



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PYD  
Title : CATALYTIC CENTERS IN THE THIAMIN DIPHOSPHATE DEPENDENT  
ENZYME PYRUVATE DECARBOXYLASE AT 2.4 ANGSTROMS RESO-  
LUTION  
Authors : Furey, W.; Dyda, F.  
Deposited on : 1993-03-23  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

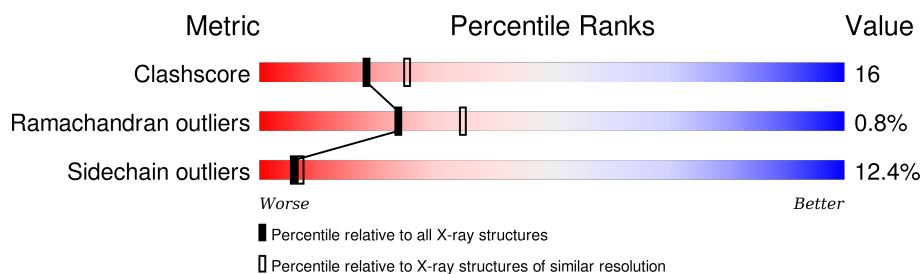
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	 51% 31% 11% • •
1	B	556	 55% 28% 10% • •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8316 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 DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			
1	B	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			

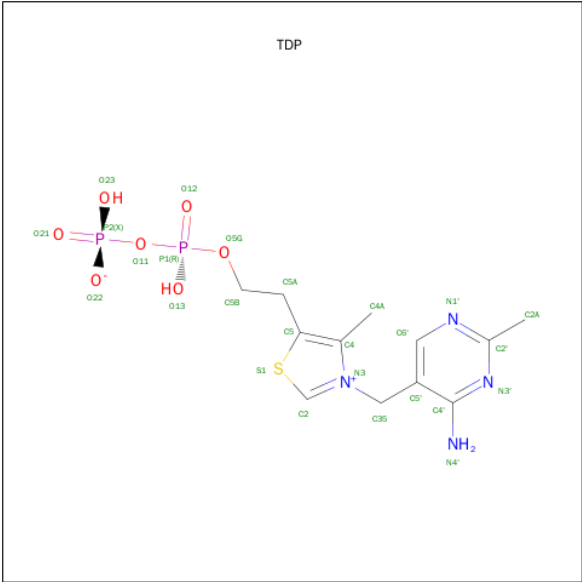
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	ARG	CONFLICT	UNP P06169
A	143	ALA	CYS	CONFLICT	UNP P06169
A	206	ALA	VAL	CONFLICT	UNP P06169
A	208	VAL	ALA	CONFLICT	UNP P06169
A	538	ILE	VAL	CONFLICT	UNP P06169
A	551	LYS	GLU	CONFLICT	UNP P06169
B	55	ALA	ARG	CONFLICT	UNP P06169
B	143	ALA	CYS	CONFLICT	UNP P06169
B	206	ALA	VAL	CONFLICT	UNP P06169
B	208	VAL	ALA	CONFLICT	UNP P06169
B	538	ILE	VAL	CONFLICT	UNP P06169
B	551	LYS	GLU	CONFLICT	UNP P06169

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		



L281	L282	L283	S284	V285	G286	A287	L288	L289	S290	D291	PHE	ASN	THR	GLY	SER	PHE	SER	TYR	SER	TYR	K302	T303	K304	N305	E308	F309	H310	K315	T316	K317	K327	F328	K332	T337	A338	D339	K342	G343	Y344	V349	P350	A351	K352	N356	P364	M370	Q373
E380	G381	D382	I385	T388	T399	F400	P401	N402	N403	T404	Q409	V410	L411	T418	T422	L423	A426	F427	E431	I432	D433	P434	K435	K436	L440	F441	D444	G445	S446	L447	V451	T456	M457	I458	R459	Y465	L466	N470	N471	D472	G473	Y474	T475	I476	E477		
K478	L479	I480	H481	G482	P483	K484	A485	Q486	Q491	L496	S497	L498	L499	P500	T501	A504	K505	D506	Y507	E508	T509	V512	E517	N518	D519	D524	K525	N528	D529	R534	N535	E537	I538	N539	L540	P541	V542	P546	Q547	N548	L549	V550	Q552	A553	K554	L555	T556

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.95Å 74.67Å 119.95Å 90.00° 116.39° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	GPRLSA, X-PLOR	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	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: MG, TDP

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	1.06	0/4215	2.24	190/5728 (3.3%)
1	B	1.04	2/4215 (0.0%)	2.27	165/5728 (2.9%)
All	All	1.05	2/8430 (0.0%)	2.26	355/11456 (3.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	39	GLU	CD-OE1	-5.29	1.19	1.25
1	B	517	GLU	CD-OE1	-5.01	1.20	1.25

