



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:42 AM UTC

PDB ID : 3FBP / pdb_00003fbp
Title : STRUCTURE REFINEMENT OF FRUCTOSE-1,6-BISPHOSPHATASE AND ITS FRUCTOSE 2,6-BISPHOSPHATE COMPLEX AT 2.8 ANGSTROMS RESOLUTION
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Deposited on : 1990-06-07
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

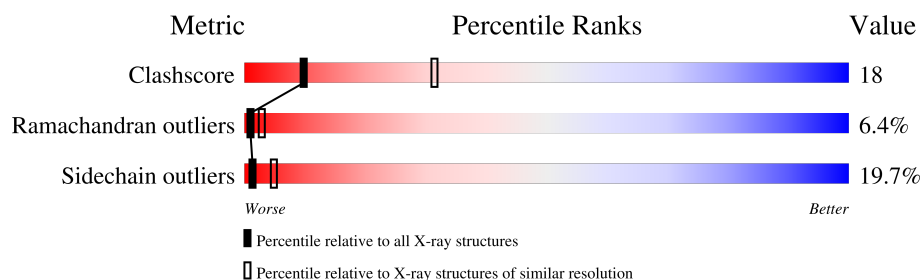
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 ≥ 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	335	
1	B	335	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5978 atoms, of which 1080 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.

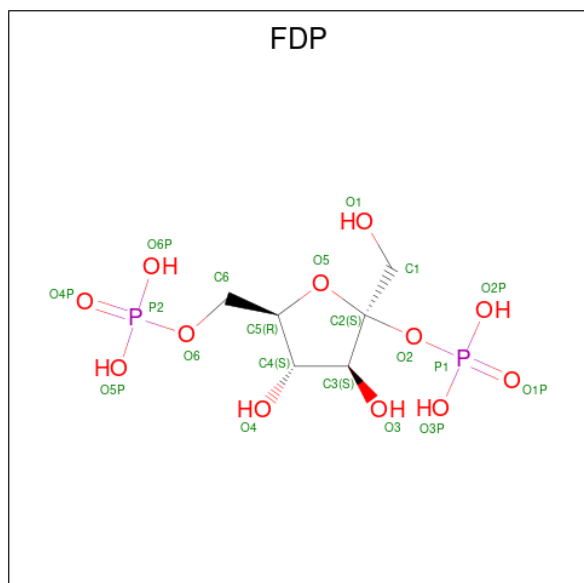
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			2967	1546	538	408	460	15			
1	B	316	Total	C	H	N	O	S	0	0	0
			2967	1546	538	408	460	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FDP) (formula: $C_6H_{14}O_{12}P_2$).



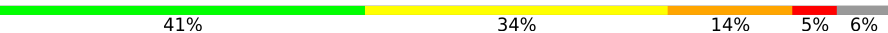
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			22	6	2	12	2		
2	B	1	Total	C	H	O	P	0	0
			22	6	2	12	2		

