



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:51 AM EDT

PDB ID : 4ALD  
Title : HUMAN MUSCLE FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE COM-  
PLEXED WITH FRUCTOSE 1,6-BISPHOSPHATE  
Authors : Dalby, A.R.; Dauter, Z.; Littlechild, J.A.  
Deposited on : 1998-07-26  
Resolution : 2.80 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

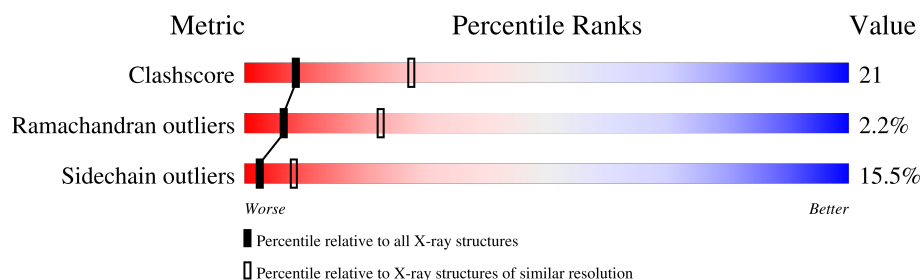
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FP	A	364	-	X	X	-

## 2 Entry composition [i](#)

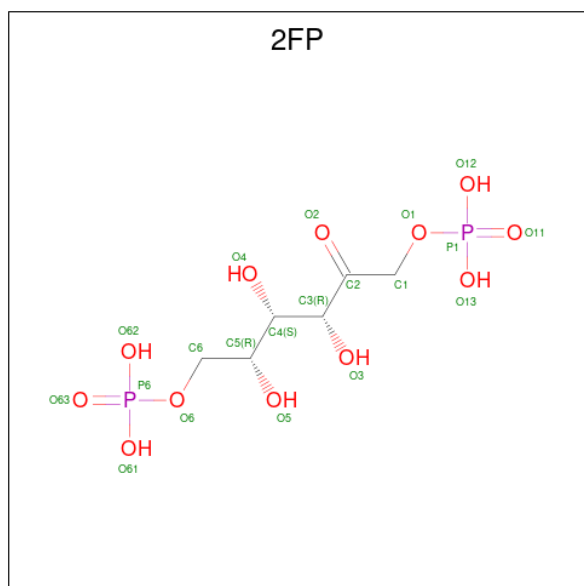
There are 2 unique types of molecules in this entry. The entry contains 2783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FRUCTOSE-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2763	1741	486	525	11			

- Molecule 2 is 1,6-FRUCTOSE DIPHOSPHATE (LINEAR FORM) (three-letter code: 2FP) (formula:  $C_6H_{14}O_{12}P_2$ ).



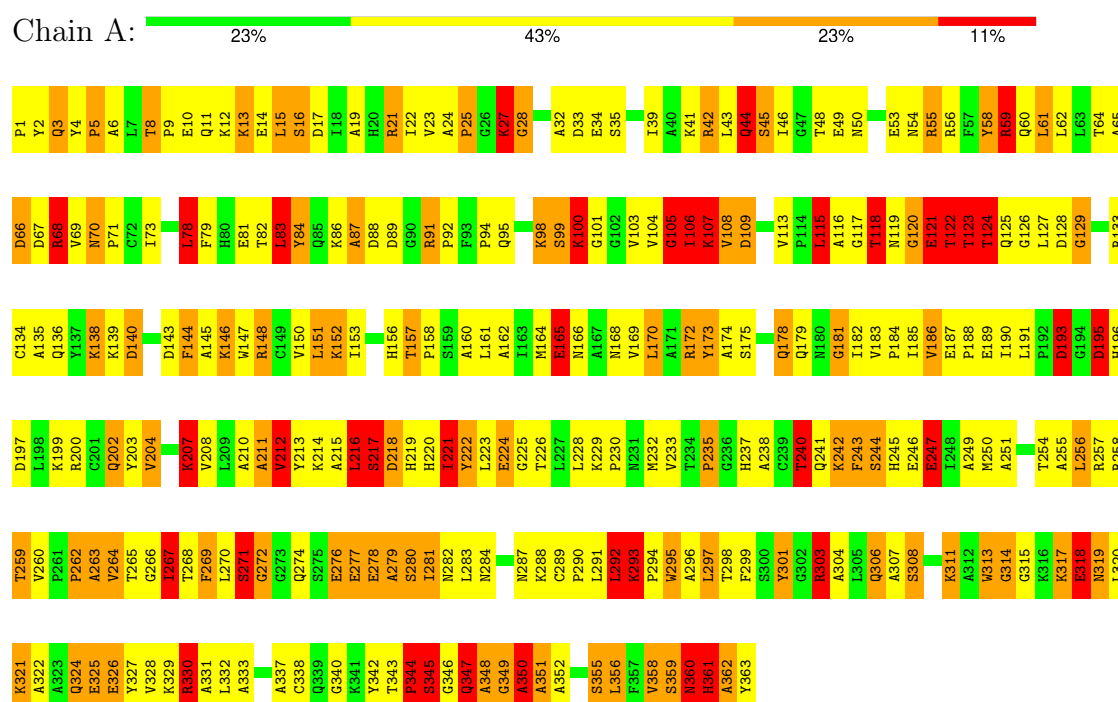
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		

### 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: FRUCTOSE-BISPHOSPHATE ALDOLASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.50Å 96.50Å 166.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.56 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (19.56-2.80)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.202 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2783	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: 2FP

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	1.39	15/2817 (0.5%)	3.37	362/3818 (9.5%)

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	59

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	SER	CB-OG	-7.49	1.32	1.42
1	A	175	SER	CB-OG	-6.14	1.34	1.42
1	A	126	GLY	N-CA	-6.12	1.36	1.46
1	A	271	SER	CB-OG	5.76	1.49	1.42
1	A	59	ARG	NE-CZ	-5.74	1.25	1.33
1	A	280	SER	CB-OG	-5.56	1.35	1.42
1	A	272	GLY	N-CA	-5.48	1.37	1.46
1	A	165	GLU	CD-OE1	5.34	1.31	1.25
1	A	244	SER	CB-OG	-5.25	1.35	1.42
1	A	165	GLU	CD-OE2	5.22	1.31	1.25
1	A	59	ARG	CD-NE	-5.19	1.37	1.46
1	A	129	GLY	N-CA	-5.13	1.38	1.46
1	A	272	GLY	C-O	5.12	1.31	1.23
1	A	258	ARG	CD-NE	5.11	1.55	1.46
1	A	28	GLY	N-CA	-5.05	1.38	1.46

