



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2018 – 12:54 AM EDT

PDB ID : 1IVR  
Title : STRUCTURE OF ASPARTATE AMINOTRANSFERASE  
Authors : Graf Von Stosch, A.  
Deposited on : 1996-10-11  
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

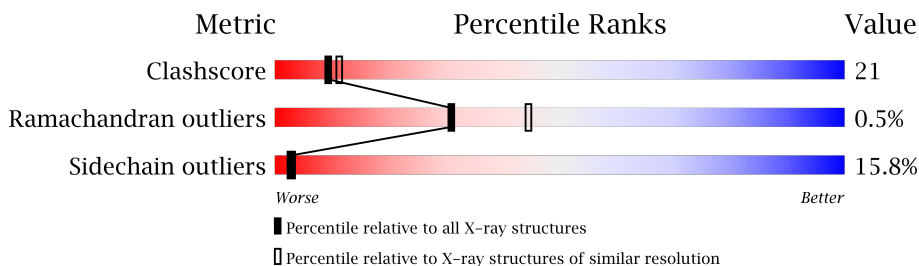
# 1 Overall quality at a glance

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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3494 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.

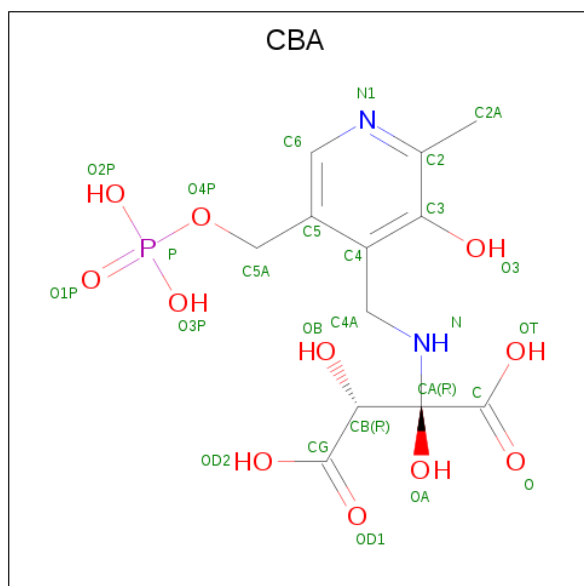
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3161	2004	558	581	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	PRO	SER	CONFLICT	UNP P00508

- Molecule 2 is N-PYRIDOXYL-2,3-DIHYDROXYASPARTIC ACID-5-MONOPHOSPHATE (three-letter code: CBA) (formula:  $C_{12}H_{17}N_2O_{11}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	26	12	2	11	1	0	0

- Molecule 3 is water.

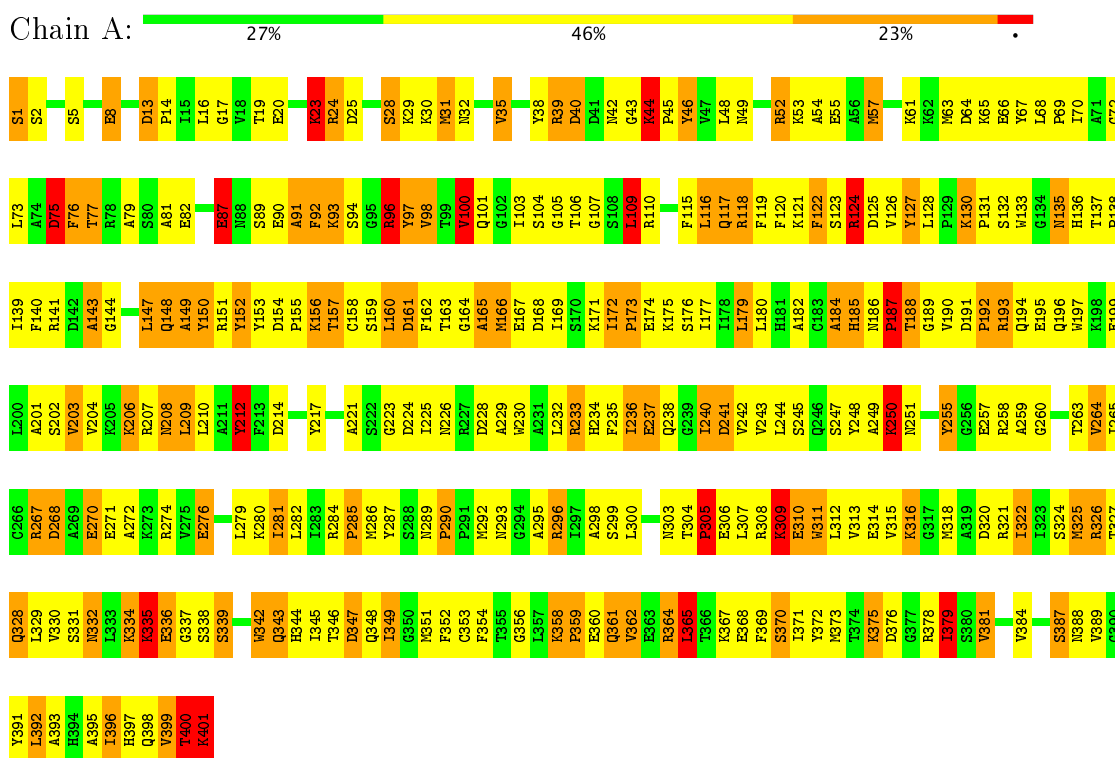
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	307	Total 307	O 307	0	0

### 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 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: ASPARTATE AMINOTRANSFERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.70Å 91.40Å 128.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, TNT	Depositor
R, $R_{free}$	0.153 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: CBA

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	1.32	1/3231 (0.0%)	3.18	396/4360 (9.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	SER	CB-OG	5.95	1.50	1.42