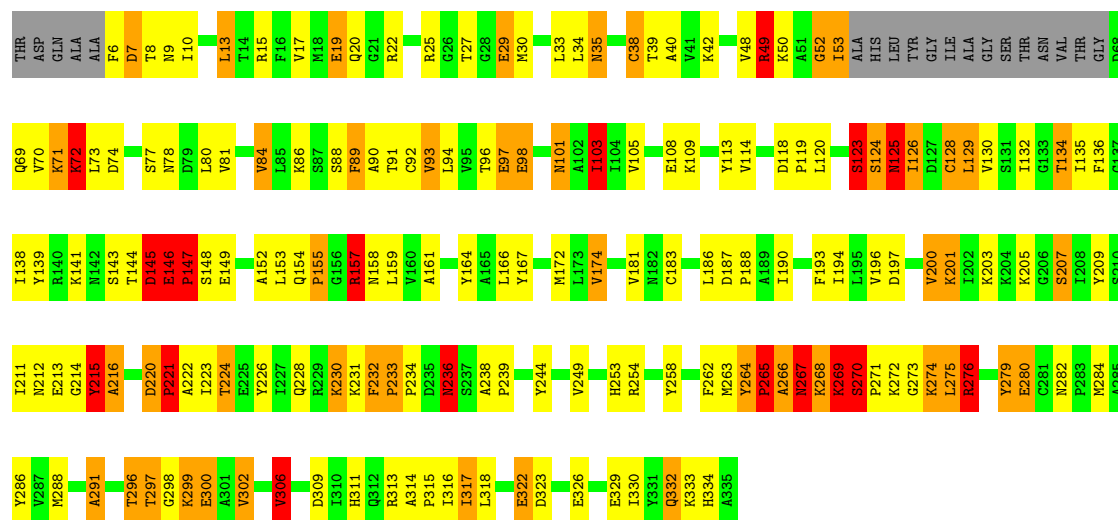
3 Residue-property plots

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.

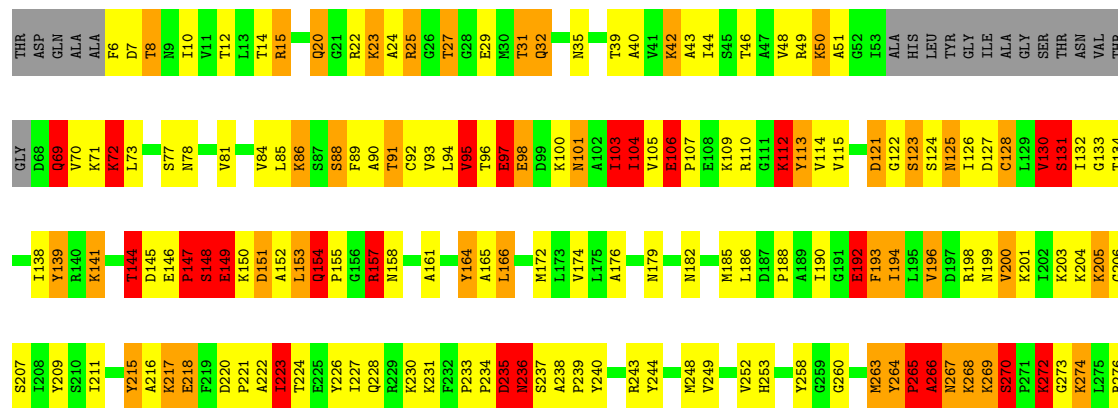
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

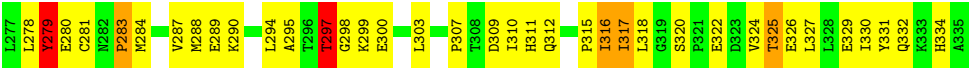
Chain A: 



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.60Å 131.60Å 68.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5978	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FDP

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	1.13	8/2469 (0.3%)	2.18	117/3337 (3.5%)
1	B	1.08	8/2469 (0.3%)	2.17	107/3337 (3.2%)
All	All	1.11	16/4938 (0.3%)	2.17	224/6674 (3.4%)

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	10
1	B	0	10
All	All	0	20

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	HIS	CD2-NE2	-7.00	1.30	1.37
1	B	334	HIS	CD2-NE2	-6.96	1.30	1.37
1	A	334	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	253	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	311	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	253	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	10	ILE	CA-CB	5.71	1.60	1.53
1	B	27	THR	CA-CB	5.62	1.60	1.52
1	A	253	HIS	CG-ND1	-5.55	1.32	1.38
1	B	216	ALA	N-CA	-5.42	1.39	1.46
1	A	103	ILE	CA-CB	5.40	1.61	1.54
1	A	233	PRO	CA-CB	-5.34	1.49	1.54
1	B	103	ILE	CA-CB	5.28	1.60	1.54
1	A	311	HIS	CG-ND1	-5.25	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	THR	CA-CB	5.21	1.62	1.53
1	B	334	HIS	CG-ND1	-5.19	1.32	1.38