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	NE-CZ-NH2	-39.92	100.34	120.30
1	A	133	ARG	NE-CZ-NH2	-30.43	105.08	120.30
1	A	56	ARG	NE-CZ-NH1	29.06	134.83	120.30
1	A	59	ARG	CD-NE-CZ	27.71	162.40	123.60
1	A	91	ARG	NE-CZ-NH2	-25.85	107.37	120.30
1	A	56	ARG	NE-CZ-NH2	-25.56	107.52	120.30
1	A	330	ARG	NE-CZ-NH2	-24.75	107.92	120.30
1	A	193	ASP	CB-CG-OD2	23.54	139.48	118.30
1	A	148	ARG	NE-CZ-NH2	-23.42	108.59	120.30
1	A	59	ARG	NE-CZ-NH2	21.38	130.99	120.30
1	A	133	ARG	NH1-CZ-NH2	19.53	140.89	119.40
1	A	21	ARG	NE-CZ-NH2	-18.89	110.86	120.30
1	A	68	ARG	NE-CZ-NH1	17.61	129.10	120.30
1	A	67	ASP	CB-CG-OD1	17.61	134.15	118.30
1	A	311	LYS	CB-CG-CD	17.44	156.95	111.60
1	A	172	ARG	NE-CZ-NH1	-17.17	111.71	120.30
1	A	107	LYS	CD-CE-NZ	16.34	149.29	111.70
1	A	67	ASP	CB-CG-OD2	-15.92	103.97	118.30
1	A	91	ARG	NH1-CZ-NH2	15.77	136.74	119.40
1	A	258	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	A	303	ARG	CG-CD-NE	14.23	141.69	111.80
1	A	148	ARG	NE-CZ-NH1	14.08	127.34	120.30
1	A	128	ASP	CB-CG-OD2	13.79	130.71	118.30
1	A	172	ARG	NE-CZ-NH2	12.75	126.67	120.30
1	A	133	ARG	NE-CZ-NH1	-12.55	114.03	120.30
1	A	68	ARG	CD-NE-CZ	-12.20	106.52	123.60
1	A	197	ASP	CB-CG-OD2	-12.13	107.38	118.30
1	A	81	GLU	OE1-CD-OE2	-11.93	108.98	123.30
1	A	197	ASP	CB-CG-OD1	11.78	128.90	118.30
1	A	158	PRO	N-CA-CB	11.31	116.87	103.30
1	A	173	TYR	CB-CG-CD1	11.14	127.68	121.00
1	A	218	ASP	CB-CG-OD1	10.96	128.16	118.30
1	A	148	ARG	CD-NE-CZ	10.90	138.86	123.60
1	A	2	TYR	CB-CG-CD1	-10.85	114.49	121.00
1	A	143	ASP	CB-CG-OD1	10.81	128.03	118.30
1	A	21	ARG	CD-NE-CZ	-10.68	108.64	123.60
1	A	2	TYR	C-N-CA	10.63	148.28	121.70
1	A	240	THR	CA-CB-CG2	-10.43	97.80	112.40
1	A	68	ARG	NH1-CZ-NH2	10.14	130.55	119.40
1	A	84	TYR	CB-CG-CD2	-10.10	114.94	121.00
1	A	174	ALA	N-CA-CB	9.94	124.02	110.10
1	A	218	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	A	91	ARG	CB-CA-C	9.72	129.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ALA	N-CA-CB	9.52	123.43	110.10
1	A	343	THR	O-C-N	9.47	139.10	121.10
1	A	242	LYS	CB-CA-C	9.47	129.34	110.40
1	A	304	ALA	CA-C-N	9.46	138.00	117.20
1	A	21	ARG	NH1-CZ-NH2	9.45	129.79	119.40
1	A	207	LYS	CD-CE-NZ	9.36	133.23	111.70
1	A	247	GLU	CG-CD-OE1	-9.34	99.62	118.30
1	A	133	ARG	CD-NE-CZ	9.32	136.65	123.60
1	A	247	GLU	CG-CD-OE2	9.32	136.95	118.30
1	A	223	LEU	CA-CB-CG	9.27	136.62	115.30
1	A	55	ARG	NE-CZ-NH2	9.15	124.88	120.30
1	A	262	PRO	CA-C-N	9.07	137.15	117.20
1	A	259	THR	CA-CB-CG2	8.95	124.93	112.40
1	A	83	LEU	CB-CG-CD1	8.94	126.20	111.00
1	A	217	SER	N-CA-CB	-8.92	97.12	110.50
1	A	91	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	258	ARG	NH1-CZ-NH2	8.86	129.15	119.40
1	A	101	GLY	CA-C-N	8.84	133.89	116.20
1	A	33	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	271	SER	C-N-CA	8.65	140.46	122.30
1	A	311	LYS	CA-CB-CG	8.63	132.40	113.40
1	A	81	GLU	O-C-N	-8.61	108.93	122.70
1	A	123	THR	N-CA-CB	8.59	126.62	110.30
1	A	53	GLU	CG-CD-OE1	8.53	135.37	118.30
1	A	281	ILE	CA-CB-CG2	8.52	127.95	110.90
1	A	113	VAL	CG1-CB-CG2	-8.45	97.39	110.90
1	A	157	THR	CA-C-O	-8.45	102.36	120.10
1	A	360	ASN	CB-CA-C	8.42	127.25	110.40
1	A	212	VAL	O-C-N	-8.42	109.23	122.70
1	A	173	TYR	CG-CD2-CE2	8.37	127.99	121.30
1	A	185	ILE	O-C-N	-8.36	109.32	122.70
1	A	170	LEU	CB-CG-CD1	8.36	125.21	111.00
1	A	6	ALA	CB-CA-C	-8.33	97.60	110.10
1	A	44	GLN	O-C-N	-8.32	109.39	122.70
1	A	279	ALA	O-C-N	-8.31	109.40	122.70
1	A	89	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	330	ARG	NH1-CZ-NH2	8.24	128.47	119.40
1	A	257	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	A	193	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	A	363	TYR	CB-CG-CD1	-8.21	116.07	121.00
1	A	208	VAL	CG1-CB-CG2	-8.19	97.80	110.90
1	A	348	ALA	N-CA-C	8.19	133.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	TYR	CB-CG-CD1	-8.16	116.11	121.00
1	A	289	CYS	N-CA-CB	-8.14	95.95	110.60
1	A	59	ARG	NH1-CZ-NH2	-8.07	110.52	119.40
1	A	123	THR	CB-CA-C	-8.07	89.82	111.60
1	A	88	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	42	ARG	CG-CD-NE	7.92	128.44	111.80
1	A	143	ASP	CB-CG-OD2	-7.92	111.18	118.30
1	A	2	TYR	CB-CG-CD2	7.88	125.72	121.00
1	A	17	ASP	N-CA-CB	7.83	124.70	110.60
1	A	224	GLU	OE1-CD-OE2	-7.82	113.92	123.30
1	A	165	GLU	CB-CG-CD	7.82	135.30	114.20
1	A	207	LYS	O-C-N	-7.75	110.31	122.70
1	A	213	TYR	CB-CG-CD2	7.63	125.58	121.00
1	A	116	ALA	CB-CA-C	-7.63	98.66	110.10
1	A	219	HIS	CG-ND1-CE1	7.63	118.88	108.20
1	A	362	ALA	N-CA-CB	7.58	120.71	110.10
1	A	351	ALA	N-CA-CB	-7.51	99.59	110.10
1	A	115	LEU	N-CA-CB	-7.50	95.40	110.40
1	A	262	PRO	O-C-N	-7.46	110.77	122.70
1	A	64	THR	CA-CB-CG2	7.46	122.84	112.40
1	A	351	ALA	O-C-N	-7.45	110.78	122.70
1	A	62	LEU	O-C-N	-7.41	110.85	122.70
1	A	43	LEU	O-C-N	-7.36	110.92	122.70
1	A	203	TYR	CZ-CE2-CD2	-7.31	113.22	119.80
1	A	33	ASP	OD1-CG-OD2	-7.30	109.44	123.30
1	A	258	ARG	CD-NE-CZ	-7.29	113.39	123.60
1	A	318	GLU	CB-CG-CD	7.29	133.89	114.20
1	A	140	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	124	THR	CA-CB-CG2	7.28	122.60	112.40
1	A	303	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	32	ALA	CB-CA-C	7.24	120.95	110.10
1	A	246	GLU	N-CA-CB	7.24	123.62	110.60
1	A	99	SER	CA-C-O	-7.21	104.95	120.10
1	A	193	ASP	OD1-CG-OD2	-7.21	109.60	123.30