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	CD-NE-CZ	28.75	163.85	123.60
1	A	296	ARG	NE-CZ-NH2	-26.39	107.11	120.30
1	A	296	ARG	NE-CZ-NH1	23.64	132.12	120.30
1	A	274	ARG	CD-NE-CZ	23.20	156.08	123.60
1	A	124	ARG	NE-CZ-NH2	-23.07	108.76	120.30
1	A	110	ARG	NE-CZ-NH2	-21.44	109.58	120.30
1	A	96	ARG	NE-CZ-NH1	19.11	129.85	120.30
1	A	224	ASP	CB-CG-OD1	18.94	135.35	118.30
1	A	207	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	284	ARG	NE-CZ-NH2	17.54	129.07	120.30
1	A	233	ARG	NE-CZ-NH1	-17.41	111.59	120.30
1	A	274	ARG	NE-CZ-NH2	-16.85	111.88	120.30
1	A	276	GLU	CA-CB-CG	16.50	149.69	113.40
1	A	124	ARG	CD-NE-CZ	16.14	146.19	123.60
1	A	141	ARG	NE-CZ-NH1	15.56	128.08	120.30
1	A	376	ASP	CB-CG-OD2	-15.55	104.30	118.30
1	A	125	ASP	CB-CG-OD2	14.53	131.38	118.30
1	A	326	ARG	NE-CZ-NH2	14.47	127.54	120.30
1	A	212	TYR	CB-CG-CD2	-14.42	112.35	121.00
1	A	241	ASP	CB-CG-OD2	-13.81	105.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NE-CZ-NH2	-12.77	113.91	120.30
1	A	336	GLU	CG-CD-OE2	12.77	143.84	118.30
1	A	75	ASP	CB-CG-OD2	-12.67	106.90	118.30
1	A	309	LYS	CA-CB-CG	12.18	140.19	113.40
1	A	364	ARG	NE-CZ-NH2	-11.85	114.37	120.30
1	A	351	MET	CG-SD-CE	11.82	119.11	100.20
1	A	141	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	A	296	ARG	CD-NE-CZ	11.74	140.04	123.60
1	A	268	ASP	CA-CB-CG	11.66	139.05	113.40
1	A	321	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	24	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	A	321	ARG	CD-NE-CZ	11.34	139.47	123.60
1	A	242	VAL	CA-CB-CG1	11.11	127.56	110.90
1	A	149	ALA	O-C-N	10.90	140.15	122.70
1	A	393	ALA	N-CA-CB	10.84	125.28	110.10
1	A	64	ASP	CB-CG-OD1	10.81	128.03	118.30
1	A	151	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	A	23	LYS	CA-CB-CG	10.62	136.77	113.40
1	A	118	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	8	GLU	OE1-CD-OE2	10.29	135.64	123.30
1	A	96	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	276	GLU	CG-CD-OE1	-10.09	98.11	118.30
1	A	127	TYR	CB-CG-CD1	-10.01	114.99	121.00
1	A	368	GLU	OE1-CD-OE2	9.89	135.17	123.30
1	A	124	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	64	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	A	217	TYR	CB-CG-CD1	9.38	126.63	121.00
1	A	364	ARG	NH1-CZ-NH2	9.19	129.51	119.40
1	A	336	GLU	OE1-CD-OE2	-9.14	112.33	123.30
1	A	20	GLU	CA-CB-CG	9.12	133.47	113.40
1	A	110	ARG	NH1-CZ-NH2	9.10	129.41	119.40
1	A	167	GLU	N-CA-CB	9.03	126.85	110.60
1	A	20	GLU	OE1-CD-OE2	-8.98	112.52	123.30
1	A	378	ARG	CD-NE-CZ	8.92	136.08	123.60
1	A	109	LEU	CA-CB-CG	8.91	135.80	115.30
1	A	167	GLU	OE1-CD-OE2	8.90	133.98	123.30
1	A	311	TRP	CZ3-CH2-CZ2	-8.75	111.10	121.60
1	A	13	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	A	339	SER	CB-CA-C	-8.61	93.75	110.10
1	A	20	GLU	CG-CD-OE2	8.56	135.42	118.30
1	A	125	ASP	OD1-CG-OD2	-8.55	107.05	123.30
1	A	141	ARG	CD-NE-CZ	8.54	135.55	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASP	O-C-N	-8.49	109.12	122.70
1	A	389	VAL	CB-CA-C	8.49	127.52	111.40
1	A	364	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	321	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	212	TYR	CB-CG-CD1	8.41	126.05	121.00
1	A	67	TYR	CB-CG-CD2	8.29	125.97	121.00
1	A	320	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	172	ILE	O-C-N	8.25	136.78	121.10
1	A	107	GLY	CA-C-O	-8.23	105.79	120.60
1	A	392	LEU	CB-CG-CD1	-8.14	97.16	111.00
1	A	304	THR	CA-CB-CG2	8.12	123.77	112.40
1	A	311	TRP	CE3-CZ3-CH2	8.10	130.11	121.20
1	A	325	MET	CA-CB-CG	8.04	126.98	113.30
1	A	118	ARG	CD-NE-CZ	8.03	134.84	123.60
1	A	55	GLU	CG-CD-OE2	-8.03	102.25	118.30
1	A	13	ASP	CA-C-O	8.01	136.93	120.10
1	A	55	GLU	OE1-CD-OE2	7.98	132.88	123.30
1	A	268	ASP	N-CA-CB	-7.98	96.23	110.60
1	A	270	GLU	CA-C-O	-7.91	103.48	120.10
1	A	367	LYS	CA-C-N	7.88	134.52	117.20
1	A	312	LEU	CB-CG-CD1	-7.87	97.61	111.00
1	A	250	LYS	O-C-N	-7.86	110.12	122.70
1	A	274	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	314	GLU	CG-CD-OE2	7.83	133.96	118.30
1	A	300	LEU	O-C-N	-7.80	110.22	122.70
1	A	153	TYR	CA-CB-CG	7.79	128.19	113.40
1	A	159	SER	N-CA-CB	7.76	122.14	110.50
1	A	376	ASP	OD1-CG-OD2	7.76	138.04	123.30
1	A	165	ALA	N-CA-CB	7.74	120.94	110.10
1	A	378	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	296	ARG	CA-CB-CG	7.68	130.29	113.40
1	A	97	TYR	CB-CG-CD1	-7.67	116.39	121.00
1	A	118	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	257	GLU	CG-CD-OE2	-7.65	103.00	118.30