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CD-NE-CZ	23.23	156.13	123.60
1	B	459	ARG	NE-CZ-NH1	22.85	131.73	120.30
1	B	459	ARG	NE-CZ-NH2	-21.18	109.71	120.30
1	B	524	ASP	CB-CG-OD2	19.94	136.25	118.30
1	A	161	ARG	NE-CZ-NH1	19.36	129.98	120.30
1	B	258	ARG	NE-CZ-NH2	-16.75	111.93	120.30
1	B	258	ARG	NE-CZ-NH1	16.63	128.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ARG	CD-NE-CZ	16.63	146.88	123.60
1	A	511	ARG	NE-CZ-NH1	16.24	128.42	120.30
1	B	65	LYS	CB-CG-CD	15.21	151.16	111.60
1	A	312	ASP	CB-CG-OD1	14.60	131.44	118.30
1	A	312	ASP	CB-CG-OD2	-14.59	105.17	118.30
1	B	151	ARG	NE-CZ-NH2	-14.53	113.04	120.30
1	A	534	ARG	NE-CZ-NH1	13.51	127.06	120.30
1	B	534	ARG	NE-CZ-NH1	-13.18	113.71	120.30
1	A	202	ASP	CB-CG-OD2	-12.69	106.88	118.30
1	A	12	GLU	OE1-CD-OE2	12.42	138.21	123.30
1	B	534	ARG	NE-CZ-NH2	12.42	126.51	120.30
1	B	219	ASP	CB-CG-OD1	12.39	129.45	118.30
1	B	35	ASP	CB-CG-OD2	-12.23	107.29	118.30
1	A	44	ARG	CD-NE-CZ	12.11	140.56	123.60
1	B	287	ALA	N-CA-CB	-12.11	93.15	110.10
1	A	459	ARG	NE-CZ-NH2	-11.77	114.41	120.30
1	B	224	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	B	524	ASP	CB-CG-OD1	-11.26	108.17	118.30
1	A	161	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	339	ASP	CB-CG-OD1	10.90	128.11	118.30
1	B	151	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	A	437	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	A	459	ARG	NE-CZ-NH1	-10.57	115.01	120.30
1	A	150	ASP	CB-CG-OD2	-10.38	108.96	118.30
1	A	317	ARG	NE-CZ-NH2	10.26	125.43	120.30
1	A	209	LYS	CA-CB-CG	10.22	135.88	113.40
1	B	25	LEU	CA-CB-CG	10.15	138.63	115.30
1	A	459	ARG	NH1-CZ-NH2	10.08	130.49	119.40
1	A	35	ASP	CB-CG-OD2	-10.04	109.27	118.30
1	A	127	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	444	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	B	226	ASP	CB-CG-OD1	9.80	127.12	118.30
1	B	332	LYS	CB-CA-C	9.74	129.87	110.40
1	B	231	THR	CA-CB-CG2	9.72	126.01	112.40
1	B	59	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	179	LYS	CA-CB-CG	9.61	134.54	113.40
1	A	280	ASP	CB-CG-OD1	9.54	126.89	118.30
1	A	236	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	444	ASP	CB-CG-OD1	9.37	126.73	118.30
1	A	405	TYR	CB-CG-CD1	9.37	126.62	121.00
1	B	436	LYS	CB-CA-C	9.36	129.12	110.40
1	A	44	ARG	NE-CZ-NH2	9.32	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLU	OE1-CD-OE2	9.26	134.41	123.30
1	A	12	GLU	CG-CD-OE1	-9.25	99.80	118.30
1	B	285	VAL	CA-C-O	9.12	139.25	120.10
1	B	202	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	B	474	TYR	CB-CG-CD1	8.97	126.38	121.00
1	B	539	MET	CG-SD-CE	8.96	114.53	100.20
1	B	534	ARG	CD-NE-CZ	8.79	135.91	123.60
1	A	219	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	141	ASP	CB-CG-OD2	8.70	126.13	118.30
1	B	431	GLU	OE1-CD-OE2	-8.65	112.92	123.30
1	A	148	GLU	OE1-CD-OE2	-8.47	113.14	123.30
1	B	115	HIS	N-CA-CB	8.42	125.76	110.60
1	B	553	ALA	CB-CA-C	-8.38	97.53	110.10
1	A	41	GLU	CA-CB-CG	8.37	131.81	113.40
1	B	474	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	A	533	ILE	CA-CB-CG2	8.15	127.20	110.90
1	A	552	GLN	CG-CD-OE1	8.08	137.76	121.60
1	B	302	LYS	CA-CB-CG	8.04	131.09	113.40
1	B	135	THR	CA-CB-CG2	8.00	123.60	112.40
1	A	542	VAL	CA-CB-CG1	7.95	122.82	110.90
1	A	508	GLU	OE1-CD-OE2	7.94	132.82	123.30
1	B	537	GLU	OE1-CD-OE2	-7.91	113.81	123.30
1	B	529	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	B	284	SER	CB-CA-C	7.86	125.03	110.10
1	B	227	VAL	CB-CA-C	7.80	126.21	111.40
1	A	38	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	A	13	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	49	ALA	CB-CA-C	7.71	121.67	110.10
1	A	405	TYR	CA-CB-CG	7.68	128.00	113.40
1	B	436	LYS	CA-CB-CG	7.67	130.28	113.40
1	A	101	VAL	N-CA-CB	-7.63	94.71	111.50
1	B	151	ARG	CD-NE-CZ	7.63	134.28	123.60
1	B	253	SER	CB-CA-C	7.58	124.50	110.10
1	B	435	LYS	CB-CG-CD	7.58	131.31	111.60
1	A	32	SER	C-N-CA	7.54	140.54	121.70
1	A	415	ILE	CA-C-N	7.53	131.26	116.20
1	A	186	ASP	CB-CG-OD2	7.47	125.02	118.30
1	B	444	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	484	LYS	CG-CD-CE	7.45	134.26	111.90
1	B	273	LYS	CA-CB-CG	7.45	129.78	113.40
1	B	121	ASP	N-CA-CB	7.36	123.85	110.60
1	A	2	SER	N-CA-CB	7.34	121.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	ARG	CD-NE-CZ	7.27	133.78	123.60
1	B	267	LEU	CA-CB-CG	7.21	131.87	115.30
1	A	508	GLU	CG-CD-OE2	-7.18	103.93	118.30
1	A	219	ASP	CA-CB-CG	7.17	129.18	113.40
1	B	519	ASP	CB-CG-OD1	7.17	124.76	118.30
1	A	41	GLU	OE1-CD-OE2	-7.16	114.71	123.30
1	B	279	ALA	N-CA-CB	7.12	120.07	110.10
1	A	86	ALA	N-CA-CB	7.06	119.99	110.10
1	A	157	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	B	431	GLU	CG-CD-OE1	7.05	132.40	118.30
1	B	161	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	127	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	A	31	LEU	CB-CG-CD1	7.01	122.92	111.00
1	A	38	TYR	CB-CG-CD2	7.00	125.20	121.00
1	A	255	GLN	O-C-N	-6.96	111.56	122.70
1	B	400	PHE	CA-CB-CG	6.95	130.57	113.90
1	B	282	ILE	O-C-N	6.94	133.81	122.70
1	A	115	HIS	N-CA-CB	6.93	123.07	110.60
1	A	117	LEU	CA-CB-CG	6.92	131.22	115.30
1	A	288	LEU	N-CA-C	-6.91	92.36	111.00
1	A	63	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	423	LEU	CB-CA-C	6.88	123.27	110.20
1	B	507	TYR	CB-CG-CD1	6.86	125.12	121.00
1	B	274	GLU	CA-CB-CG	6.85	128.46	113.40
1	B	286	GLY	CA-C-N	-6.82	102.20	117.20
1	A	433	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	477	GLU	OE1-CD-OE2	6.78	131.44	123.30
1	A	380	GLU	OE1-CD-OE2	-6.76	115.18	123.30