1	A	16	SER	CB-CA-C	7.19	123.76	110.10
1	A	185	ILE	CA-C-N	7.14	132.91	117.20
1	A	44	GLN	CA-C-O	7.14	135.09	120.10
1	A	118	THR	N-CA-CB	-7.12	96.77	110.30
1	A	220	HIS	CA-CB-CG	-7.10	101.54	113.60
1	A	237	HIS	O-C-N	-7.09	111.35	122.70
1	A	347	GLN	N-CA-CB	-7.03	97.95	110.60
1	A	2	TYR	O-C-N	-7.03	111.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	SER	N-CA-CB	-7.03	99.96	110.50
1	A	189	GLU	OE1-CD-OE2	-6.99	114.92	123.30
1	A	16	SER	N-CA-CB	-6.98	100.03	110.50
1	A	121	GLU	O-C-N	-6.98	111.54	122.70
1	A	49	GLU	OE1-CD-OE2	6.96	131.65	123.30
1	A	207	LYS	CB-CG-CD	6.95	129.67	111.60
1	A	88	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	313	TRP	CE3-CZ3-CH2	-6.89	113.62	121.20
1	A	278	GLU	OE1-CD-OE2	6.86	131.53	123.30
1	A	333	ALA	CB-CA-C	6.86	120.39	110.10
1	A	45	SER	CB-CA-C	6.85	123.11	110.10
1	A	81	GLU	CG-CD-OE2	6.83	131.95	118.30
1	A	33	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	179	GLN	CG-CD-OE1	-6.80	108.00	121.60
1	A	120	GLY	O-C-N	-6.78	111.86	122.70
1	A	345	SER	CA-C-O	6.77	134.31	120.10
1	A	350	ALA	C-N-CA	6.75	138.57	121.70
1	A	91	ARG	N-CA-CB	-6.74	98.47	110.60
1	A	326	GLU	CB-CG-CD	6.71	132.32	114.20
1	A	62	LEU	CB-CG-CD2	6.70	122.39	111.00
1	A	17	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	42	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	157	THR	O-C-N	6.69	133.81	121.10
1	A	1	PRO	O-C-N	-6.68	112.02	122.70
1	A	181	GLY	CA-C-O	-6.67	108.59	120.60
1	A	356	LEU	CB-CG-CD2	-6.67	99.66	111.00
1	A	301	TYR	CB-CG-CD1	6.67	125.00	121.00
1	A	245	HIS	CA-CB-CG	6.66	124.93	113.60
1	A	237	HIS	N-CA-CB	-6.65	98.63	110.60
1	A	264	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	A	224	GLU	CG-CD-OE2	6.63	131.56	118.30
1	A	186	VAL	O-C-N	-6.62	112.10	122.70
1	A	95	GLN	O-C-N	-6.62	112.11	122.70
1	A	330	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	170	LEU	CB-CG-CD2	-6.60	99.77	111.00
1	A	268	THR	OG1-CB-CG2	-6.57	94.89	110.00
1	A	66	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	161	LEU	N-CA-CB	-6.54	97.32	110.40
1	A	199	LYS	CA-CB-CG	-6.54	99.02	113.40
1	A	128	ASP	C-N-CA	6.52	135.99	122.30
1	A	329	LYS	O-C-N	-6.51	112.29	122.70
1	A	53	GLU	CG-CD-OE2	-6.49	105.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	PRO	O-C-N	-6.49	112.32	122.70
1	A	43	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	115	LEU	CA-C-N	6.42	131.33	117.20
1	A	216	LEU	N-CA-CB	-6.41	97.58	110.40
1	A	202	GLN	OE1-CD-NE2	-6.40	107.18	121.90
1	A	306	GLN	CA-C-N	6.40	131.27	117.20
1	A	168	ASN	CB-CG-OD1	-6.39	108.81	121.60
1	A	215	ALA	CB-CA-C	6.39	119.69	110.10
1	A	272	GLY	O-C-N	-6.37	112.37	123.20
1	A	101	GLY	CA-C-O	-6.36	109.14	120.60
1	A	304	ALA	CA-C-O	-6.35	106.77	120.10
1	A	346	GLY	N-CA-C	-6.34	97.25	113.10
1	A	348	ALA	CB-CA-C	-6.33	100.61	110.10
1	A	216	LEU	CB-CG-CD1	6.31	121.73	111.00
1	A	348	ALA	O-C-N	-6.30	112.48	123.20
1	A	117	GLY	CA-C-O	6.29	131.92	120.60
1	A	2	TYR	CA-C-O	6.28	133.28	120.10
1	A	108	VAL	CA-CB-CG2	-6.27	101.50	110.90
1	A	265	THR	O-C-N	-6.27	112.55	123.20
1	A	345	SER	CA-C-N	-6.26	103.69	116.20
1	A	62	LEU	CA-C-N	6.25	130.94	117.20
1	A	246	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	A	17	ASP	CA-C-O	-6.24	107.00	120.10
1	A	27	LYS	CA-CB-CG	6.21	127.06	113.40
1	A	158	PRO	CA-N-CD	-6.21	102.81	111.50
1	A	150	VAL	CA-C-N	6.21	130.85	117.20
1	A	45	SER	O-C-N	-6.19	112.79	122.70
1	A	202	GLN	CG-CD-NE2	6.19	131.56	116.70
1	A	213	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
1	A	243	PHE	O-C-N	-6.18	112.81	122.70
1	A	61	LEU	N-CA-CB	6.14	122.68	110.40
1	A	54	ASN	CB-CG-OD1	-6.13	109.34	121.60
1	A	87	ALA	O-C-N	-6.06	113.00	122.70
1	A	363	TYR	CB-CG-CD2	6.05	124.63	121.00
1	A	14	GLU	CG-CD-OE2	6.03	130.37	118.30
1	A	276	GLU	N-CA-CB	-6.03	99.75	110.60
1	A	62	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	269	PHE	O-C-N	-6.02	113.07	122.70
1	A	105	GLY	O-C-N	-6.01	113.08	122.70
1	A	73	ILE	CA-C-N	6.01	128.22	116.20
1	A	133	ARG	CA-C-N	6.00	130.41	117.20
1	A	127	LEU	CA-C-O	-5.98	107.54	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	SER	C-N-CA	-5.96	106.79	121.70
1	A	68	ARG	CB-CG-CD	-5.93	96.18	111.60
1	A	100	LYS	CD-CE-NZ	5.93	125.33	111.70
1	A	157	THR	CA-CB-CG2	-5.92	104.11	112.40
1	A	138	LYS	C-N-CA	5.91	136.48	121.70
1	A	313	TRP	CZ3-CH2-CZ2	5.91	128.69	121.60
1	A	293	LYS	CB-CG-CD	5.91	126.96	111.60
1	A	10	GLU	OE1-CD-OE2	5.91	130.39	123.30
1	A	360	ASN	C-N-CA	5.89	136.43	121.70
1	A	162	ALA	N-CA-CB	5.89	118.34	110.10
1	A	327	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	347	GLN	C-N-CA	5.86	136.34	121.70
1	A	249	ALA	O-C-N	-5.85	113.34	122.70
1	A	238	ALA	CB-CA-C	-5.83	101.35	110.10
1	A	271	SER	CA-CB-OG	5.83	126.94	111.20
1	A	193	ASP	O-C-N	-5.81	113.33	123.20
1	A	127	LEU	O-C-N	5.80	131.99	122.70
1	A	15	LEU	O-C-N	-5.80	113.42	122.70
1	A	61	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	237	HIS	CA-C-N	5.80	129.96	117.20
1	A	79	PHE	CB-CG-CD2	-5.79	116.74	120.80
1	A	121	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	44	GLN	CA-CB-CG	5.78	126.12	113.40
1	A	301	TYR	CG-CD2-CE2	5.77	125.92	121.30
1	A	168	ASN	N-CA-CB	-5.77	100.21	110.60
1	A	84	TYR	CD1-CG-CD2	5.76	124.23	117.90
1	A	107	LYS	CG-CD-CE	5.76	129.17	111.90
1	A	116	ALA	CA-C-O	-5.75	108.01	120.10