1	A	96	ARG	CB-CG-CD	7.65	131.49	111.60
1	A	300	LEU	CA-CB-CG	7.63	132.84	115.30
1	A	210	LEU	N-CA-CB	7.55	125.50	110.40
1	A	282	LEU	CB-CA-C	7.55	124.55	110.20
1	A	87	GLU	CG-CD-OE2	7.53	133.37	118.30
1	A	166	MET	CB-CG-SD	-7.51	89.87	112.40
1	A	322	ILE	O-C-N	7.50	134.70	122.70
1	A	337	GLY	O-C-N	7.48	134.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	A	188	THR	N-CA-CB	-7.46	96.14	110.30
1	A	153	TYR	CZ-CE2-CD2	7.41	126.47	119.80
1	A	272	ALA	N-CA-CB	7.38	120.44	110.10
1	A	327	THR	CA-CB-CG2	7.38	122.73	112.40
1	A	136	HIS	N-CA-CB	7.37	123.87	110.60
1	A	248	TYR	O-C-N	7.37	134.49	122.70
1	A	237	GLU	CB-CG-CD	7.33	133.98	114.20
1	A	82	GLU	CG-CD-OE2	-7.28	103.74	118.30
1	A	166	MET	CG-SD-CE	-7.28	88.56	100.20
1	A	307	LEU	CB-CA-C	7.28	124.03	110.20
1	A	163	THR	CA-CB-OG1	-7.27	93.73	109.00
1	A	46	TYR	CB-CG-CD2	7.26	125.35	121.00
1	A	136	HIS	CA-C-O	-7.26	104.86	120.10
1	A	336	GLU	CG-CD-OE1	-7.24	103.82	118.30
1	A	372	TYR	O-C-N	-7.23	111.13	122.70
1	A	122	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	A	75	ASP	OD1-CG-OD2	7.20	136.97	123.30
1	A	314	GLU	CG-CD-OE1	-7.18	103.93	118.30
1	A	270	GLU	N-CA-CB	7.18	123.53	110.60
1	A	310	GLU	O-C-N	-7.17	111.23	122.70
1	A	242	VAL	CG1-CB-CG2	-7.16	99.45	110.90
1	A	191	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	194	GLN	CG-CD-NE2	-7.13	99.60	116.70
1	A	342	TRP	O-C-N	7.12	134.10	122.70
1	A	258	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	337	GLY	CA-C-O	-7.10	107.82	120.60
1	A	157	THR	CA-CB-OG1	-7.08	94.13	109.00
1	A	206	LYS	N-CA-CB	-7.07	97.87	110.60
1	A	367	LYS	CA-C-O	-7.07	105.25	120.10
1	A	66	GLU	O-C-N	7.03	133.94	122.70
1	A	308	ARG	CB-CG-CD	-7.01	93.38	111.60
1	A	28	SER	C-N-CA	7.00	139.21	121.70
1	A	152	TYR	CB-CG-CD2	6.97	125.18	121.00
1	A	228	ASP	CA-CB-CG	6.96	128.72	113.40
1	A	364	ARG	CB-CA-C	-6.95	96.50	110.40
1	A	339	SER	O-C-N	6.94	133.80	122.70
1	A	332	ASN	O-C-N	6.93	133.79	122.70
1	A	395	ALA	CB-CA-C	6.92	120.48	110.10
1	A	308	ARG	CG-CD-NE	-6.88	97.36	111.80
1	A	185	HIS	C-N-CA	6.84	138.81	121.70
1	A	232	LEU	O-C-N	6.84	133.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	SER	O-C-N	6.82	133.61	122.70
1	A	148	GLN	OE1-CD-NE2	-6.81	106.23	121.90
1	A	127	TYR	CB-CG-CD2	6.78	125.07	121.00
1	A	251	ASN	CB-CA-C	6.78	123.96	110.40
1	A	140	PHE	CB-CG-CD1	-6.78	116.06	120.80
1	A	296	ARG	CG-CD-NE	6.78	126.03	111.80
1	A	289	ASN	CB-CA-C	6.77	123.94	110.40
1	A	223	GLY	C-N-CA	6.75	138.59	121.70
1	A	279	LEU	O-C-N	-6.75	111.90	122.70
1	A	270	GLU	CB-CG-CD	6.74	132.41	114.20
1	A	91	ALA	CA-C-O	6.71	134.19	120.10
1	A	247	SER	N-CA-CB	6.68	120.52	110.50
1	A	55	GLU	CB-CA-C	-6.67	97.05	110.40
1	A	326	ARG	NH1-CZ-NH2	-6.67	112.06	119.40
1	A	120	PHE	CZ-CE2-CD2	6.67	128.11	120.10
1	A	276	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	A	241	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	392	LEU	CB-CG-CD2	6.63	122.27	111.00
1	A	214	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	248	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	176	SER	O-C-N	-6.59	112.15	122.70
1	A	151	ARG	NH1-CZ-NH2	-6.58	112.17	119.40
1	A	229	ALA	N-CA-CB	-6.54	100.94	110.10
1	A	224	ASP	OD1-CG-OD2	-6.54	110.88	123.30
1	A	194	GLN	N-CA-CB	-6.52	98.87	110.60
1	A	264	VAL	CA-CB-CG1	6.51	120.67	110.90
1	A	392	LEU	CA-C-O	6.51	133.77	120.10
1	A	25	ASP	CB-CA-C	6.51	123.42	110.40
1	A	40	ASP	CB-CA-C	6.50	123.41	110.40
1	A	331	SER	CA-C-O	-6.50	106.45	120.10
1	A	365	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	249	ALA	CA-C-O	6.49	133.72	120.10
1	A	180	LEU	O-C-N	6.47	133.05	122.70
1	A	194	GLN	C-N-CA	6.44	137.80	121.70
1	A	233	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	A	313	VAL	CB-CA-C	6.43	123.62	111.40
1	A	96	ARG	O-C-N	-6.42	112.43	122.70
1	A	161	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	354	PHE	CB-CG-CD1	6.39	125.28	120.80
1	A	70	ILE	CA-C-O	-6.37	106.73	120.10
1	A	100	VAL	N-CA-CB	-6.36	97.50	111.50
1	A	96	ARG	CA-CB-CG	6.36	127.39	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LYS	CG-CD-CE	6.35	130.96	111.90
1	A	245	SER	O-C-N	-6.34	112.55	122.70
1	A	271	GLU	CG-CD-OE1	6.34	130.98	118.30
1	A	144	GLY	CA-C-O	-6.32	109.22	120.60
1	A	148	GLN	CG-CD-NE2	6.29	131.81	116.70
1	A	66	GLU	CG-CD-OE2	6.29	130.88	118.30
1	A	52	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	399	VAL	N-CA-CB	-6.28	97.68	111.50
1	A	285	PRO	N-CA-CB	6.28	110.83	103.30