1	B	95	VAL	CA-CB-CG1	-6.76	100.77	110.90
1	A	176	VAL	N-CA-CB	-6.75	96.65	111.50
1	B	143	ALA	N-CA-CB	6.75	119.55	110.10
1	A	280	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	545	ALA	CB-CA-C	6.73	120.19	110.10
1	B	154	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	209	LYS	N-CA-CB	-6.70	98.53	110.60
1	B	344	TYR	O-C-N	6.70	133.42	122.70
1	A	258	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	556	THR	CA-C-O	6.69	134.15	120.10
1	B	155	THR	CA-CB-OG1	-6.61	95.11	109.00
1	A	545	ALA	N-CA-CB	-6.61	100.84	110.10
1	A	540	LEU	N-CA-CB	-6.61	97.19	110.40
1	A	441	PHE	N-CA-CB	6.58	122.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	506	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	453	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	65	LYS	CA-CB-CG	6.53	127.76	113.40
1	A	61	TYR	CB-CG-CD1	6.52	124.91	121.00
1	B	280	ASP	CB-CG-OD2	-6.50	112.44	118.30
1	A	352	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	287	ALA	CA-C-O	6.50	133.75	120.10
1	B	496	LEU	CB-CA-C	6.49	122.54	110.20
1	A	303	THR	CA-CB-CG2	6.49	121.48	112.40
1	B	472	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	506	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	B	224	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	264	VAL	N-CA-C	-6.44	93.62	111.00
1	A	275	ALA	CB-CA-C	6.42	119.72	110.10
1	B	445	GLY	C-N-CA	6.41	137.73	121.70
1	A	251	SER	CA-CB-OG	-6.38	93.98	111.20
1	B	277	GLU	CG-CD-OE1	6.38	131.06	118.30
1	A	511	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	305	ASN	CB-CA-C	-6.33	97.74	110.40
1	A	493	TRP	N-CA-CB	6.32	121.98	110.60
1	B	227	VAL	CG1-CB-CG2	6.31	121.00	110.90
1	A	264	VAL	CA-CB-CG2	6.30	120.34	110.90
1	A	493	TRP	O-C-N	6.28	132.74	122.70
1	A	533	ILE	N-CA-CB	6.27	125.22	110.80
1	B	266	THR	CA-CB-CG2	6.27	121.17	112.40
1	B	280	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	4	ILE	CA-CB-CG2	6.25	123.41	110.90
1	B	426	ALA	CB-CA-C	6.23	119.44	110.10
1	A	56	TYR	CA-CB-CG	6.21	125.19	113.40
1	B	115	HIS	N-CA-C	-6.20	94.25	111.00
1	A	405	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	533	ILE	CB-CA-C	-6.19	99.23	111.60
1	B	267	LEU	O-C-N	6.18	132.59	122.70
1	B	5	THR	CA-CB-CG2	6.17	121.04	112.40
1	A	230	GLU	OE1-CD-OE2	6.17	130.70	123.30
1	B	259	TYR	CB-CG-CD2	6.17	124.70	121.00
1	B	486	GLN	CB-CG-CD	6.16	127.61	111.60
1	B	210	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	506	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	B	51	GLU	CA-CB-CG	6.12	126.87	113.40
1	B	446	SER	N-CA-CB	6.12	119.68	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	304	LYS	N-CA-C	6.09	127.44	111.00
1	A	226	ASP	CA-CB-CG	6.08	126.76	113.40
1	A	247	MET	N-CA-CB	6.06	121.50	110.60
1	A	317	ARG	NH1-CZ-NH2	-6.03	112.76	119.40
1	A	338	ALA	N-CA-CB	6.03	118.54	110.10
1	B	220	ALA	N-CA-CB	-6.03	101.66	110.10
1	B	459	ARG	CA-CB-CG	6.01	126.63	113.40
1	B	207	LEU	CA-CB-CG	6.00	129.10	115.30
1	B	286	GLY	O-C-N	5.98	132.27	122.70
1	A	217	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	188	SER	N-CA-CB	5.97	119.45	110.50
1	A	33	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	349	VAL	N-CA-CB	-5.96	98.40	111.50
1	A	189	LEU	CA-CB-CG	5.95	128.99	115.30
1	B	528	ASN	CB-CG-OD1	-5.95	109.70	121.60
1	A	141	ASP	CA-CB-CG	5.95	126.49	113.40
1	A	304	LYS	C-N-CA	5.93	136.53	121.70
1	A	312	ASP	O-C-N	5.93	132.19	122.70
1	A	496	LEU	CB-CA-C	5.93	121.47	110.20
1	A	515	THR	N-CA-CB	-5.92	99.05	110.30
1	B	34	LEU	CB-CA-C	5.92	121.45	110.20
1	B	304	LYS	CB-CG-CD	5.92	126.98	111.60
1	A	529	ASP	CB-CA-C	5.92	122.23	110.40
1	B	339	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	142	ILE	N-CA-CB	5.88	124.32	110.80
1	B	150	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	552	GLN	OE1-CD-NE2	-5.86	108.43	121.90
1	B	399	THR	N-CA-CB	5.85	121.42	110.30
1	B	235	ILE	CA-CB-CG2	5.83	122.55	110.90
1	A	528	ASN	CA-CB-CG	-5.83	100.58	113.40
1	B	435	LYS	CA-CB-CG	5.83	126.22	113.40
1	A	289	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	517	GLU	CG-CD-OE1	5.80	129.90	118.30
1	A	531	SER	N-CA-CB	-5.80	101.81	110.50
1	A	73	THR	OG1-CB-CG2	5.79	123.32	110.00
1	A	453	GLU	CG-CD-OE1	5.79	129.88	118.30
1	B	277	GLU	CB-CG-CD	5.78	129.81	114.20
1	A	468	VAL	CA-CB-CG1	5.77	119.55	110.90
1	B	234	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	199	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	A	103	SER	N-CA-CB	-5.73	101.91	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ASP	CA-CB-CG	5.73	126.00	113.40
1	A	306	ILE	O-C-N	5.72	131.86	122.70
1	A	148	GLU	CG-CD-OE2	5.72	129.75	118.30
1	B	47	GLY	CA-C-O	-5.72	110.30	120.60
1	A	542	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	B	3	GLU	CG-CD-OE2	-5.69	106.91	118.30
1	A	210	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	332	LYS	N-CA-CB	-5.69	100.36	110.60
1	A	43	MET	CG-SD-CE	-5.68	91.11	100.20
1	B	422	THR	N-CA-CB	5.68	121.09	110.30
1	A	155	THR	CA-CB-CG2	5.67	120.34	112.40
1	A	104	ILE	N-CA-CB	5.67	123.84	110.80
1	A	519	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	230	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	B	470	ASN	O-C-N	5.66	131.75	122.70
1	B	56	TYR	CB-CG-CD2	5.65	124.39	121.00
1	B	427	PHE	CA-CB-CG	5.65	127.46	113.90
1	A	44	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	154	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	179	LYS	N-CA-CB	-5.62	100.48	110.60
1	B	388	THR	CA-CB-CG2	5.62	120.27	112.40
1	B	199	GLU	CA-CB-CG	5.61	125.73	113.40
1	B	315	LYS	O-C-N	5.59	131.65	122.70
1	A	287	ALA	C-N-CA	5.58	135.66	121.70