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	HIS	N-CA-C	18.14	131.13	111.36
1	B	334	HIS	CA-CB-CG	-12.96	100.84	113.80
1	A	302	VAL	N-CA-C	11.11	121.95	110.62
1	B	179	ASN	CA-CB-CG	10.59	123.19	112.60
1	B	269	LYS	N-CA-C	-10.18	87.23	107.69
1	B	266	ALA	N-CA-C	10.08	132.27	110.80
1	B	8	THR	N-CA-C	9.75	131.57	110.80
1	B	88	SER	N-CA-C	-9.61	93.78	108.67
1	B	149	GLU	N-CA-C	9.53	131.10	110.80
1	B	270	SER	N-CA-C	9.17	130.07	109.81
1	A	149	GLU	N-CA-C	9.08	124.49	110.42
1	A	9	ASN	N-CA-C	-8.78	93.29	108.56
1	B	15	ARG	N-CA-C	-8.74	101.33	111.03
1	A	269	LYS	N-CA-C	-8.68	92.32	110.80
1	A	98	GLU	N-CA-C	8.41	123.27	112.34
1	A	13	LEU	CB-CA-C	-8.40	98.02	110.96
1	B	274	LYS	N-CA-C	-8.33	101.99	112.90
1	B	125	ASN	CA-CB-CG	8.29	120.89	112.60
1	B	235	ASP	CA-CB-CG	8.21	120.81	112.60
1	A	215	TYR	CA-CB-CG	8.21	128.67	113.90
1	A	154	GLN	CA-C-N	8.17	128.67	119.93
1	A	154	GLN	C-N-CA	8.17	128.67	119.93
1	A	49	ARG	CA-CB-CG	8.10	130.29	114.10
1	A	266	ALA	N-CA-C	8.00	127.85	110.80
1	B	281	CYS	N-CA-C	7.95	120.94	111.33
1	B	25	ARG	CA-CB-CG	7.89	129.88	114.10
1	B	69	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	B	151	ASP	N-CA-C	-7.80	102.47	110.97
1	B	98	GLU	N-CA-C	7.77	120.44	111.11
1	A	268	LYS	O-C-N	7.72	132.01	123.13
1	A	268	LYS	CA-C-O	7.67	129.03	120.43
1	A	72	LYS	N-CA-C	7.64	127.08	110.80
1	B	317	ILE	N-CA-C	-7.58	97.49	108.11
1	A	146	GLU	CA-C-N	7.50	129.21	119.84
1	A	146	GLU	C-N-CA	7.50	129.21	119.84
1	A	88	SER	N-CA-C	-7.49	97.38	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	O-C-N	7.46	131.83	123.40
1	B	6	PHE	CA-CB-CG	7.42	121.22	113.80
1	A	174	VAL	N-CA-C	-7.27	97.97	108.36
1	B	113	TYR	N-CA-C	7.22	121.44	109.95
1	A	236	ASN	CA-CB-CG	7.22	119.82	112.60
1	B	196	VAL	CA-CB-CG2	-7.10	98.33	110.40
1	A	309	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	282	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	A	7	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	213	GLU	CA-CB-CG	-6.97	100.15	114.10
1	A	239	PRO	N-CA-C	6.97	122.20	111.11
1	A	89	PHE	N-CA-CB	-6.97	102.03	110.53
1	A	69	GLN	N-CA-C	6.96	125.63	110.80
1	B	69	GLN	CG-CD-NE2	6.95	126.82	116.40
1	A	93	VAL	N-CA-C	-6.94	98.18	108.45
1	A	274	LYS	N-CA-C	-6.93	96.04	110.80
1	B	69	GLN	CB-CG-CD	6.83	124.22	112.60
1	A	113	TYR	N-CA-C	6.82	120.79	109.95
1	B	157	ARG	CA-CB-CG	6.79	127.67	114.10
1	A	39	THR	N-CA-C	-6.78	103.97	111.36