1	A	284	ARG	NH1-CZ-NH2	-6.27	112.50	119.40
1	A	116	LEU	O-C-N	-6.25	112.70	122.70
1	A	359	PRO	N-CD-CG	-6.25	93.83	103.20
1	A	77	THR	CB-CA-C	6.23	128.43	111.60
1	A	75	ASP	C-N-CA	-6.22	106.14	121.70
1	A	235	PHE	CA-C-N	-6.22	103.50	117.20
1	A	369	PHE	CZ-CE2-CD2	-6.22	112.64	120.10
1	A	257	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	A	130	LYS	CA-CB-CG	-6.18	99.81	113.40
1	A	265	ILE	N-CA-CB	6.15	124.95	110.80
1	A	289	ASN	OD1-CG-ND2	6.14	136.02	121.90
1	A	173	PRO	C-N-CA	6.13	137.03	121.70
1	A	31	MET	CA-C-O	-6.13	107.22	120.10
1	A	372	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
1	A	66	GLU	CG-CD-OE1	-6.12	106.06	118.30
1	A	17	GLY	CA-C-N	6.12	130.66	117.20
1	A	201	ALA	N-CA-CB	6.12	118.67	110.10
1	A	54	ALA	CB-CA-C	6.11	119.26	110.10
1	A	276	GLU	CG-CD-OE2	6.11	130.51	118.30
1	A	135	ASN	CB-CA-C	6.10	122.60	110.40
1	A	282	LEU	CB-CG-CD1	-6.10	100.64	111.00
1	A	105	GLY	CA-C-O	-6.08	109.66	120.60
1	A	122	PHE	CA-C-O	-6.07	107.35	120.10
1	A	271	GLU	CA-CB-CG	6.06	126.73	113.40
1	A	204	VAL	CA-CB-CG1	6.05	119.98	110.90
1	A	197	TRP	CA-C-O	-6.04	107.41	120.10
1	A	370	SER	O-C-N	6.03	132.35	122.70
1	A	392	LEU	N-CA-CB	-6.03	98.35	110.40
1	A	401	LYS	CB-CA-C	-6.03	98.35	110.40
1	A	105	GLY	O-C-N	6.02	132.33	122.70
1	A	164	GLY	O-C-N	6.00	132.30	122.70
1	A	182	ALA	CB-CA-C	5.99	119.08	110.10
1	A	233	ARG	CB-CG-CD	-5.98	96.06	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ALA	C-N-CA	5.96	134.81	122.30
1	A	308	ARG	CB-CA-C	5.96	122.31	110.40
1	A	48	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	A	352	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	A	149	ALA	CB-CA-C	-5.94	101.19	110.10
1	A	289	ASN	CB-CG-OD1	-5.94	109.72	121.60
1	A	311	TRP	CH2-CZ2-CE2	5.94	123.34	117.40
1	A	98	VAL	N-CA-CB	5.94	124.56	111.50
1	A	38	TYR	O-C-N	5.93	132.19	122.70
1	A	79	ALA	N-CA-CB	5.93	118.41	110.10
1	A	392	LEU	CB-CA-C	5.93	121.47	110.20
1	A	124	ARG	NH1-CZ-NH2	5.92	125.92	119.40
1	A	158	CYS	N-CA-CB	5.92	121.27	110.60
1	A	312	LEU	CB-CG-CD2	5.92	121.06	111.00
1	A	316	LYS	CG-CD-CE	5.90	129.61	111.90
1	A	280	LYS	O-C-N	5.89	132.13	122.70
1	A	384	VAL	CB-CA-C	5.88	122.58	111.40
1	A	334	LYS	C-N-CA	5.88	136.40	121.70
1	A	285	PRO	C-N-CA	5.88	136.40	121.70
1	A	306	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	69	PRO	N-CA-CB	5.87	110.35	103.30
1	A	209	LEU	O-C-N	5.86	132.08	122.70
1	A	110	ARG	CB-CG-CD	-5.84	96.41	111.60
1	A	208	ASN	N-CA-CB	-5.84	100.09	110.60
1	A	103	ILE	CA-CB-CG1	-5.83	99.92	111.00
1	A	150	TYR	CB-CG-CD2	5.82	124.49	121.00
1	A	193	ARG	CD-NE-CZ	-5.82	115.45	123.60
1	A	143	ALA	O-C-N	-5.80	113.33	123.20
1	A	396	ILE	CA-CB-CG1	5.80	122.02	111.00
1	A	249	ALA	O-C-N	-5.79	113.43	122.70
1	A	1	SER	O-C-N	5.79	131.96	122.70
1	A	214	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	39	ARG	CG-CD-NE	5.75	123.88	111.80
1	A	207	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
1	A	321	ARG	CB-CG-CD	5.74	126.53	111.60
1	A	368	GLU	CB-CA-C	-5.74	98.91	110.40
1	A	150	TYR	CB-CA-C	5.74	121.88	110.40
1	A	392	LEU	O-C-N	-5.72	113.54	122.70
1	A	313	VAL	CA-CB-CG1	5.71	119.47	110.90
1	A	217	TYR	C-N-CA	5.70	135.95	121.70
1	A	379	ILE	CA-CB-CG2	5.70	122.30	110.90
1	A	268	ASP	O-C-N	5.70	131.81	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	LYS	N-CA-CB	5.69	120.84	110.60
1	A	49	ASN	CB-CG-OD1	-5.68	110.23	121.60
1	A	24	ARG	CB-CA-C	-5.68	99.03	110.40
1	A	335	LYS	CG-CD-CE	5.68	128.95	111.90
1	A	356	GLY	O-C-N	5.68	131.78	122.70
1	A	87	GLU	CG-CD-OE1	-5.67	106.95	118.30
1	A	375	LYS	N-CA-CB	5.67	120.81	110.60
1	A	271	GLU	CB-CG-CD	5.67	129.50	114.20
1	A	195	GLU	CG-CD-OE2	5.67	129.63	118.30
1	A	326	ARG	C-N-CA	5.66	135.86	121.70
1	A	156	LYS	CB-CG-CD	-5.65	96.92	111.60
1	A	290	PRO	N-CA-CB	-5.61	96.42	102.60
1	A	45	PRO	O-C-N	5.60	131.67	122.70
1	A	182	ALA	O-C-N	-5.60	113.74	122.70
1	A	194	GLN	OE1-CD-NE2	5.60	134.78	121.90
1	A	259	ALA	CA-C-O	-5.60	108.33	120.10
1	A	255	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	A	343	GLN	CB-CA-C	5.58	121.56	110.40
1	A	185	HIS	CG-ND1-CE1	5.55	115.97	108.20
1	A	236	ILE	CA-C-O	-5.55	108.45	120.10
1	A	106	THR	O-C-N	5.54	132.63	123.20
1	A	195	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	177	ILE	CA-CB-CG2	5.53	121.96	110.90
1	A	379	ILE	N-CA-CB	5.52	123.49	110.80
1	A	384	VAL	CA-CB-CG2	5.51	119.16	110.90
1	A	260	GLY	CA-C-O	-5.50	110.70	120.60
1	A	376	ASP	N-CA-CB	5.50	120.49	110.60
