1	A	264	LEU
1	A	274	ILE
1	A	278	LEU
1	A	300	GLU
1	A	306	THR
1	A	323	GLN
1	A	328	LYS
1	A	335	GLU
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	354	GLU
1	A	356	ILE
1	A	374	LYS
1	A	380	LYS
1	A	382	LYS
1	A	398	ASP
1	A	418	ARG
1	A	420	ILE
1	A	433	ILE
1	A	434	GLU
1	A	456	GLN
1	A	464	SER
1	A	472	LYS
1	A	479	GLN
1	A	502	LEU
1	A	506	LEU
1	A	509	LYS
1	A	519	ILE
1	A	524	ARG
1	A	529	GLU
1	A	533	ARG
1	A	558	GLU
1	A	561	LYS
1	A	638	LEU
1	A	654	ASN
1	A	685	VAL
1	A	692	LEU
1	A	739	ARG
1	A	747	LYS
1	A	780	LEU
1	A	801	THR
1	A	858	LYS
1	A	859	ARG
1	A	861	GLU
1	A	867	VAL
1	A	880	LYS
1	A	882	ASN
1	A	885	LEU
1	B	67	GLU
1	B	70	GLU
1	B	76	GLU
1	B	77	LEU

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Mol	Chain	Res	Type
1	B	79	ARG
1	B	90	ILE
1	B	94	LEU
1	B	98	LYS
1	B	106	HIS
1	B	192	VAL
1	B	196	LEU
1	B	199	ILE
1	B	234	ASP
1	B	250	LEU
1	B	252	ASN
1	B	262	GLN
1	B	263	ARG
1	B	264	LEU
1	B	274	ILE
1	B	278	LEU
1	B	300	GLU
1	B	304	LYS
1	B	326	LYS
1	B	327	SER
1	B	334	ARG
1	B	343	GLU
1	B	382	LYS
1	B	385	VAL
1	B	391	ILE
1	B	392	LYS
1	B	396	MET
1	B	398	ASP
1	B	414	MET
1	B	415	ASP
1	B	417	VAL
1	B	418	ARG
1	B	420	ILE
1	B	422	ASP
1	B	423	ARG
1	B	428	VAL
1	B	429	SER
1	B	430	ASP
1	B	432	ASP
1	B	433	ILE
1	B	434	GLU
1	B	466	GLN

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Mol	Chain	Res	Type
1	B	475	LEU
1	B	503	ASN
1	B	509	LYS
1	B	519	ILE
1	B	522	GLU
1	B	534	GLN
1	B	537	ILE
1	B	539	SER
1	B	560	GLU
1	B	572	LEU
1	B	610	LEU
1	B	638	LEU
1	B	654	ASN
1	B	685	VAL
1	B	692	LEU
1	B	719	ILE
1	B	723	LYS
1	B	725	LYS
1	B	758	VAL
1	B	776	MET
1	B	777	LEU
1	B	780	LEU
1	B	781	GLU
1	B	818	ASP
1	B	843	VAL
1	B	859	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	68	GLN
1	A	106	HIS
1	A	123	HIS
1	A	129	ASN
1	A	140	GLN
1	A	159	GLN
1	A	164	ASN
1	A	167	GLN
1	A	179	HIS
1	A	252	ASN
1	A	288	ASN

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	323	GLN
1	A	364	HIS
1	A	425	ASN
1	A	452	HIS
1	A	454	GLN
1	A	503	ASN
1	A	508	ASN
1	A	534	GLN
1	A	563	GLN
1	A	605	GLN
1	A	639	GLN
1	A	646	HIS
1	A	654	ASN
1	A	727	GLN
1	A	737	HIS
1	A	793	ASN
1	A	810	GLN
1	A	840	HIS
1	A	882	ASN
1	B	58	ASN
1	B	68	GLN
1	B	106	HIS
1	B	123	HIS
1	B	167	GLN
1	B	252	ASN
1	B	262	GLN
1	B	323	GLN
1	B	336	HIS
1	B	364	HIS
1	B	377	GLN
1	B	452	HIS
1	B	454	GLN
1	B	534	GLN
1	B	646	HIS
1	B	654	ASN
1	B	682	GLN
1	B	727	GLN
1	B	737	HIS
1	B	790	GLN
1	B	836	ASN
1	B	840	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
3	TPP	A	887	2	26,27,27	1.44	4 (15%)	38,40,40	0.93	1 (2%)
3	TPP	B	887	2	26,27,27	1.47	4 (15%)	38,40,40	0.90	1 (2%)