1	A	10	ILE	CB-CA-C	6.76	119.84	111.25
1	B	7	ASP	N-CA-C	6.75	121.04	107.41
1	A	125	ASN	CA-CB-CG	6.74	119.34	112.60
1	B	297	THR	N-CA-C	-6.70	104.59	112.89
1	B	146	GLU	CA-CB-CG	6.69	127.48	114.10
1	A	35	ASN	CA-CB-CG	-6.63	105.97	112.60
1	B	272	LYS	CA-C-O	6.61	129.96	120.51
1	B	131	SER	CA-CB-OG	-6.59	97.91	111.10
1	A	332	GLN	CB-CG-CD	6.58	123.78	112.60
1	A	270	SER	N-CA-C	6.58	124.34	109.81
1	A	38	CYS	N-CA-C	6.53	119.23	111.33
1	B	101	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	B	31	THR	CA-C-O	-6.52	114.16	121.00
1	A	129	LEU	N-CA-C	6.51	120.49	111.90
1	A	20	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	A	232	PHE	CA-C-N	6.43	124.29	119.66
1	A	232	PHE	C-N-CA	6.43	124.29	119.66
1	A	297	THR	CA-CB-OG1	-6.41	99.98	109.60
1	B	228	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	216	ALA	N-CA-C	-6.39	103.44	111.11
1	A	306	VAL	N-CA-C	-6.39	100.92	107.89
1	B	179	ASN	OD1-CG-ND2	-6.39	116.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	CA-C-O	-6.36	113.99	121.05
1	A	273	GLY	N-CA-C	-6.34	104.62	111.21
1	B	278	LEU	N-CA-C	6.33	118.99	111.33
1	A	152	ALA	CA-C-N	6.31	131.43	121.72
1	A	152	ALA	C-N-CA	6.31	131.43	121.72
1	A	200	VAL	N-CA-C	6.19	118.03	109.80
1	B	325	THR	CA-CB-OG1	-6.19	100.32	109.60
1	B	70	VAL	N-CA-C	-6.18	104.31	113.39
1	B	236	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	264	TYR	CA-C-N	6.16	127.54	119.84
1	B	264	TYR	C-N-CA	6.16	127.54	119.84
1	A	145	ASP	CA-C-O	6.13	127.87	121.06
1	B	112	LYS	N-CA-C	6.13	120.60	113.18
1	B	329	GLU	CB-CG-CD	6.13	123.03	112.60
1	A	10	ILE	N-CA-CB	-6.10	103.81	111.31
1	B	86	LYS	N-CA-C	6.09	118.70	111.33
1	A	19	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	53	ILE	N-CA-C	-6.03	94.13	111.00
1	A	136	PHE	CA-C-N	6.01	125.74	121.65
1	A	136	PHE	C-N-CA	6.01	125.74	121.65
1	B	35	ASN	CA-CB-CG	-5.98	106.62	112.60
1	B	106	GLU	CA-C-N	5.98	125.45	119.24
1	B	106	GLU	C-N-CA	5.98	125.45	119.24
1	A	39	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	70	VAL	N-CA-C	5.96	116.15	110.42
1	B	205	LYS	CA-CB-CG	5.95	126.00	114.10
1	A	291	ALA	N-CA-C	-5.95	105.67	113.17
1	A	155	PRO	N-CA-C	5.94	120.94	111.26
1	B	264	TYR	CA-CB-CG	-5.94	103.21	113.90
1	B	39	THR	CA-CB-OG1	-5.93	100.70	109.60
1	B	236	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	123	SER	CA-CB-OG	5.92	122.94	111.10
1	B	121	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	272	LYS	CA-CB-CG	5.89	125.89	114.10