1	A	423	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	263	TYR	C-N-CA	5.57	135.62	121.70
1	B	465	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	305	ASN	N-CA-CB	5.55	120.59	110.60
1	B	35	ASP	OD1-CG-OD2	5.54	133.83	123.30
1	A	262	VAL	CA-CB-CG2	5.52	119.18	110.90
1	A	526	SER	CA-CB-OG	-5.52	96.30	111.20
1	B	447	LEU	CB-CG-CD2	5.52	120.38	111.00
1	A	488	ASN	N-CA-CB	5.51	120.51	110.60
1	A	510	HIS	O-C-N	5.50	131.50	122.70
1	B	499	LEU	CB-CA-C	5.50	120.65	110.20
1	A	515	THR	OG1-CB-CG2	5.50	122.64	110.00
1	B	284	SER	N-CA-CB	-5.50	102.25	110.50
1	A	517	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	B	230	GLU	CA-CB-CG	5.49	125.47	113.40
1	A	209	LYS	N-CA-CB	5.48	120.46	110.60
1	B	285	VAL	N-CA-C	-5.48	96.21	111.00
1	A	274	GLU	CG-CD-OE2	-5.47	107.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	N-CA-CB	5.46	120.43	110.60
1	B	535	MET	CG-SD-CE	5.45	108.92	100.20
1	B	266	THR	CA-CB-OG1	-5.45	97.56	109.00
1	A	101	VAL	CB-CA-C	5.43	121.71	111.40
1	B	202	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	415	ILE	CA-C-O	-5.41	108.74	120.10
1	B	121	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	99	VAL	CA-CB-CG1	5.39	118.99	110.90
1	A	234	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	193	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	B	537	GLU	CA-CB-CG	5.39	125.27	113.40
1	B	157	TYR	CA-CB-CG	-5.39	103.16	113.40
1	A	514	THR	CA-C-N	-5.38	105.35	117.20
1	B	61	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	265	GLY	O-C-N	5.36	131.27	122.70
1	B	175	ASN	CB-CG-ND2	5.36	129.55	116.70
1	B	283	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	185	ILE	O-C-N	5.34	131.25	122.70
1	A	330	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	239	GLN	N-CA-CB	5.34	120.20	110.60
1	A	553	ALA	CB-CA-C	-5.33	102.10	110.10
1	B	441	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	A	99	VAL	CA-CB-CG2	5.32	118.87	110.90
1	A	325	GLN	CB-CG-CD	5.32	125.42	111.60
1	A	535	MET	CA-CB-CG	-5.31	104.27	113.30
1	A	306	ILE	CA-CB-CG1	-5.31	100.91	111.00
1	A	440	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	127	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	B	382	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	508	GLU	O-C-N	5.29	131.17	122.70
1	B	285	VAL	CA-C-N	-5.29	105.62	116.20
1	A	319	ALA	CB-CA-C	-5.29	102.17	110.10
1	A	415	ILE	CA-CB-CG2	-5.29	100.33	110.90
1	A	102	PRO	C-N-CA	5.28	134.90	121.70
1	B	508	GLU	CB-CA-C	-5.27	99.85	110.40
1	A	173	ASP	O-C-N	5.27	131.13	122.70
1	A	333	LEU	CA-CB-CG	5.26	127.41	115.30
1	B	285	VAL	CA-CB-CG1	-5.26	103.02	110.90
1	A	389	GLY	N-CA-C	-5.25	99.97	113.10
1	A	344	TYR	CA-C-O	5.25	131.13	120.10
1	B	227	VAL	CA-CB-CG1	5.25	118.78	110.90
1	B	509	THR	CA-CB-OG1	-5.25	97.98	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	GLN	C-N-CA	5.24	134.79	121.70
1	B	271	GLU	CG-CD-OE2	-5.23	107.85	118.30
1	A	35	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	497	SER	N-CA-CB	5.22	118.33	110.50
1	A	472	ASP	N-CA-CB	-5.22	101.20	110.60
1	A	217	LEU	CB-CG-CD2	5.22	119.88	111.00
1	B	504	ALA	C-N-CA	5.21	134.73	121.70
1	B	304	LYS	N-CA-CB	-5.21	101.22	110.60
1	A	31	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	553	ALA	N-CA-CB	-5.20	102.83	110.10
1	A	274	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	B	277	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	B	409	GLN	CB-CA-C	5.16	120.71	110.40
1	B	154	ARG	CG-CD-NE	-5.15	100.99	111.80
1	A	21	THR	N-CA-CB	5.14	120.07	110.30
1	A	145	ALA	CB-CA-C	5.14	117.81	110.10
1	A	187	MET	CA-CB-CG	5.14	122.04	113.30
1	A	230	GLU	O-C-N	5.14	130.92	122.70
1	B	83	ASN	OD1-CG-ND2	5.13	133.69	121.90
1	A	287	ALA	O-C-N	-5.12	114.50	122.70
1	A	556	THR	OG1-CB-CG2	-5.12	98.22	110.00
1	A	531	SER	CA-CB-OG	-5.12	97.37	111.20
1	A	151	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	534	ARG	CG-CD-NE	5.12	122.55	111.80
1	A	338	ALA	O-C-N	5.12	130.88	122.70
1	B	57	ALA	N-CA-CB	5.11	117.26	110.10
1	B	138	MET	N-CA-CB	5.11	119.80	110.60
1	B	447	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	491	GLN	N-CA-C	-5.10	97.22	111.00
1	B	433	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	101	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	479	LEU	CB-CA-C	5.10	119.88	110.20
1	B	539	MET	CB-CA-C	5.09	120.58	110.40
1	A	417	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	A	82	LEU	CB-CA-C	5.08	119.84	110.20
1	B	59	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	119	ASN	N-CA-CB	-5.07	101.47	110.60
1	B	235	ILE	CB-CA-C	5.07	121.75	111.60
1	B	342	LYS	CA-CB-CG	5.07	124.56	113.40
1	B	258	ARG	CB-CA-C	-5.07	100.27	110.40
1	B	554	LYS	O-C-N	5.07	130.80	122.70
1	B	477	GLU	CG-CD-OE2	-5.06	108.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	553	ALA	CA-C-N	-5.06	106.07	117.20
1	A	290	SER	CB-CA-C	5.04	119.68	110.10
1	A	144	THR	N-CA-CB	-5.03	100.74	110.30
1	B	174	LEU	CB-CA-C	5.03	119.76	110.20
1	A	200	VAL	CG1-CB-CG2	5.03	118.95	110.90
1	B	539	MET	N-CA-CB	-5.03	101.55	110.60
1	A	468	VAL	O-C-N	-5.01	114.68	122.70
1	B	117	LEU	N-CA-CB	-5.01	100.37	110.40
1	A	499	LEU	CB-CA-C	5.01	119.72	110.20
1	A	323	GLY	CA-C-O	-5.01	111.58	120.60
1	A	97	HIS	C-N-CA	5.00	134.21	121.70
1	A	534	ARG	NH1-CZ-NH2	-5.00	113.90	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ARG	Sidechain
1	B	154	ARG	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	4130	0	4150	139	1
1	B	4130	0	4151	126	1
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	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8316	0	8333	260	1