1	A	243	PHE	CZ-CE2-CD2	-5.75	113.19	120.10
1	A	166	ASN	CA-CB-CG	-5.75	100.74	113.40
1	A	125	GLN	CA-C-N	5.75	127.69	116.20
1	A	95	GLN	CB-CA-C	5.74	121.87	110.40
1	A	106	ILE	O-C-N	-5.73	113.53	122.70
1	A	228	LEU	O-C-N	-5.72	113.54	122.70
1	A	277	GLU	CG-CD-OE2	5.71	129.73	118.30
1	A	173	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	58	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	219	HIS	ND1-CG-CD2	-5.70	98.03	106.00
1	A	296	ALA	C-N-CA	5.69	135.93	121.70
1	A	210	ALA	CB-CA-C	5.69	118.63	110.10
1	A	122	THR	CA-C-O	-5.68	108.16	120.10
1	A	78	LEU	C-N-CA	5.67	135.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ALA	O-C-N	-5.66	113.64	122.70
1	A	277	GLU	N-CA-CB	-5.66	100.42	110.60
1	A	83	LEU	N-CA-CB	5.64	121.69	110.40
1	A	199	LYS	CA-C-N	5.64	129.62	117.20
1	A	19	ALA	N-CA-CB	-5.64	102.20	110.10
1	A	195	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	351	ALA	CA-C-O	5.63	131.93	120.10
1	A	295	TRP	CA-CB-CG	5.62	124.39	113.70
1	A	178	GLN	CB-CG-CD	5.62	126.22	111.60
1	A	246	GLU	CB-CG-CD	5.62	129.37	114.20
1	A	199	LYS	CB-CG-CD	5.61	126.18	111.60
1	A	296	ALA	CA-C-N	5.59	129.50	117.20
1	A	340	GLY	O-C-N	-5.59	113.76	122.70
1	A	321	LYS	O-C-N	-5.58	113.77	122.70
1	A	186	VAL	CA-C-O	5.58	131.82	120.10
1	A	3	GLN	CA-C-O	5.58	131.82	120.10
1	A	251	ALA	N-CA-CB	5.57	117.90	110.10
1	A	292	LEU	O-C-N	-5.55	113.82	122.70
1	A	83	LEU	CB-CA-C	-5.54	99.67	110.20
1	A	293	LYS	CA-CB-CG	-5.54	101.21	113.40
1	A	318	GLU	CA-C-O	-5.52	108.51	120.10
1	A	42	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	235	PRO	N-CA-CB	5.52	109.92	103.30
1	A	343	THR	N-CA-CB	5.50	120.75	110.30
1	A	17	ASP	CA-C-N	5.50	129.30	117.20
1	A	125	GLN	C-N-CA	5.49	133.82	122.30
1	A	342	TYR	CG-CD2-CE2	-5.48	116.91	121.30
1	A	330	ARG	CA-C-N	5.48	129.25	117.20
1	A	200	ARG	CD-NE-CZ	-5.47	115.94	123.60
1	A	21	ARG	CG-CD-NE	-5.47	100.31	111.80
1	A	196	HIS	CG-ND1-CE1	5.47	115.86	108.20
1	A	41	LYS	CA-CB-CG	5.46	125.41	113.40
1	A	306	GLN	O-C-N	-5.46	113.97	122.70
1	A	347	GLN	CB-CA-C	5.45	121.31	110.40
1	A	213	TYR	CA-CB-CG	-5.45	103.05	113.40
1	A	267	ILE	CB-CA-C	5.44	122.47	111.60
1	A	88	ASP	C-N-CA	5.43	135.28	121.70
1	A	293	LYS	CD-CE-NZ	5.43	124.18	111.70
1	A	304	ALA	CB-CA-C	5.41	118.21	110.10
1	A	267	ILE	CA-CB-CG2	5.40	121.70	110.90
1	A	151	LEU	CB-CA-C	5.40	120.46	110.20
1	A	318	GLU	CA-CB-CG	5.40	125.28	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	210	ALA	N-CA-CB	-5.39	102.55	110.10
1	A	221	ILE	CA-CB-CG1	-5.38	100.78	111.00
1	A	166	ASN	O-C-N	-5.38	114.10	122.70
1	A	179	GLN	OE1-CD-NE2	5.37	134.26	121.90
1	A	258	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	133	ARG	CG-CD-NE	-5.36	100.55	111.80
1	A	218	ASP	C-N-CA	5.35	135.08	121.70
1	A	225	GLY	CA-C-N	5.35	128.97	117.20
1	A	25	PRO	N-CA-CB	5.35	109.72	103.30
1	A	325	GLU	CA-CB-CG	-5.34	101.66	113.40
1	A	153	ILE	CA-CB-CG2	-5.31	100.28	110.90
1	A	332	LEU	CA-C-O	5.30	131.23	120.10
1	A	217	SER	O-C-N	-5.28	114.25	122.70
1	A	150	VAL	CA-C-O	-5.28	109.02	120.10
1	A	136	GLN	CG-CD-OE1	-5.28	111.05	121.60
1	A	301	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	222	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
1	A	145	ALA	CB-CA-C	5.27	118.00	110.10
1	A	211	ALA	CA-C-N	5.27	128.79	117.20
1	A	240	THR	CA-C-O	-5.25	109.08	120.10
1	A	355	SER	N-CA-CB	-5.25	102.63	110.50
1	A	232	MET	CA-C-N	5.24	128.73	117.20
1	A	5	PRO	C-N-CA	5.24	134.79	121.70
1	A	360	ASN	CA-C-O	5.22	131.07	120.10
1	A	207	LYS	CA-C-N	5.22	128.69	117.20
1	A	297	LEU	CA-C-O	5.21	131.04	120.10
1	A	358	VAL	CA-CB-CG2	5.21	118.72	110.90
1	A	128	ASP	OD1-CG-OD2	-5.20	113.42	123.30
1	A	319	ASN	O-C-N	-5.20	114.38	122.70
1	A	199	LYS	O-C-N	-5.20	114.38	122.70
1	A	108	VAL	O-C-N	5.20	131.01	122.70
1	A	84	TYR	N-CA-CB	-5.18	101.27	110.60
1	A	160	ALA	N-CA-CB	5.18	117.36	110.10
1	A	151	LEU	CA-C-N	5.16	128.55	117.20
1	A	215	ALA	O-C-N	-5.15	114.46	122.70
1	A	256	LEU	O-C-N	-5.15	114.46	122.70
1	A	269	PHE	N-CA-C	5.14	124.89	111.00
1	A	58	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	A	115	LEU	O-C-N	-5.14	114.47	122.70
1	A	263	ALA	N-CA-CB	5.13	117.29	110.10
1	A	324	GLN	CG-CD-OE1	5.12	131.83	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ARG	O-C-N	-5.12	114.52	122.70
1	A	232	MET	O-C-N	-5.09	114.55	122.70
1	A	108	VAL	CA-C-N	-5.08	106.02	117.20
1	A	48	THR	N-CA-CB	-5.08	100.65	110.30
1	A	337	ALA	O-C-N	-5.08	114.58	122.70
1	A	135	ALA	CB-CA-C	-5.07	102.49	110.10
1	A	278	GLU	N-CA-CB	5.07	119.72	110.60
1	A	294	PRO	C-N-CA	5.07	134.37	121.70
1	A	343	THR	CA-C-O	-5.07	109.46	120.10
1	A	144	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	109	ASP	CA-C-O	-5.06	109.47	120.10
1	A	32	ALA	O-C-N	-5.05	114.61	122.70
1	A	361	HIS	C-N-CA	5.05	134.32	121.70
1	A	135	ALA	CA-C-O	-5.05	109.50	120.10
1	A	115	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	267	ILE	CA-CB-CG1	-5.04	101.43	111.00
1	A	14	GLU	N-CA-CB	5.03	119.65	110.60
1	A	58	TYR	CA-CB-CG	-5.02	103.86	113.40
1	A	245	HIS	ND1-CG-CD2	-5.02	98.97	106.00
1	A	79	PHE	C-N-CA	5.02	134.24	121.70
1	A	225	GLY	O-C-N	-5.01	114.68	122.70
1	A	99	SER	CA-C-N	5.01	128.22	117.20
1	A	100	LYS	O-C-N	-5.01	114.69	123.20
1	A	204	VAL	CA-C-N	5.01	128.22	117.20
1	A	238	ALA	CA-C-O	-5.01	109.58	120.10