1	A	90	GLU	OE1-CD-OE2	5.49	129.89	123.30
1	A	77	THR	N-CA-CB	-5.49	99.87	110.30
1	A	187	PRO	N-CA-CB	-5.49	96.56	102.60
1	A	328	GLN	CG-CD-NE2	-5.48	103.54	116.70
1	A	298	ALA	N-CA-CB	5.48	117.77	110.10
1	A	155	PRO	CA-C-O	-5.46	107.08	120.20
1	A	44	LYS	N-CA-CB	-5.46	100.78	110.60
1	A	109	LEU	CB-CA-C	5.45	120.56	110.20
1	A	271	GLU	CG-CD-OE2	-5.44	107.42	118.30
1	A	24	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	73	LEU	N-CA-CB	-5.44	99.52	110.40
1	A	182	ALA	C-N-CA	5.43	135.28	121.70
1	A	354	PHE	C-N-CA	5.43	135.27	121.70
1	A	268	ASP	CB-CA-C	-5.43	99.54	110.40
1	A	35	VAL	CA-C-O	5.42	131.48	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	PRO	N-CA-C	5.42	126.19	112.10
1	A	115	PHE	CB-CA-C	5.41	121.23	110.40
1	A	64	ASP	CB-CA-C	5.41	121.22	110.40
1	A	236	ILE	CB-CG1-CD1	-5.39	98.80	113.90
1	A	339	SER	CA-CB-OG	-5.39	96.64	111.20
1	A	28	SER	CB-CA-C	5.39	120.34	110.10
1	A	28	SER	O-C-N	-5.38	114.09	122.70
1	A	87	GLU	O-C-N	-5.36	114.12	122.70
1	A	303	ASN	CA-C-N	5.35	128.97	117.20
1	A	156	LYS	CA-CB-CG	-5.34	101.66	113.40
1	A	233	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	387	SER	CA-C-O	-5.33	108.90	120.10
1	A	46	TYR	CB-CA-C	5.33	121.05	110.40
1	A	174	GLU	CA-CB-CG	5.29	125.05	113.40
1	A	13	ASP	O-C-N	-5.29	111.04	121.10
1	A	191	ASP	OD1-CG-OD2	-5.29	113.25	123.30
1	A	97	TYR	CB-CG-CD2	5.28	124.17	121.00
1	A	207	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	221	ALA	CB-CA-C	-5.28	102.19	110.10
1	A	293	ASN	CB-CG-OD1	-5.27	111.07	121.60
1	A	307	LEU	N-CA-C	-5.27	96.78	111.00
1	A	270	GLU	O-C-N	5.26	131.12	122.70
1	A	328	GLN	CA-C-N	5.26	128.77	117.20
1	A	203	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	A	184	ALA	CB-CA-C	5.25	117.98	110.10
1	A	248	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	338	SER	N-CA-CB	5.24	118.36	110.50
1	A	25	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	224	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	82	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	A	67	TYR	CA-CB-CG	5.22	123.33	113.40
1	A	166	MET	N-CA-CB	5.22	120.01	110.60
1	A	236	ILE	O-C-N	5.22	131.06	122.70
1	A	282	LEU	N-CA-CB	-5.22	99.96	110.40
1	A	42	ASN	CB-CG-OD1	-5.21	111.18	121.60
1	A	126	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	A	378	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	A	195	GLU	N-CA-CB	5.20	119.96	110.60
1	A	176	SER	C-N-CA	5.19	134.68	121.70
1	A	57	MET	CG-SD-CE	-5.19	91.90	100.20
1	A	316	LYS	CB-CG-CD	-5.18	98.12	111.60
1	A	103	ILE	CA-C-O	5.18	130.97	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	CA-C-O	5.17	130.96	120.10
1	A	228	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	381	VAL	CB-CA-C	5.16	121.19	111.40
1	A	347	ASP	C-N-CA	5.15	134.58	121.70
1	A	287	TYR	CG-CD1-CE1	5.14	125.42	121.30
1	A	119	PHE	CD1-CE1-CZ	-5.14	113.93	120.10
1	A	5	SER	CB-CA-C	5.14	119.86	110.10
1	A	335	LYS	CA-C-O	-5.13	109.32	120.10
1	A	208	ASN	CB-CG-OD1	-5.13	111.34	121.60
1	A	188	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	217	TYR	CG-CD1-CE1	5.13	125.40	121.30
1	A	400	THR	OG1-CB-CG2	5.13	121.79	110.00
1	A	164	GLY	CA-C-O	-5.12	111.38	120.60
1	A	193	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	393	ALA	O-C-N	5.12	130.89	122.70
1	A	214	ASP	CB-CA-C	5.12	120.64	110.40
1	A	120	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	A	147	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	160	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	131	PRO	CA-C-N	-5.11	105.96	117.20
1	A	65	LYS	CB-CA-C	-5.11	100.19	110.40
1	A	336	GLU	CA-C-O	5.11	130.82	120.10
1	A	369	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	A	127	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	A	329	LEU	CB-CG-CD2	5.08	119.63	111.00
1	A	314	GLU	CA-C-O	-5.07	109.45	120.10
1	A	92	PHE	O-C-N	-5.06	114.60	122.70
1	A	235	PHE	CD1-CE1-CZ	-5.06	114.03	120.10
1	A	274	ARG	CA-C-O	-5.06	109.48	120.10
1	A	292	MET	CA-CB-CG	5.06	121.89	113.30
1	A	168	ASP	O-C-N	5.05	130.78	122.70
1	A	362	VAL	CA-CB-CG1	5.05	118.48	110.90
1	A	358	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	A	217	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	A	388	ASN	OD1-CG-ND2	5.04	133.50	121.90
1	A	356	GLY	CA-C-O	-5.04	111.53	120.60
1	A	130	LYS	CG-CD-CE	-5.03	96.81	111.90
1	A	120	PHE	CB-CG-CD2	5.03	124.32	120.80
1	A	240	ILE	CA-CB-CG2	5.02	120.93	110.90
1	A	197	TRP	CD1-CG-CD2	-5.00	102.30	106.30