1	A	7	ASP	N-CA-C	-5.87	98.30	110.80
1	A	97	GLU	CA-CB-CG	5.85	125.80	114.10
1	A	238	ALA	CA-C-N	5.83	125.84	119.89
1	A	238	ALA	C-N-CA	5.83	125.84	119.89
1	B	20	GLN	N-CA-C	-5.83	105.01	111.36
1	A	13	LEU	N-CA-CB	5.80	118.38	109.91
1	A	221	PRO	N-CA-C	5.72	124.25	112.47
1	A	268	LYS	CA-C-N	5.71	132.44	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	C-N-CA	5.71	132.44	121.54
1	A	267	ASN	N-CA-C	5.67	122.89	110.80
1	B	20	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	101	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	314	ALA	CA-C-N	5.65	126.10	119.99
1	A	314	ALA	C-N-CA	5.65	126.10	119.99
1	B	194	ILE	N-CA-CB	-5.64	102.78	110.56
1	A	317	ILE	N-CA-C	-5.62	99.96	108.17
1	B	298	GLY	N-CA-C	-5.62	106.94	114.25
1	A	89	PHE	N-CA-C	-5.61	101.20	109.62
1	B	101	ASN	CB-CG-ND2	5.59	124.79	116.40
1	B	125	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	B	193	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	302	VAL	CA-C-O	-5.58	115.15	120.95
1	B	50	LYS	O-C-N	-5.56	115.64	122.20
1	A	201	LYS	CA-C-O	-5.55	114.96	121.46
1	A	276	ARG	CA-C-O	5.55	127.30	120.92
1	B	238	ALA	CA-C-N	5.54	125.54	119.89
1	B	238	ALA	C-N-CA	5.54	125.54	119.89
1	B	91	THR	N-CA-CB	-5.53	102.24	111.20
1	B	97	GLU	N-CA-C	-5.52	104.12	111.24
1	A	279	TYR	N-CA-C	5.52	120.89	113.72
1	B	235	ASP	N-CA-C	-5.51	99.06	110.80
1	B	299	LYS	N-CA-C	-5.50	99.07	110.80
1	B	196	VAL	CA-CB-CG1	5.50	119.74	110.40
1	B	223	ILE	N-CA-CB	-5.47	102.20	111.23
1	B	104	ILE	CA-CB-CG2	-5.46	101.23	110.50
1	B	263	MET	N-CA-C	5.45	118.07	108.75
1	A	268	LYS	CA-CB-CG	-5.44	103.23	114.10
1	B	43	ALA	N-CA-C	5.44	117.91	111.33
1	B	112	LYS	CA-CB-CG	5.42	124.93	114.10
1	B	125	ASN	N-CA-C	-5.42	104.56	113.50
1	A	334	HIS	N-CA-C	-5.41	102.27	108.49
1	B	134	THR	CA-CB-OG1	-5.41	101.48	109.60
1	B	126	ILE	CB-CA-C	-5.39	104.86	112.14
1	A	39	THR	CA-CB-CG2	5.38	119.65	110.50
1	B	7	ASP	CA-C-N	5.38	131.82	121.54
1	B	7	ASP	C-N-CA	5.38	131.82	121.54
1	B	270	SER	CA-C-O	-5.37	112.80	120.16
1	A	215	TYR	N-CA-C	5.36	122.22	110.80
1	A	315	PRO	CA-C-N	-5.36	114.65	122.58
1	A	315	PRO	C-N-CA	-5.36	114.65	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	151	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	159	LEU	CA-C-O	-5.32	115.91	121.55
1	A	158	ASN	CB-CG-ND2	5.32	124.37	116.40
1	A	158	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	128	CYS	CA-C-N	5.31	129.88	122.08