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 16.

All (260) 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)
3:B:557:TDP:H2	3:B:557:TDP:C2	0.97	1.49
3:A:557:TDP:C2	3:A:557:TDP:H2	0.97	1.46
1:B:267:LEU:HD11	1:B:552:GLN:HB2	1.47	0.93
1:B:4:ILE:HD11	1:B:8:LYS:HG2	1.56	0.86
1:B:505:LYS:H	1:B:505:LYS:HD2	1.45	0.81
1:A:345:LYS:HD3	1:A:345:LYS:H	1.45	0.81
1:A:553:ALA:O	1:A:556:THR:HG22	1.81	0.81
1:A:267:LEU:HD21	1:A:552:GLN:NE2	1.96	0.80
1:A:158:VAL:HG23	1:A:187:MET:CE	2.11	0.80
1:B:159:THR:HG22	1:B:161:ARG:HB2	1.63	0.79
1:A:132:ILE:HG22	1:B:117:LEU:HD21	1.67	0.76
1:A:12:GLU:HG2	1:A:181:LEU:HD13	1.67	0.75
1:A:287:ALA:HB1	1:A:289:LEU:HB3	1.68	0.75
1:B:476:ILE:HD12	1:B:549:LEU:HD21	1.67	0.75
1:B:126:HIS:HE1	1:B:136:THR:OG1	1.71	0.74
1:B:65:LYS:HD2	1:B:432:ILE:HD11	1.71	0.72
1:A:280:ASP:HA	1:A:304:LYS:HE2	1.71	0.72
1:A:327:LYS:O	1:A:331:GLN:HG3	1.90	0.71
1:B:271:GLU:HG2	1:B:350:PRO:HB3	1.74	0.70
1:A:473:GLY:HA2	1:A:490:ILE:HG12	1.73	0.70
1:B:476:ILE:HD12	1:B:549:LEU:CD2	2.22	0.69
1:A:505:LYS:HD3	1:A:505:LYS:H	1.57	0.69
1:A:491:GLN:HB2	1:B:459:ARG:HG2	1.75	0.67
1:A:505:LYS:CD	1:A:505:LYS:H	2.07	0.67
1:A:241:PRO:HB3	1:A:349:VAL:HG12	1.77	0.66
1:B:553:ALA:O	1:B:554:LYS:C	2.33	0.66
1:B:525:LYS:H	1:B:525:LYS:HD2	1.61	0.66
1:A:158:VAL:HG23	1:A:187:MET:HE2	1.77	0.65
1:A:302:LYS:HZ3	1:A:304:LYS:HD3	1.62	0.65
1:A:505:LYS:HD3	1:A:506:ASP:H	1.62	0.65
1:A:114:HIS:N	1:A:116:THR:HG1	1.95	0.65
1:B:546:PRO:HB2	1:B:548:ASN:ND2	2.12	0.64
1:B:342:LYS:HD2	1:B:342:LYS:O	1.98	0.64
1:B:525:LYS:H	1:B:525:LYS:CD	2.11	0.63
1:A:157:TYR:HB3	1:A:187:MET:HE1	1.81	0.63
1:A:4:ILE:CG1	1:A:8:LYS:HD3	2.28	0.63
1:B:95:VAL:O	1:B:162:PRO:HA	2.00	0.62
1:B:21:THR:HG22	1:B:431:GLU:OE2	1.99	0.62
1:A:553:ALA:C	1:A:556:THR:HG22	2.20	0.62
1:B:480:ILE:HG12	1:B:556:THR:HG23	1.82	0.61
1:A:302:LYS:NZ	1:A:304:LYS:NZ	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:HIS:CE1	1:B:136:THR:OG1	2.53	0.61
1:A:369:TRP:CH2	1:A:373:GLN:HG2	2.36	0.61
1:A:212:LYS:O	1:A:345:LYS:HE2	2.00	0.61
1:B:287:ALA:HB1	1:B:288:LEU:HD12	1.82	0.61
1:B:553:ALA:HA	1:B:556:THR:HG22	1.83	0.61
1:A:4:ILE:HG12	1:A:8:LYS:HD3	1.82	0.61
1:B:288:LEU:H	1:B:288:LEU:HD12	1.65	0.61
1:B:103:SER:O	1:B:105:SER:N	2.34	0.61
1:A:104:ILE:HG22	1:A:104:ILE:O	2.00	0.60
1:B:385:ILE:HG22	1:B:418:THR:HG22	1.83	0.59
1:B:480:ILE:HG12	1:B:556:THR:CG2	2.32	0.59
1:A:79:LEU:HA	1:A:82:LEU:HD22	1.83	0.59
1:A:218:ALA:HB2	1:A:252:ILE:HD11	1.84	0.59
1:A:499:LEU:HD22	1:A:533:ILE:HD12	1.83	0.59
1:A:200:VAL:O	1:A:204:ILE:HG13	2.02	0.58
1:A:426:ALA:HA	1:A:438:VAL:HG21	1.83	0.58
1:B:235:ILE:HD11	1:B:258:ARG:HB2	1.85	0.58
1:B:555:LEU:HD12	1:B:555:LEU:O	2.04	0.58
3:A:557:TDP:N1'	1:B:51:GLU:OE2	2.37	0.58
1:B:339:ASP:O	1:B:342:LYS:HG3	2.03	0.57
1:B:145:ALA:HB3	1:B:146:PRO:HD3	1.85	0.57
1:A:267:LEU:HD21	1:A:552:GLN:HE22	1.68	0.57
1:A:51:GLU:HB2	1:A:80:SER:HB2	1.86	0.57
1:B:190:LYS:HD2	1:B:191:PRO:HD2	1.87	0.57
1:A:232:LYS:HE3	1:A:252:ILE:HA	1.87	0.56
1:A:71:ILE:HA	1:A:98:VAL:O	2.04	0.56
1:A:496:LEU:HD22	1:A:509:THR:HB	1.86	0.56
1:A:262:VAL:O	1:A:272:VAL:HG11	2.05	0.56
1:A:95:VAL:O	1:A:162:PRO:HA	2.04	0.56
1:B:380:GLU:HG3	1:B:402:ASN:O	2.06	0.56
1:A:244:VAL:O	1:A:262:VAL:HA	2.05	0.56
1:A:345:LYS:CD	1:A:345:LYS:H	2.11	0.56
1:B:475:THR:HG21	1:B:542:VAL:O	2.06	0.55
1:B:65:LYS:HD2	1:B:432:ILE:CD1	2.37	0.55
1:A:380:GLU:HG2	1:A:401:PRO:HB2	1.89	0.55
1:B:228:LYS:HD3	1:B:229:ALA:H	1.71	0.54
1:A:218:ALA:CB	1:A:252:ILE:HD11	2.37	0.54
1:A:152:CYS:HB3	1:A:163:VAL:HG11	1.90	0.54
1:A:13:ARG:HG3	1:A:185:ILE:HD11	1.89	0.54
1:A:139:ILE:HG21	1:A:145:ALA:HB2	1.90	0.54
1:A:415:ILE:O	1:A:446:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:CD1	1:B:8:LYS:HG2	2.34	0.53
1:A:92:HIS:O	1:A:224:ARG:HG2	2.07	0.53
1:A:22:VAL:HG11	1:A:71:ILE:HD12	1.91	0.53
1:B:505:LYS:HD2	1:B:506:ASP:H	1.72	0.53