There are no chirality outliers.



There are no planarity outliers.

## 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	3161	0	3155	134	2
2	A	26	0	13	5	0
3	A	307	0	0	29	6
All	All	3494	0	3168	134	6

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 21.

All (134) 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:19:THR:O	1:A:23:LYS:HG2	1.75	0.86
1:A:396:ILE:O	1:A:400:THR:HB	1.77	0.85
1:A:276:GLU:HG3	3:A:678:HOH:O	1.84	0.78
1:A:165:ALA:O	1:A:169:ILE:HG13	1.86	0.76
1:A:325:MET:HE3	3:A:727:HOH:O	1.90	0.71
1:A:93:LYS:HE2	3:A:552:HOH:O	1.89	0.71
1:A:188:THR:HG23	1:A:190:VAL:HG23	1.73	0.71
1:A:311:TRP:O	1:A:315:VAL:HG23	1.92	0.69
1:A:157:THR:HG21	3:A:429:HOH:O	1.91	0.69
1:A:361:GLN:HG3	3:A:686:HOH:O	1.92	0.69
1:A:53:LYS:HE3	1:A:310:GLU:OE1	1.92	0.69
1:A:398:GLN:NE2	1:A:401:LYS:HE2	2.10	0.67
1:A:185:HIS:ND1	1:A:188:THR:HB	2.10	0.67
1:A:188:THR:HG22	1:A:190:VAL:H	1.60	0.66
1:A:325:MET:CE	1:A:328:GLN:HE22	2.08	0.66
1:A:87:GLU:O	1:A:93:LYS:HD3	1.96	0.65
1:A:398:GLN:HE22	1:A:401:LYS:HE2	1.62	0.65
1:A:169:ILE:HA	1:A:172:ILE:HD12	1.82	0.62
1:A:75:ASP:N	1:A:75:ASP:OD1	2.33	0.61
1:A:57:MET:O	1:A:61:LYS:HB2	2.01	0.61
1:A:124:ARG:HE	1:A:124:ARG:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:OD2	1:A:157:THR:HB	2.00	0.60
1:A:335:LYS:HE2	3:A:506:HOH:O	2.02	0.60
1:A:199:GLU:HG3	3:A:578:HOH:O	2.00	0.60
1:A:94:SER:OG	1:A:96:ARG:HG3	2.02	0.59
1:A:250:LYS:CE	2:A:402:CBA:H4A2	2.32	0.59
1:A:225:ILE:HG13	1:A:226:ASN:N	2.17	0.59
1:A:334:LYS:HG3	3:A:543:HOH:O	2.02	0.58
1:A:172:ILE:HG22	1:A:209:LEU:HD22	1.85	0.58
1:A:2:SER:HA	3:A:706:HOH:O	2.05	0.57
1:A:137:THR:HB	1:A:138:PRO:HD3	1.85	0.57
1:A:397:HIS:O	1:A:401:LYS:N	2.35	0.57
1:A:43:GLY:HA2	3:A:697:HOH:O	2.05	0.56
1:A:358:LYS:HE3	1:A:361:GLN:OE1	2.06	0.56
1:A:31:MET:HE2	1:A:371:ILE:HG12	1.86	0.56
1:A:250:LYS:HE3	2:A:402:CBA:H4A2	1.88	0.56
1:A:91:ALA:HA	1:A:96:ARG:HD3	1.87	0.56
1:A:237:GLU:OE1	3:A:617:HOH:O	2.18	0.56
1:A:175:LYS:HB2	3:A:619:HOH:O	2.06	0.55
1:A:325:MET:CE	1:A:328:GLN:NE2	2.69	0.55
1:A:365:LEU:HD23	1:A:373:MET:CE	2.37	0.55
1:A:23:LYS:HB2	3:A:526:HOH:O	2.06	0.55
1:A:31:MET:CE	1:A:371:ILE:HG12	2.37	0.55
1:A:225:ILE:HG13	1:A:226:ASN:H	1.72	0.54
1:A:361:GLN:HB3	1:A:399:VAL:CG1	2.37	0.54
1:A:44:LYS:NZ	3:A:760:HOH:O	2.40	0.54
1:A:128:LEU:HD11	1:A:147:LEU:HD22	1.90	0.53
1:A:233:ARG:O	3:A:752:HOH:O	2.18	0.53
1:A:130:LYS:HG3	1:A:150:TYR:O	2.09	0.52
1:A:330:VAL:HG21	1:A:346:THR:HG23	1.91	0.52
1:A:186:ASN:ND2	2:A:402:CBA:O3	2.39	0.52
1:A:234:HIS:HE1	3:A:549:HOH:O	1.92	0.52
1:A:328:GLN:O	1:A:332:ASN:OD1	2.27	0.52
1:A:318:MET:O	1:A:322:ILE:HG13	2.09	0.52
1:A:72:GLY:HA3	1:A:101:GLN:HB2	1.93	0.51
1:A:172:ILE:HG22	1:A:209:LEU:CD2	2.41	0.51
1:A:53:LYS:O	1:A:57:MET:HG3	2.11	0.51
1:A:353:CYS:HB3	1:A:379:ILE:CD1	2.41	0.50
1:A:124:ARG:CA	1:A:124:ARG:HE	2.20	0.50
1:A:127:TYR:CE2	1:A:172:ILE:HG12	2.46	0.50
1:A:375:LYS:NZ	3:A:602:HOH:O	2.40	0.50
1:A:117:GLN:HG3	1:A:143:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD23	1:A:373:MET:HE3	1.92	0.49