1	A	128	CYS	C-N-CA	5.31	129.88	122.08
1	A	265	PRO	CA-C-N	5.29	131.65	121.54
1	A	265	PRO	C-N-CA	5.29	131.65	121.54
1	A	196	VAL	N-CA-CB	-5.29	102.49	111.23
1	B	217	LYS	N-CA-C	5.28	117.72	111.33
1	B	220	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	216	ALA	N-CA-C	-5.27	99.57	110.80
1	A	89	PHE	CB-CA-C	5.26	120.01	112.12
1	B	123	SER	CA-C-O	5.26	125.82	119.61
1	A	29	GLU	N-CA-C	5.25	121.99	110.80
1	A	134	THR	CA-C-O	-5.25	114.66	120.38
1	A	233	PRO	N-CA-CB	5.25	105.95	103.22
1	B	332	GLN	N-CA-C	-5.25	105.47	111.14
1	A	276	ARG	CB-CG-CD	5.24	123.35	111.30
1	A	297	THR	CA-CB-CG2	5.22	119.38	110.50
1	A	157	ARG	N-CA-C	-5.22	106.88	113.20
1	A	143	SER	CA-C-N	5.21	131.49	121.54
1	A	143	SER	C-N-CA	5.21	131.49	121.54
1	B	51	ALA	CA-C-O	5.20	126.59	120.98
1	A	284	MET	CG-SD-CE	-5.19	89.47	100.90
1	B	300	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	207	SER	N-CA-C	5.17	121.81	110.80
1	B	154	GLN	O-C-N	-5.17	115.38	121.32
1	B	7	ASP	N-CA-CB	-5.16	100.96	110.56
1	B	23	LYS	N-CA-CB	-5.15	102.35	110.49
1	B	42	LYS	N-CA-C	-5.15	105.35	110.97
1	A	124	SER	CA-C-O	5.14	127.94	122.13
1	B	32	GLN	CA-CB-CG	5.12	124.35	114.10
1	B	31	THR	O-C-N	-5.12	116.71	122.03
1	B	149	GLU	O-C-N	-5.11	115.80	122.59
1	A	30	MET	CG-SD-CE	-5.11	89.66	100.90
1	B	148	SER	N-CA-C	5.10	121.66	110.80
1	A	101	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	B	77	SER	CB-CA-C	-5.09	102.34	110.79
1	B	95	VAL	CB-CA-C	-5.08	103.21	110.12
1	B	128	CYS	CA-C-N	5.08	129.35	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	CYS	C-N-CA	5.08	129.35	122.19
1	B	134	THR	O-C-N	-5.07	117.45	123.22
1	A	154	GLN	CA-C-O	-5.06	115.83	120.94
1	B	192	GLU	N-CA-C	5.06	116.89	109.24
1	B	199	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	220	ASP	N-CA-C	5.06	117.63	110.24
1	A	126	ILE	CB-CA-C	-5.05	104.93	111.20
1	A	269	LYS	N-CA-CB	5.05	119.03	110.49
1	A	280	GLU	N-CA-C	-5.05	105.21	112.13
1	A	118	ASP	N-CA-C	-5.05	99.45	109.10
1	A	22	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	B	22	ARG	N-CA-C	-5.04	105.78	111.28
1	A	52	GLY	CA-C-N	5.04	130.77	121.70
1	A	52	GLY	C-N-CA	5.04	130.77	121.70
1	A	8	THR	CB-CA-C	5.03	117.47	109.02
1	B	130	VAL	CA-C-N	5.02	131.14	121.54
1	B	130	VAL	C-N-CA	5.02	131.14	121.54
1	A	86	LYS	CB-CG-CD	-5.02	99.75	111.30
1	B	224	THR	CA-C-O	-5.02	115.55	120.82
1	B	23	LYS	CA-CB-CG	5.01	124.12	114.10