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LYS	Mainchain
1	A	103	VAL	Mainchain
1	A	105	GLY	Mainchain
1	A	108	VAL	Mainchain
1	A	119	ASN	Mainchain
1	A	121	GLU	Mainchain
1	A	122	THR	Mainchain
1	A	124	THR	Mainchain
1	A	129	GLY	Mainchain
1	A	138	LYS	Mainchain
1	A	139	LYS	Mainchain
1	A	140	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	15	LEU	Mainchain
1	A	156	HIS	Mainchain
1	A	157	THR	Mainchain
1	A	164	MET	Mainchain
1	A	181	GLY	Mainchain
1	A	190	ILE	Mainchain
1	A	195	ASP	Mainchain
1	A	204	VAL	Mainchain
1	A	207	LYS	Mainchain
1	A	212	VAL	Mainchain
1	A	217	SER	Mainchain
1	A	221	ILE	Mainchain
1	A	23	VAL	Mainchain
1	A	235	PRO	Mainchain
1	A	240	THR	Mainchain
1	A	242	LYS	Mainchain
1	A	256	LEU	Mainchain
1	A	259	THR	Mainchain
1	A	260	VAL	Mainchain
1	A	262	PRO	Mainchain
1	A	264	VAL	Mainchain
1	A	266	GLY	Mainchain
1	A	272	GLY	Mainchain
1	A	279	ALA	Mainchain
1	A	281	ILE	Mainchain
1	A	282	ASN	Mainchain
1	A	287	ASN	Mainchain
1	A	290	PRO	Mainchain
1	A	292	LEU	Mainchain
1	A	301	TYR	Mainchain
1	A	307	ALA	Mainchain
1	A	314	GLY	Mainchain
1	A	330	ARG	Mainchain
1	A	331	ALA	Mainchain
1	A	338	CYS	Mainchain
1	A	348	ALA	Mainchain
1	A	350	ALA	Peptide
1	A	360	ASN	Mainchain
1	A	4	TYR	Mainchain
1	A	5	PRO	Mainchain
1	A	50	ASN	Mainchain
1	A	68	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	78	LEU	Peptide
1	A	8	THR	Mainchain
1	A	83	LEU	Mainchain
1	A	84	TYR	Mainchain
1	A	99	SER	Mainchain