1:A:98:VAL:O	1:A:263:THR:HA	2.11	0.49
1:A:135:ASN:O	1:A:139:ILE:HG13	2.12	0.49
1:A:76:PHE:HB2	1:A:299:SER:HB2	1.93	0.49
1:A:179:LEU:HA	1:A:212:TYR:O	2.13	0.49
1:A:325:MET:HE1	1:A:328:GLN:NE2	2.28	0.49
1:A:154:ASP:OD2	1:A:157:THR:CB	2.61	0.49
1:A:332:ASN:O	1:A:336:GLU:HG2	2.13	0.49
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.43	0.48
1:A:365:LEU:HD22	1:A:399:VAL:HG11	1.93	0.48
1:A:30:LYS:CB	1:A:370:SER:HB3	2.43	0.48
1:A:40:ASP:HB3	1:A:46:TYR:HB2	1.95	0.48
1:A:8:GLU:HB3	3:A:565:HOH:O	2.12	0.48
1:A:243:VAL:HG12	1:A:264:VAL:HG13	1.95	0.48
1:A:184:ALA:O	1:A:185:HIS:C	2.48	0.48
1:A:133:TRP:CH2	2:A:402:CBA:H5A1	2.49	0.48
1:A:189:GLY:O	1:A:349:ILE:HG13	2.14	0.47
1:A:96:ARG:NH2	1:A:241:ASP:OD1	2.46	0.47
1:A:230:TRP:O	1:A:234:HIS:N	2.43	0.47
1:A:361:GLN:HB3	1:A:399:VAL:HG13	1.96	0.47
1:A:250:LYS:HE2	2:A:402:CBA:H4A2	1.97	0.47
1:A:362:VAL:HG11	1:A:375:LYS:HA	1.96	0.47
1:A:30:LYS:HA	1:A:370:SER:O	2.15	0.46
1:A:392:LEU:O	1:A:396:ILE:HD12	2.16	0.46
1:A:193:ARG:O	1:A:196:GLN:N	2.49	0.46
1:A:305:PRO:O	1:A:309:LYS:HG3	2.15	0.46
1:A:24:ARG:NH2	3:A:448:HOH:O	2.49	0.46
1:A:401:LYS:OXT	1:A:401:LYS:HG2	2.15	0.46
1:A:124:ARG:HB3	3:A:597:HOH:O	2.14	0.46
1:A:39:ARG:HB2	3:A:697:HOH:O	2.15	0.46
1:A:109:LEU:HA	1:A:212:TYR:OH	2.16	0.45
1:A:100:VAL:HG12	1:A:100:VAL:O	2.17	0.45
1:A:81:ALA:CB	1:A:97:TYR:CE2	3.00	0.45
1:A:162:PHE:CE1	1:A:196:GLN:HB3	2.52	0.45
1:A:154:ASP:HB2	1:A:161:ASP:HB2	1.99	0.44
1:A:238:GLN:NE2	3:A:584:HOH:O	2.41	0.44
1:A:28:SER:HB3	3:A:421:HOH:O	2.17	0.44
1:A:326:ARG:HD3	1:A:345:ILE:O	2.18	0.44
1:A:172:ILE:CG2	1:A:209:LEU:HD22	2.46	0.44
1:A:116:LEU:O	1:A:117:GLN:C	2.56	0.44
1:A:118:ARG:HB2	3:A:703:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:O	3:A:544:HOH:O	2.21	0.43
1:A:89:SER:HB3	1:A:92:PHE:HB3	2.00	0.43
1:A:360:GLU:O	1:A:364:ARG:HG3	2.18	0.43
1:A:152:TYR:OH	1:A:192:PRO:HD3	2.18	0.43
1:A:325:MET:HE2	1:A:328:GLN:NE2	2.33	0.43
1:A:188:THR:O	1:A:348:GLN:HG2	2.18	0.43
1:A:281:ILE:O	1:A:285:PRO:HD3	2.19	0.43
1:A:13:ASP:O	1:A:14:PRO:C	2.57	0.43
1:A:186:ASN:HA	1:A:187:PRO:HA	1.80	0.42
1:A:101:GLN:NE2	1:A:295:ALA:HB2	2.34	0.42
1:A:391:TYR:O	1:A:392:LEU:C	2.58	0.42
1:A:203:VAL:HG22	3:A:559:HOH:O	2.18	0.42
1:A:236:ILE:HA	1:A:240:ILE:O	2.19	0.42
1:A:137:THR:HB	1:A:138:PRO:CD	2.50	0.42
1:A:342:TRP:HB3	1:A:345:ILE:HD12	2.01	0.42
1:A:53:LYS:NZ	3:A:698:HOH:O	2.24	0.42
1:A:185:HIS:CE1	1:A:188:THR:HB	2.55	0.42
1:A:137:THR:CB	1:A:138:PRO:CD	2.98	0.42
1:A:358:LYS:CB	1:A:359:PRO:CD	2.98	0.41
1:A:171:LYS:HB2	1:A:171:LYS:NZ	2.35	0.41
1:A:392:LEU:HA	1:A:392:LEU:HD12	1.74	0.41
1:A:344:HIS:HA	1:A:347:ASP:HB2	2.03	0.41
1:A:166:MET:HE1	3:A:578:HOH:O	2.21	0.41
1:A:172:ILE:HA	1:A:173:PRO:HD3	1.94	0.41
1:A:137:THR:CB	1:A:138:PRO:HD3	2.51	0.41
1:A:53:LYS:CE	1:A:310:GLU:OE1	2.65	0.40
1:A:122:PHE:O	1:A:123:SER:HB2	2.21	0.40
1:A:98:VAL:HG21	1:A:276:GLU:HB2	2.02	0.40
1:A:130:LYS:CG	1:A:149:ALA:HB1	2.51	0.40
1:A:364:ARG:NH2	3:A:719:HOH:O	2.54	0.40
1:A:52:ARG:HA	1:A:52:ARG:HD3	1.91	0.40