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
3	TPP	A	887	2	-	1/17/17/17	0/2/2/2
3	TPP	B	887	2	-	3/17/17/17	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TPP	C4'-N3'	3.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	887	TPP	C5'-C4'	3.74	1.49	1.42
3	B	887	TPP	C5'-C4'	3.43	1.48	1.42
3	A	887	TPP	C4'-N3'	3.30	1.39	1.35
3	A	887	TPP	C2'-N1'	2.70	1.38	1.34
3	B	887	TPP	C2'-N1'	2.67	1.38	1.34
3	B	887	TPP	PA-O3A	2.29	1.62	1.59
3	A	887	TPP	PA-O3A	2.05	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	887	TPP	C6'-N1'-C2'	2.56	120.28	116.07
3	B	887	TPP	C6'-N1'-C2'	2.51	120.20	116.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	887	TPP	PB-O3A-PA-O7
3	B	887	TPP	C5-C6-C7-O7
3	A	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O2B

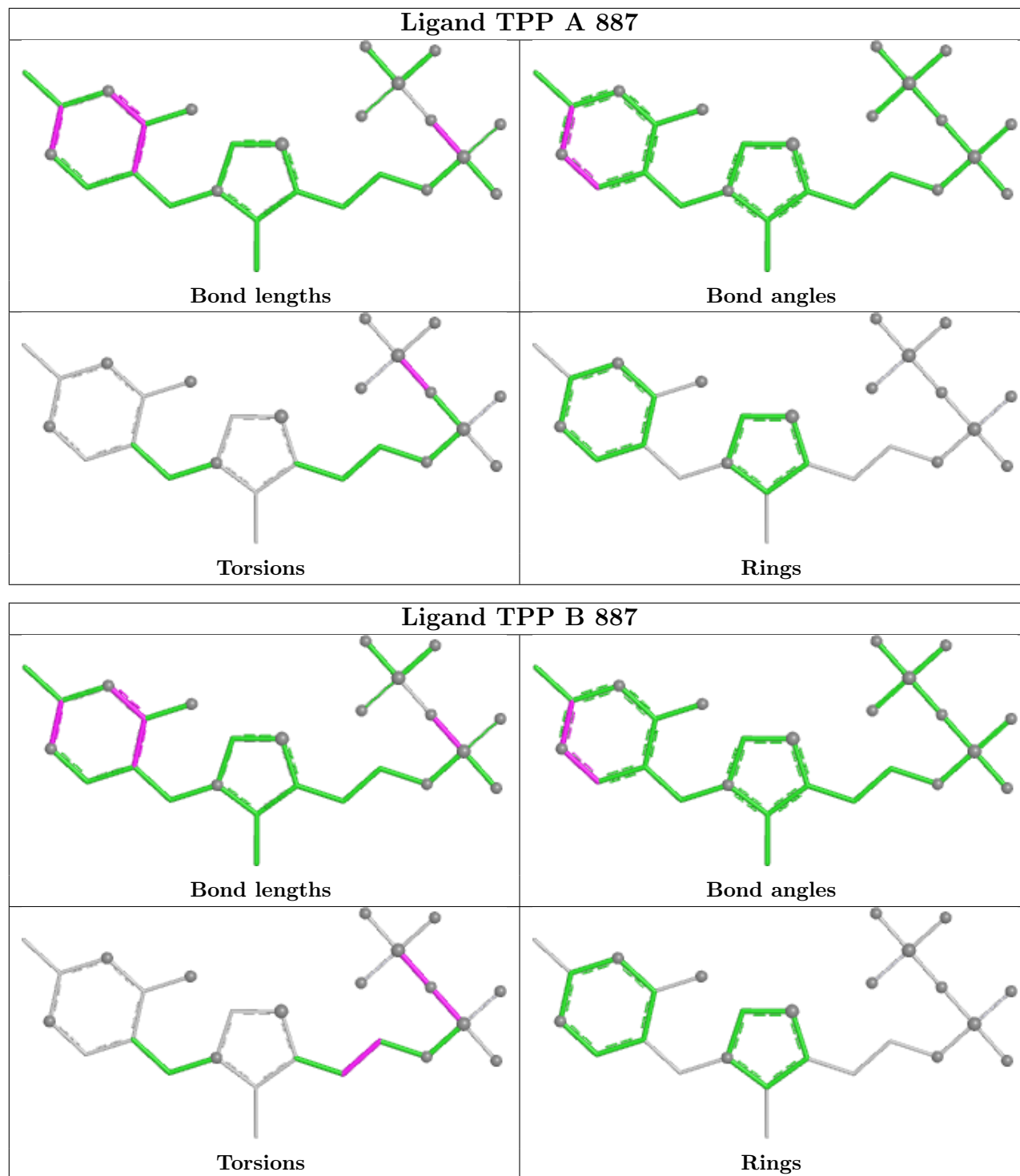
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TPP	3	0
3	B	887	TPP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.