## 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	2763	0	2781	114	0
2	A	20	0	9	9	0
All	All	2783	0	2790	116	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 21.

All (116) 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)
2:A:364:2FP:C5	2:A:364:2FP:O5	1.68	1.42
1:A:178:GLN:HE22	1:A:222:TYR:H	0.97	0.96
1:A:311:LYS:HE2	1:A:351:ALA:HB2	1.58	0.84
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.58	0.83
1:A:94:PRO:O	1:A:98:LYS:HD3	1.83	0.78
1:A:124:THR:HG21	1:A:148:ARG:O	1.83	0.76
1:A:244:SER:OG	1:A:247:GLU:HG3	1.85	0.76
1:A:186:VAL:O	1:A:188:PRO:HD3	1.90	0.71
1:A:118:THR:HG23	1:A:121:GLU:H	1.54	0.70
1:A:86:LYS:HA	1:A:92:PRO:HA	1.79	0.65
1:A:292:LEU:HD12	1:A:293:LYS:N	2.12	0.63
1:A:317:LYS:HG2	1:A:318:GLU:OE1	1.99	0.63
1:A:292:LEU:HD12	1:A:292:LEU:C	2.19	0.62
1:A:107:LYS:NZ	2:A:364:2FP:O61	2.32	0.62
1:A:267:ILE:HD11	1:A:269:PHE:CZ	2.35	0.61
1:A:267:ILE:HG12	1:A:297:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HG	1:A:221:ILE:HG12	1.82	0.61
1:A:123:THR:HG21	1:A:165:GLU:OE2	2.00	0.61
1:A:221:ILE:HD12	1:A:221:ILE:C	2.20	0.61
1:A:35:SER:N	2:A:364:2FP:O61	2.34	0.61
1:A:78:LEU:O	1:A:106:ILE:HA	2.01	0.60
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.36	0.60
1:A:146:LYS:NZ	2:A:364:2FP:H4	2.18	0.59
1:A:92:PRO:HB2	1:A:94:PRO:HD2	1.86	0.58
1:A:193:ASP:OD2	1:A:360:ASN:HB2	2.04	0.57
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.36	0.56
1:A:277:GLU:HG2	1:A:330:ARG:NH2	2.20	0.55
1:A:106:ILE:HD12	1:A:107:LYS:N	2.22	0.55
1:A:250:MET:HE1	1:A:291:LEU:CD1	2.38	0.54
1:A:195:ASP:OD1	1:A:195:ASP:C	2.45	0.54
1:A:284:ASN:ND2	1:A:288:LYS:HE2	2.22	0.53
1:A:358:VAL:HG12	1:A:359:SER:N	2.24	0.53
1:A:65:ALA:O	1:A:100:LYS:NZ	2.35	0.52
1:A:12:LYS:HG2	1:A:222:TYR:CE1	2.45	0.51
1:A:303:ARG:NH2	1:A:356:LEU:HD22	2.25	0.51
1:A:134:CYS:HB3	1:A:182:ILE:HD12	1.93	0.51
1:A:221:ILE:CD1	1:A:226:THR:HG21	2.41	0.51
1:A:178:GLN:HE22	1:A:222:TYR:N	1.83	0.51
2:A:364:2FP:C5	2:A:364:2FP:HO5	2.11	0.51
1:A:115:LEU:O	1:A:118:THR:HB	2.11	0.51
1:A:324:GLN:O	1:A:325:GLU:C	2.49	0.50
1:A:241:GLN:HB3	1:A:243:PHE:CE2	2.47	0.50
1:A:8:THR:O	1:A:11:GLN:N	2.45	0.50
1:A:283:LEU:CD2	1:A:299:PHE:HB3	2.42	0.50
1:A:60:GLN:OE1	1:A:87:ALA:HA	2.12	0.50
1:A:319:ASN:O	1:A:320:LEU:C	2.50	0.49
1:A:58:TYR:OH	1:A:306:GLN:NE2	2.34	0.49
1:A:98:LYS:HD2	1:A:104:VAL:HG23	1.94	0.49
1:A:8:THR:O	1:A:9:PRO:C	2.51	0.49
1:A:221:ILE:HD11	1:A:226:THR:HG21	1.96	0.48
1:A:267:ILE:HG13	1:A:267:ILE:O	2.09	0.48
1:A:254:THR:O	1:A:255:ALA:C	2.50	0.48
1:A:172:ARG:HH11	1:A:172:ARG:HD2	1.31	0.48
1:A:12:LYS:HG2	1:A:222:TYR:CZ	2.49	0.48
1:A:359:SER:OG	1:A:361:HIS:HB2	2.13	0.48
1:A:330:ARG:HD3	1:A:330:ARG:HA	1.46	0.48
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASP:OD1	1:A:68:ARG:HD3	2.15	0.47
1:A:303:ARG:CZ	1:A:356:LEU:HD22	2.45	0.47
1:A:244:SER:OG	1:A:247:GLU:CG	2.61	0.46
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.50	0.46
1:A:221:ILE:HD12	1:A:222:TYR:N	2.30	0.46
1:A:311:LYS:HE2	1:A:351:ALA:CB	2.37	0.46
1:A:146:LYS:HZ1	2:A:364:2FP:H4	1.78	0.46
1:A:271:SER:N	2:A:364:2FP:O11	2.46	0.46
1:A:44:GLN:O	1:A:45:SER:C	2.50	0.46
1:A:66:ASP:OD2	1:A:68:ARG:NH1	2.48	0.45
1:A:283:LEU:HD22	1:A:299:PHE:HB3	1.98	0.45
1:A:276:GLU:HB2	1:A:352:ALA:HA	1.98	0.45
1:A:115:LEU:HD22	1:A:122:THR:O	2.16	0.45
1:A:267:ILE:HD11	1:A:269:PHE:CE2	2.52	0.45
1:A:187:GLU:HG3	1:A:229:LYS:O	2.17	0.45
1:A:267:ILE:HD11	1:A:269:PHE:CE1	2.51	0.45
1:A:70:ASN:ND2	1:A:100:LYS:HB3	2.31	0.44
1:A:105:GLY:HA2	1:A:144:PHE:O	2.18	0.44
1:A:59:ARG:HG2	1:A:82:THR:HG21	1.99	0.44
1:A:120:GLY:O	1:A:152:LYS:HE2	2.18	0.44
1:A:24:ALA:O	1:A:25:PRO:C	2.56	0.44
1:A:34:GLU:HA	2:A:364:2FP:O61	2.18	0.44
1:A:118:THR:HG23	1:A:121:GLU:N	2.29	0.44
1:A:21:ARG:HH11	1:A:21:ARG:HD2	1.38	0.43
1:A:21:ARG:O	1:A:22:ILE:C	2.53	0.43
1:A:274:GLN:HB3	1:A:278:GLU:HB3	2.00	0.43
1:A:8:THR:HG23	1:A:11:GLN:OE1	2.18	0.43
1:A:12:LYS:HG2	1:A:222:TYR:CD1	2.54	0.43
1:A:250:MET:HE3	1:A:250:MET:HA	2.01	0.43
1:A:170:LEU:HD22	1:A:186:VAL:HG13	2.01	0.43
1:A:349:GLY:O	1:A:350:ALA:CB	2.67	0.42
1:A:118:THR:HG21	1:A:121:GLU:HB2	2.01	0.42
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.89	0.42
1:A:224:GLU:HG3	1:A:263:ALA:O	2.19	0.42
1:A:321:LYS:O	1:A:322:ALA:C	2.54	0.42
1:A:193:ASP:OD1	1:A:193:ASP:N	2.29	0.42
1:A:217:SER:O	1:A:218:ASP:C	2.58	0.42
1:A:276:GLU:OE1	1:A:352:ALA:HA	2.19	0.42
1:A:277:GLU:HG2	1:A:330:ARG:HH22	1.81	0.42
1:A:298:THR:OG1	1:A:299:PHE:N	2.47	0.42
1:A:13:LYS:O	1:A:13:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:O	1:A:216:LEU:HB2	2.20	0.42
1:A:191:LEU:HD13	1:A:360:ASN:HB3	2.02	0.41
1:A:147:TRP:HB3	1:A:173:TYR:CE2	2.55	0.41
1:A:250:MET:HE1	1:A:291:LEU:HD11	2.02	0.41
1:A:211:ALA:O	1:A:212:VAL:C	2.57	0.41
1:A:344:PRO:O	1:A:345:SER:C	2.59	0.41
1:A:70:ASN:HD21	1:A:100:LYS:HB3	1.86	0.41
1:A:271:SER:HB3	2:A:364:2FP:O11	2.21	0.41
1:A:46:ILE:HB	1:A:314:GLY:HA2	2.02	0.41
1:A:27:LYS:HD3	1:A:71:PRO:O	2.21	0.41
1:A:39:ILE:HG21	1:A:55:ARG:HD2	2.01	0.41
1:A:70:ASN:ND2	1:A:100:LYS:HE3	2.36	0.41
1:A:344:PRO:O	1:A:347:GLN:HB2	2.20	0.41
1:A:68:ARG:CZ	1:A:328:VAL:HG11	2.51	0.40
1:A:151:LEU:HD12	1:A:151:LEU:N	2.36	0.40
1:A:183:VAL:HA	1:A:184:PRO:HD3	1.83	0.40
1:A:202:GLN:HB2	1:A:233:VAL:HG11	2.03	0.40
1:A:303:ARG:CZ	1:A:356:LEU:HB3	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/363 (99%)	323 (90%)	30 (8%)	8 (2%)	6	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	A	350	ALA
1	A	361	HIS