1:A:27:GLY:HA2	3:B:557:TDP:H351	1.91	0.53
1:A:267:LEU:CD2	1:A:552:GLN:NE2	2.69	0.53
1:A:203:THR:O	1:A:206:ALA:HB3	2.08	0.53
1:A:264:VAL:O	1:A:268:SER:OG	2.26	0.53
1:B:440:LEU:HD12	1:B:466:LEU:HD12	1.90	0.52
1:B:221:CYS:H	1:B:287:ALA:CB	2.21	0.52
1:B:284:SER:C	1:B:286:GLY:H	2.13	0.52
1:B:440:LEU:HD22	1:B:441:PHE:N	2.25	0.52
1:A:227:VAL:HG21	1:A:330:LEU:HD23	1.90	0.52
1:A:158:VAL:HG23	1:A:187:MET:HE3	1.91	0.52
1:A:385:ILE:HG12	1:A:407:ILE:HD12	1.92	0.52
1:B:144:THR:O	1:B:147:ALA:HB3	2.10	0.52
1:A:514:THR:OG1	1:A:517:GLU:HG3	2.10	0.52
1:B:235:ILE:CD1	1:B:258:ARG:HB2	2.40	0.51
1:B:499:LEU:HB2	1:B:500:PRO:HD3	1.91	0.51
1:A:228:LYS:O	1:A:232:LYS:HG2	2.10	0.51
1:A:440:LEU:HD12	1:A:466:LEU:HD22	1.92	0.51
1:B:33:LEU:HD13	1:B:71:ILE:HD13	1.92	0.51
1:A:249:LYS:HE3	1:A:400:PHE:CZ	2.45	0.51
1:B:302:LYS:O	1:B:303:THR:OG1	2.26	0.51
1:B:401:PRO:HD2	1:B:404:THR:OG1	2.10	0.51
1:B:214:PRO:HG2	1:B:240:PHE:CE1	2.45	0.51
1:B:214:PRO:HG2	1:B:240:PHE:CD1	2.46	0.51
1:A:550:VAL:O	1:A:554:LYS:HB2	2.11	0.51
1:B:497:SER:O	1:B:500:PRO:HD2	2.11	0.50
1:B:123:THR:O	1:B:127:ARG:HG3	2.11	0.50
1:A:498:LEU:HD13	1:B:501:THR:HG21	1.93	0.50
1:B:552:GLN:HG3	1:B:552:GLN:O	2.08	0.50
1:A:302:LYS:HZ1	1:A:304:LYS:HZ3	1.60	0.50
1:B:207:LEU:CD1	1:B:305:ASN:HD21	2.24	0.50
3:A:557:TDP:H351	1:B:27:GLY:HA2	1.93	0.50
1:B:154:ARG:NH2	1:B:188:SER:O	2.45	0.50
1:A:471:ASN:O	1:A:542:VAL:HG22	2.11	0.50
1:B:456:THR:HA	1:B:459:ARG:HG3	1.92	0.50
1:B:221:CYS:SG	1:B:287:ALA:HB1	2.52	0.50
1:A:71:ILE:HG12	1:A:98:VAL:HB	1.93	0.50
1:B:154:ARG:O	1:B:158:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:OD2	1:B:481:HIS:HE1	1.95	0.49
1:A:511:ARG:NH2	1:A:537:GLU:OE1	2.45	0.49
1:B:221:CYS:HA	1:B:224:ARG:HB2	1.94	0.49
1:B:207:LEU:HG	1:B:305:ASN:ND2	2.27	0.49
1:A:4:ILE:HG13	1:A:8:LYS:HD3	1.93	0.49
1:B:547:GLN:O	1:B:550:VAL:HB	2.13	0.49
1:B:139:ILE:HG22	1:B:171:LEU:CD1	2.43	0.49
1:B:155:THR:O	1:B:159:THR:HB	2.13	0.49
1:A:222:CYS:O	1:A:227:VAL:HG13	2.13	0.49
1:A:148:GLU:OE2	1:A:151:ARG:NH1	2.46	0.49
1:B:302:LYS:HA	1:B:302:LYS:HE2	1.94	0.49
1:A:13:ARG:HD3	1:A:181:LEU:CD2	2.43	0.49
1:A:302:LYS:CE	1:A:304:LYS:HZ2	2.26	0.49
1:A:499:LEU:HD22	1:A:533:ILE:CD1	2.43	0.49
1:B:221:CYS:SG	1:B:288:LEU:CD1	3.01	0.48
1:B:497:SER:C	1:B:500:PRO:HD2	2.34	0.48
1:A:157:TYR:HD2	1:A:187:MET:HE2	1.78	0.48
1:A:254:GLU:HB2	1:A:400:PHE:O	2.13	0.48
1:B:114:HIS:N	1:B:116:THR:HG1	2.12	0.48
1:A:243:PHE:HA	1:A:261:GLY:O	2.14	0.48
1:B:549:LEU:O	1:B:553:ALA:HB2	2.14	0.48
1:A:6:LEU:O	1:A:9:TYR:HB3	2.14	0.47
1:A:142:ILE:H	1:A:142:ILE:HD12	1.79	0.47
1:B:509:THR:HA	1:B:535:MET:O	2.15	0.47
1:A:273:LYS:HD2	1:A:277:GLU:OE1	2.14	0.47
1:B:458:ILE:HG23	1:B:505:LYS:NZ	2.30	0.47
1:B:505:LYS:CD	1:B:506:ASP:H	2.28	0.47
1:B:271:GLU:CG	1:B:350:PRO:HB3	2.43	0.47
1:A:302:LYS:HZ3	1:A:304:LYS:CD	2.28	0.47
1:A:414:SER:HB2	1:B:76:VAL:HG12	1.95	0.47
1:A:361:ALA:HA	1:A:515:THR:HG22	1.97	0.47
1:B:101:VAL:O	1:B:168:PRO:HA	2.15	0.46
1:A:302:LYS:NZ	1:A:304:LYS:HZ2	2.14	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HB2	1.76	0.46
1:B:21:THR:HB	1:B:44:ARG:HG3	1.97	0.46
1:A:317:ARG:NH1	1:A:317:ARG:HB2	2.30	0.46
1:A:117:LEU:HD22	1:A:124:VAL:HG11	1.96	0.46
1:B:356:ASN:ND2	1:B:373:GLN:OE1	2.48	0.46
1:A:505:LYS:CD	1:A:506:ASP:H	2.29	0.46
1:B:435:LYS:HG3	1:B:435:LYS:O	2.15	0.46
1:A:62:ALA:HB2	1:A:68:SER:HG	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HG	1:B:89:TYR:CD2	2.51	0.46
1:B:221:CYS:H	1:B:287:ALA:HB2	1.81	0.45
1:B:234:LEU:HD21	1:B:337:ILE:HD13	1.97	0.45
1:B:553:ALA:O	1:B:556:THR:HG22	2.15	0.45
1:A:228:LYS:O	1:A:232:LYS:CG	2.65	0.45
1:A:289:LEU:HD12	1:A:291:ASP:OD1	2.17	0.45
1:A:83:ASN:HD21	1:B:76:VAL:HA	1.82	0.45
1:B:512:VAL:HG22	1:B:517:GLU:HB3	1.98	0.45
1:A:179:LYS:O	1:A:182:GLN:HG2	2.16	0.45
1:B:302:LYS:HB3	1:B:303:THR:H	1.50	0.45