All (6) 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)
3:A:673:HOH:O	3:A:673:HOH:O[3_655]	0.87	1.33
3:A:485:HOH:O	3:A:485:HOH:O[3_655]	1.33	0.87
3:A:428:HOH:O	3:A:428:HOH:O[3_655]	1.42	0.78
3:A:404:HOH:O	3:A:404:HOH:O[3_655]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:OD2	3:A:758:HOH:O[3_655]	2.07	0.13
1:A:156:LYS:O	3:A:668:HOH:O[8_556]	2.09	0.11

## 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	399/401 (100%)	372 (93%)	25 (6%)	2 (0%)	31 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	TYR
1	A	305	PRO

### 5.3.2 Protein sidechains [i](#)

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	335/335 (100%)	282 (84%)	53 (16%)	3 3

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	16	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	23	LYS
1	A	29	LYS
1	A	32	ASN
1	A	35	VAL
1	A	44	LYS
1	A	63	MET
1	A	68	LEU
1	A	75	ASP
1	A	76	PHE
1	A	77	THR
1	A	87	GLU
1	A	93	LYS
1	A	96	ARG
1	A	100	VAL
1	A	104	SER
1	A	109	LEU
1	A	117	GLN
1	A	121	LYS
1	A	124	ARG
1	A	132	SER
1	A	148	GLN
1	A	160	LEU
1	A	179	LEU
1	A	187	PRO
1	A	192	PRO
1	A	206	LYS
1	A	208	ASN
1	A	212	TYR
1	A	244	LEU
1	A	250	LYS
1	A	267	ARG
1	A	268	ASP
1	A	270	GLU
1	A	281	ILE
1	A	290	PRO
1	A	296	ARG
1	A	305	PRO
1	A	309	LYS
1	A	316	LYS
1	A	324	SER
1	A	335	LYS
1	A	339	SER

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	349	ILE
1	A	361	GLN
1	A	365	LEU
1	A	379	ILE
1	A	381	VAL
1	A	387	SER
1	A	400	THR
1	A	401	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	117	GLN
1	A	208	ASN
1	A	226	ASN
1	A	234	HIS
1	A	238	GLN
1	A	328	GLN
1	A	398	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CBA	A	402	-	17,26,26	1.91	6 (35%)	21,39,39	3.38	10 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBA	A	402	-	-	0/11/28/28	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	CBA	O4P-C5A	-2.26	1.36	1.44
2	A	402	CBA	P-O2P	-2.07	1.46	1.54
2	A	402	CBA	C6-C5	2.41	1.42	1.37
2	A	402	CBA	C2-N1	2.83	1.39	1.33
2	A	402	CBA	P-O1P	2.86	1.60	1.50
2	A	402	CBA	C6-N1	3.77	1.42	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	CBA	OA-CA-CB	-8.11	96.25	109.27
2	A	402	CBA	C2A-C2-C3	-5.86	113.98	120.96
2	A	402	CBA	O3-C3-C2	-4.76	107.81	117.78
2	A	402	CBA	O3P-P-O1P	-2.21	101.98	110.60
2	A	402	CBA	C4A-C4-C5	2.31	122.36	119.71
2	A	402	CBA	O3-C3-C4	3.13	127.31	118.13
2	A	402	CBA	C4-C3-C2	3.16	124.88	120.01
2	A	402	CBA	O4P-P-O1P	4.53	119.19	106.47
2	A	402	CBA	C2A-C2-N1	4.61	127.00	117.86
2	A	402	CBA	O4P-C5A-C5	5.40	119.78	109.39



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	CBA	5	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

### 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.