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Mol	Chain	Res	Type
1	A	362	ALA
1	A	347	GLN
1	A	344	PRO
1	A	349	GLY
1	A	230	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	291/291 (100%)	246 (84%)	45 (16%)	<b>2</b> <b>8</b>

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LYS
1	A	16	SER
1	A	27	LYS
1	A	42	ARG
1	A	44	GLN
1	A	59	ARG
1	A	61	LEU
1	A	69	VAL
1	A	70	ASN
1	A	83	LEU
1	A	91	ARG
1	A	98	LYS
1	A	100	LYS
1	A	106	ILE
1	A	107	LYS
1	A	109	ASP
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	124	THR

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Mol	Chain	Res	Type
1	A	146	LYS
1	A	152	LYS
1	A	165	GLU
1	A	169	VAL
1	A	193	ASP
1	A	207	LYS
1	A	214	LYS
1	A	216	LEU
1	A	221	ILE
1	A	240	THR
1	A	247	GLU
1	A	267	ILE
1	A	270	LEU
1	A	271	SER
1	A	280	SER
1	A	292	LEU
1	A	293	LYS
1	A	295	TRP
1	A	303	ARG
1	A	308	SER
1	A	317	LYS
1	A	318	GLU
1	A	326	GLU
1	A	355	SER