1:A:12:GLU:HG2	1:A:181:LEU:CD1	2.42	0.45
1:A:384:VAL:HG11	1:A:395:ILE:HD11	1.98	0.45
1:A:142:ILE:N	1:A:142:ILE:HD12	2.32	0.45
1:A:435:LYS:N	1:A:435:LYS:HD2	2.32	0.45
1:A:311:SER:HA	1:A:326:MET:HG2	1.99	0.45
1:B:553:ALA:HA	1:B:556:THR:CG2	2.47	0.45
1:B:222:CYS:HA	1:B:227:VAL:HG12	1.99	0.45
1:B:553:ALA:CA	1:B:556:THR:HG22	2.47	0.45
1:A:59:ASP:O	1:A:62:ALA:HB3	2.17	0.45
1:A:459:ARG:HH11	1:A:459:ARG:HD2	1.55	0.45
1:B:538:ILE:HG22	1:B:540:LEU:HG	1.98	0.45
1:A:475:THR:HB	1:A:542:VAL:O	2.17	0.44
1:A:134:GLU:HB2	1:A:161:ARG:HB3	1.99	0.44
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.82	0.44
1:A:540:LEU:HA	1:A:541:PRO:HD3	1.76	0.44
1:A:302:LYS:HD3	1:A:304:LYS:HD3	1.98	0.44
1:B:315:LYS:HE2	1:B:317:ARG:O	2.16	0.44
1:A:365:LEU:HD13	1:A:538:ILE:HG23	1.98	0.44
1:A:349:VAL:HG23	1:A:352:ARG:HH21	1.83	0.44
1:A:249:LYS:HE2	1:A:395:ILE:O	2.18	0.44
1:A:515:THR:HG22	1:A:516:GLY:N	2.32	0.44
1:B:422:THR:OG1	1:B:440:LEU:HG	2.18	0.44
1:A:273:LYS:HD2	1:A:277:GLU:CD	2.38	0.44
1:A:176:VAL:HA	1:A:177:PRO:HD3	1.93	0.44
1:B:483:PRO:C	1:B:484:LYS:HG2	2.39	0.44
1:A:147:ALA:O	1:A:150:ASP:HB2	2.18	0.43
1:A:467:PHE:HB3	1:A:538:ILE:HD11	2.00	0.43
1:B:220:ALA:HB3	1:B:288:LEU:HD13	1.99	0.43
1:A:365:LEU:HD11	1:A:512:VAL:HG13	2.00	0.43
1:B:190:LYS:CD	1:B:191:PRO:HD2	2.48	0.43
1:B:475:THR:CG2	1:B:542:VAL:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HD11	1:B:165:LEU:HD11	2.00	0.43
1:B:308:GLU:HB3	1:B:310:HIS:NE2	2.33	0.43
1:B:352:ARG:HG3	1:B:352:ARG:NH1	2.33	0.43
1:B:221:CYS:SG	1:B:288:LEU:HD11	2.59	0.43
1:A:315:LYS:HA	1:A:319:ALA:O	2.19	0.43
1:A:365:LEU:HD13	1:A:538:ILE:CG2	2.49	0.43
1:B:555:LEU:O	1:B:556:THR:O	2.37	0.42
1:B:90:ALA:HB1	1:B:411:LEU:HD22	2.01	0.42
1:A:267:LEU:CD2	1:A:552:GLN:HE22	2.30	0.42
1:B:139:ILE:CD1	1:B:165:LEU:HD11	2.50	0.42
1:A:267:LEU:HD21	1:A:552:GLN:HE21	1.77	0.42
1:B:555:LEU:O	1:B:556:THR:C	2.56	0.42
1:B:221:CYS:SG	1:B:288:LEU:HD12	2.59	0.42
1:B:411:LEU:HD23	1:B:411:LEU:C	2.40	0.42
1:A:349:VAL:CG2	1:A:352:ARG:HH21	2.33	0.42
1:B:496:LEU:HD22	1:B:509:THR:HB	2.01	0.42
1:A:416:GLY:HA3	1:A:450:THR:HG23	2.02	0.42
1:A:469:LEU:CD2	1:A:538:ILE:HD12	2.49	0.42
1:A:135:THR:O	1:A:163:VAL:HG13	2.19	0.42
1:A:72:THR:O	1:A:99:VAL:HA	2.20	0.42
1:B:14:LEU:HA	1:B:14:LEU:HD12	1.96	0.42
3:B:557:TDP:H2	3:B:557:TDP:C35	2.46	0.41
1:A:553:ALA:O	1:A:556:THR:CG2	2.60	0.41
1:A:336:ASN:N	1:A:336:ASN:ND2	2.68	0.41
1:B:508:GLU:HB2	1:B:534:ARG:HG2	2.00	0.41
1:B:268:SER:O	1:B:269:LYS:C	2.59	0.41
1:B:400:PHE:HA	1:B:401:PRO:HD3	1.84	0.41
1:A:345:LYS:HE3	1:A:345:LYS:O	2.20	0.41
1:A:304:LYS:HB3	1:A:305:ASN:H	1.61	0.41
1:A:3:GLU:O	1:A:4:ILE:HD12	2.21	0.41
1:B:247:MET:HG3	1:B:410:VAL:HB	2.03	0.41
1:A:360:PRO:HG2	1:A:363:THR:OG1	2.20	0.41
1:B:171:LEU:O	1:B:174:LEU:HB2	2.20	0.41
1:A:447:LEU:HD11	1:A:451:VAL:HG23	2.02	0.41
1:A:214:PRO:HD2	1:A:344:TYR:CE1	2.55	0.41
1:B:505:LYS:CD	1:B:505:LYS:H	2.14	0.41
1:B:352:ARG:HD3	1:B:399:THR:HG21	2.02	0.41
1:A:27:GLY:O	1:A:31:LEU:HD13	2.21	0.41
1:A:302:LYS:HE2	1:A:304:LYS:HZ2	1.86	0.41
1:B:239:GLN:O	1:B:258:ARG:HD3	2.21	0.41
1:A:62:ALA:HB2	1:A:68:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:O	1:B:451:VAL:HB	2.21	0.41
1:A:266:THR:HG22	1:A:273:LYS:NZ	2.36	0.41
1:B:234:LEU:CD2	1:B:337:ILE:HD13	2.51	0.41
1:B:433:ASP:HA	1:B:434:PRO:HD3	1.96	0.41
1:A:227:VAL:O	1:A:227:VAL:HG22	2.21	0.40
1:B:92:HIS:HD2	1:B:225:HIS:HE1	1.69	0.40
1:A:35:ASP:OD2	1:B:481:HIS:CE1	2.74	0.40
1:B:269:LYS:O	1:B:272:VAL:HB	2.21	0.40
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.87	0.40
1:A:23:PHE:O	1:A:70:ILE:HA	2.21	0.40
1:B:220:ALA:HB3	1:B:288:LEU:CD1	2.51	0.40
1:B:328:PHE:O	1:B:332:LYS:HB2	2.22	0.40
1:A:227:VAL:CG2	1:A:330:LEU:HD23	2.52	0.40
1:A:555:LEU:HG	1:A:555:LEU:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:NH1	1:B:199:GLU:OE2[2_555]	2.08	0.12

## 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	531/556 (96%)	490 (92%)	37 (7%)	4 (1%)	24	35
1	B	531/556 (96%)	492 (93%)	34 (6%)	5 (1%)	21	30
All	All	1062/1112 (96%)	982 (92%)	71 (7%)	9 (1%)	24	35

All (9) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	103	SER
1	A	227	VAL
1	A	304	LYS
1	B	288	LEU
1	B	289	LEU
1	B	104	ILE
1	A	417	PHE
1	B	303	THR
1	B	342	LYS

### 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	447/464 (96%)	389 (87%)	58 (13%)	5	6
1	B	447/464 (96%)	394 (88%)	53 (12%)	6	8
All	All	894/928 (96%)	783 (88%)	111 (12%)	6	7

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	13	ARG
1	A	14	LEU
1	A	31	LEU
1	A	33	LEU
1	A	34	LEU
1	A	52	LEU
1	A	70	ILE
1	A	82	LEU
1	A	99	VAL
1	A	102	PRO
1	A	103	SER
1	A	114	HIS
1	A	117	LEU
1	A	126	HIS

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Mol	Chain	Res	Type
1	A	135	THR
1	A	142	ILE
1	A	144	THR
1	A	161	ARG
1	A	165	LEU
1	A	176	VAL
1	A	179	LYS
1	A	196	SER
1	A	199	GLU
1	A	207	LEU
1	A	224	ARG
1	A	232	LYS
1	A	233	LYS
1	A	237	LEU
1	A	264	VAL
1	A	267	LEU
1	A	271	GLU
1	A	273	LYS
1	A	274	GLU
1	A	289	LEU
1	A	291	ASP
1	A	302	LYS
1	A	303	THR
1	A	304	LYS
1	A	330	LEU
1	A	336	ASN
1	A	345	LYS
1	A	359	VAL
1	A	362	SER
1	A	391	SER
1	A	405	TYR
1	A	440	LEU
1	A	453	GLU
1	A	475	THR
1	A	479	LEU
1	A	498	LEU
1	A	505	LYS
1	A	512	VAL
1	A	515	THR
1	A	520	LYS
1	A	525	LYS
1	A	533	ILE

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Mol	Chain	Res	Type
1	A	555	LEU
1	B	2	SER
1	B	14	LEU
1	B	21	THR
1	B	25	LEU
1	B	33	LEU
1	B	34	LEU
1	B	52	LEU
1	B	70	ILE
1	B	142	ILE
1	B	161	ARG
1	B	167	LEU
1	B	174	LEU
1	B	176	VAL
1	B	179	LYS
1	B	183	THR
1	B	189	LEU
1	B	190	LYS
1	B	198	LYS
1	B	199	GLU
1	B	207	LEU
1	B	215	VAL
1	B	223	SER
1	B	224	ARG
1	B	227	VAL
1	B	228	LYS
1	B	232	LYS
1	B	234	LEU
1	B	235	ILE
1	B	281	LEU
1	B	289	LEU
1	B	291	ASP
1	B	302	LYS
1	B	304	LYS
1	B	305	ASN
1	B	327	LYS
1	B	342	LYS
1	B	349	VAL
1	B	352	ARG
1	B	364	PRO
1	B	370	MET
1	B	423	LEU

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Mol	Chain	Res	Type
1	B	435	LYS
1	B	440	LEU
1	B	447	LEU
1	B	466	LEU
1	B	475	THR
1	B	476	ILE
1	B	479	LEU
1	B	484	LYS
1	B	505	LYS
1	B	512	VAL
1	B	525	LYS
1	B	548	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	126	HIS
1	A	255	GLN
1	A	403	ASN
1	A	523	GLN
1	A	552	GLN
1	B	20	ASN
1	B	83	ASN
1	B	126	HIS
1	B	131	ASN
1	B	213	ASN
1	B	225	HIS
1	B	376	ASN
1	B	548	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	TDP	A	557	2	21,27,27	1.09	1 (4%)	31,40,40	1.31	5 (16%)
3	TDP	B	557	2	21,27,27	1.19	1 (4%)	31,40,40	1.67	7 (22%)

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	TDP	A	557	2	-	0/16/17/17	0/2/2/2
3	TDP	B	557	2	-	0/16/17/17	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	557	TDP	C2'-N3'	-2.28	1.29	1.34
3	A	557	TDP	C35-N3	2.37	1.53	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	557	TDP	C4A-C4-C5	-3.49	121.05	128.90
3	B	557	TDP	O11-P2-O21	-3.08	98.09	107.70
3	B	557	TDP	N1'-C2'-N3'	-2.12	121.67	125.60
3	A	557	TDP	N1'-C2'-N3'	-2.09	121.73	125.60
3	B	557	TDP	C2A-C2'-N1'	2.00	119.43	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	TDP	C5-C4-N3	2.09	112.30	107.69
3	B	557	TDP	C5-C4-N3	2.21	112.56	107.69
3	A	557	TDP	P1-O5G-C5B	2.34	134.87	121.50
3	B	557	TDP	C4A-C4-N3	2.81	126.34	122.59
3	A	557	TDP	C2A-C2'-N1'	3.02	120.66	117.03
3	A	557	TDP	C5A-C5-C4	3.30	130.52	127.56
3	B	557	TDP	C5A-C5-C4	3.76	130.93	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	TDP	3	0
3	B	557	TDP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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