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

Mol	Chain	Res	Type
1	A	70	ASN
1	A	119	ASN
1	A	178	GLN
1	A	245	HIS
1	A	287	ASN
1	A	306	GLN
1	A	324	GLN
1	A	339	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	2FP	A	364	-	19,19,19	7.35	16 (84%)	21,28,28	4.56	11 (52%)

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	2FP	A	364	-	-	15/24/24/24	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	364	2FP	O2-C2	20.46	1.55	1.21
2	A	364	2FP	O5-C5	11.97	1.68	1.43
2	A	364	2FP	O1-C1	-10.08	1.33	1.43
2	A	364	2FP	O3-C3	8.67	1.59	1.42
2	A	364	2FP	C6-C5	7.79	1.62	1.51
2	A	364	2FP	P6-O63	6.71	1.71	1.50
2	A	364	2FP	P1-O11	6.30	1.70	1.50
2	A	364	2FP	P6-O62	5.14	1.73	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	364	2FP	C1-C2	-4.96	1.43	1.51
2	A	364	2FP	C5-C4	4.90	1.62	1.53
2	A	364	2FP	P1-O12	4.16	1.70	1.54
2	A	364	2FP	P1-O13	3.39	1.67	1.54
2	A	364	2FP	P6-O6	3.18	1.70	1.60
2	A	364	2FP	P1-O1	3.17	1.70	1.60
2	A	364	2FP	O4-C4	2.91	1.50	1.43
2	A	364	2FP	P6-O61	2.16	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	364	2FP	C5-C4-C3	12.33	132.28	112.05
2	A	364	2FP	O61-P6-O6	10.34	133.62	106.67
2	A	364	2FP	O4-C4-C5	-8.46	89.70	108.93
2	A	364	2FP	O4-C4-C3	-5.56	99.31	109.29
2	A	364	2FP	O5-C5-C6	4.12	119.07	109.99
2	A	364	2FP	O13-P1-O1	3.41	115.55	106.67
2	A	364	2FP	O3-C3-C4	3.14	117.19	110.38
2	A	364	2FP	O1-P1-O11	2.73	113.82	106.44
2	A	364	2FP	O61-P6-O63	-2.70	100.31	110.83
2	A	364	2FP	O13-P1-O11	-2.39	101.54	110.83
2	A	364	2FP	O62-P6-O61	-2.19	99.58	107.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	364	2FP	C6-O6-P6-O61
2	A	364	2FP	O5-C5-C6-O6
2	A	364	2FP	C4-C5-C6-O6
2	A	364	2FP	O4-C4-C5-C6
2	A	364	2FP	C3-C4-C5-C6
2	A	364	2FP	O4-C4-C5-O5
2	A	364	2FP	O2-C2-C3-O3
2	A	364	2FP	C1-O1-P1-O11
2	A	364	2FP	C1-O1-P1-O12
2	A	364	2FP	C1-O1-P1-O13
2	A	364	2FP	C3-C4-C5-O5
2	A	364	2FP	C5-C6-O6-P6
2	A	364	2FP	C6-O6-P6-O62
2	A	364	2FP	C6-O6-P6-O63

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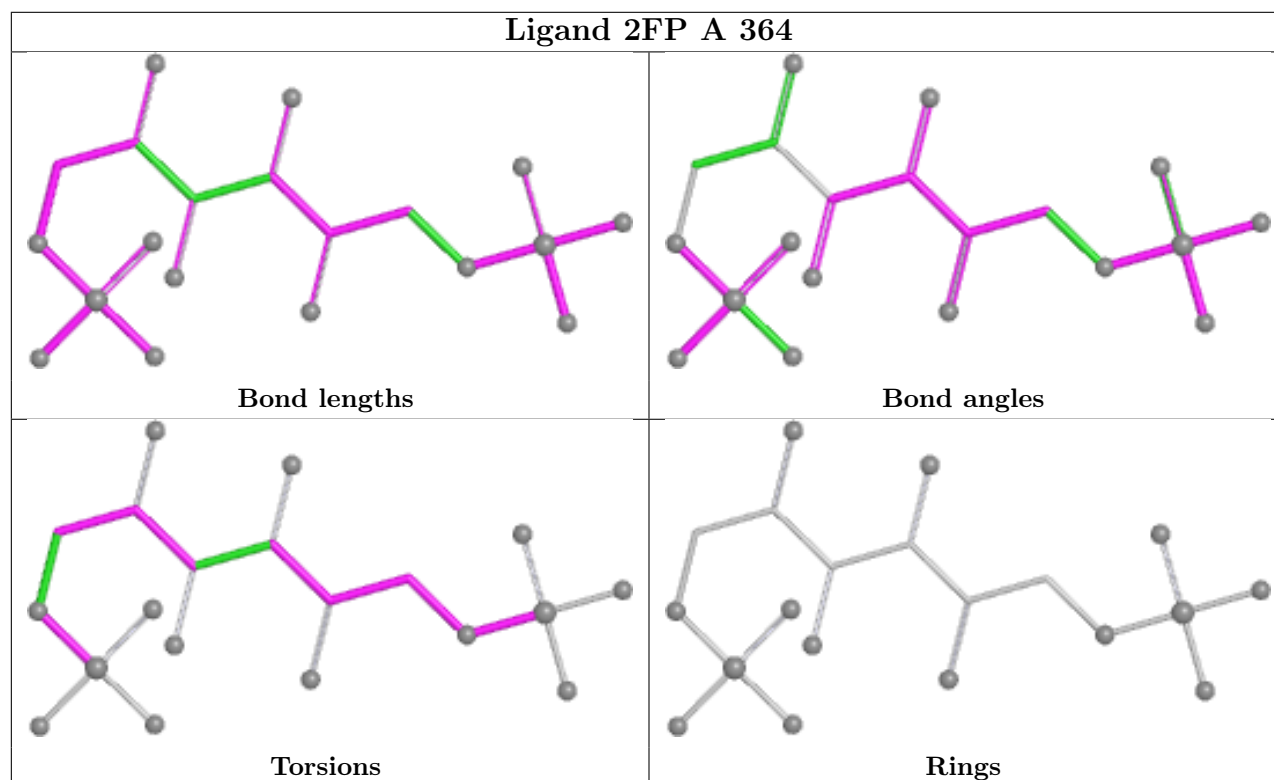
Mol	Chain	Res	Type	Atoms
2	A	364	2FP	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	364	2FP	9	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 [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.