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLU	Peptide
1	A	193	PHE	Sidechain
1	A	209	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	262	PHE	Sidechain
1	A	264	TYR	Sidechain
1	A	270	SER	Peptide
1	A	279	TYR	Sidechain
1	A	286	TYR	Sidechain
1	A	6	PHE	Peptide
1	B	106	GLU	Peptide
1	B	139	TYR	Sidechain
1	B	164	TYR	Sidechain
1	B	209	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	244	TYR	Sidechain
1	B	270	SER	Peptide
1	B	279	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2429	538	2486	86	0
1	B	2429	538	2486	97	0
2	A	20	2	10	2	0
2	B	20	2	10	0	0
All	All	4898	1080	4992	174	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 18.

All (174) 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:141:LYS:HE3	1:A:148:SER:HA	1.45	0.96
1:A:270:SER:HA	1:A:272:LYS:HG3	1.55	0.88
1:A:188:PRO:HD2	1:B:50:LYS:HD3	1.65	0.78
1:B:223:ILE:HD13	1:B:265:PRO:HG3	1.65	0.76
1:B:94:LEU:HB2	1:B:103:ILE:HG23	1.69	0.74
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.71	0.72
1:B:176:ALA:HB2	1:B:287:VAL:HG22	1.69	0.72
1:B:96:THR:HG22	1:B:98:GLU:N	2.04	0.71
1:B:190:ILE:HD11	1:B:194:ILE:HD11	1.72	0.70
1:A:96:THR:HG23	1:A:119:PRO:HD3	1.73	0.70
1:A:329:GLU:O	1:A:332:GLN:HG2	1.92	0.70
1:B:104:ILE:HG13	1:B:149:GLU:HG3	1.73	0.70
1:A:183:CYS:HB2	1:A:197:ASP:HB3	1.75	0.68
1:A:80:LEU:O	1:A:84:VAL:HB	1.94	0.68
1:B:130:VAL:HG13	1:B:131:SER:H	1.58	0.67
1:A:91:THR:HG23	1:A:105:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HD2	1:A:223:ILE:HD12	1.79	0.65
1:B:269:LYS:O	1:B:272:LYS:HA	1.96	0.65
1:B:107:PRO:HA	1:B:110:ARG:HD2	1.79	0.65
1:B:166:LEU:HD23	1:B:249:VAL:HG12	1.80	0.63
1:A:187:ASP:HB2	1:A:194:ILE:HD12	1.79	0.63
1:B:29:GLU:HB2	1:B:113:TYR:HE1	1.63	0.63
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.80	0.62
1:A:223:ILE:HD11	1:A:265:PRO:HG2	1.82	0.62
1:A:215:TYR:HD1	1:A:216:ALA:H	1.48	0.62
1:B:40:ALA:O	1:B:44:ILE:HG13	2.00	0.61
1:B:69:GLN:HG2	1:B:72:LYS:HB2	1.83	0.61
1:A:215:TYR:HD1	1:A:216:ALA:N	1.99	0.61
1:B:81:VAL:O	1:B:85:LEU:HG	2.01	0.61
1:A:96:THR:HG22	1:A:98:GLU:H	1.65	0.60
1:A:129:LEU:HD11	1:B:172:MET:HB2	1.84	0.60
1:A:190:ILE:HD11	1:A:194:ILE:HD11	1.84	0.60
1:A:52:GLY:O	1:A:53:ILE:HG13	2.01	0.60
1:A:267:ASN:HA	1:A:272:LYS:HG2	1.82	0.60
1:A:329:GLU:HA	1:A:332:GLN:NE2	2.18	0.59
1:B:316:ILE:HD12	1:B:318:LEU:HD23	1.84	0.58
1:B:264:TYR:HD2	1:B:273:GLY:HA2	1.66	0.58
1:A:155:PRO:HD3	1:A:306:VAL:HG22	1.84	0.58
1:B:252:VAL:HG11	1:B:284:MET:SD	2.43	0.58
1:A:128:CYS:HG	1:B:258:TYR:HE2	1.53	0.57
1:B:91:THR:HG23	1:B:105:VAL:HG21	1.87	0.57
1:A:94:LEU:HD12	1:A:103:ILE:HD11	1.88	0.56
1:A:276:ARG:NH2	2:A:336:FDP:H11	2.21	0.56
1:B:264:TYR:CD2	1:B:273:GLY:HA2	2.40	0.56
1:B:288:MET:HE2	1:B:318:LEU:HD13	1.87	0.56
1:B:205:LYS:NZ	1:B:322:GLU:HB3	2.20	0.56
1:B:153:LEU:HD21	1:B:310:ILE:HG22	1.88	0.56
1:A:329:GLU:HA	1:A:332:GLN:HE21	1.70	0.55
1:A:13:LEU:CD1	1:A:38:CYS:SG	2.95	0.55
1:B:252:VAL:HG22	1:B:318:LEU:HD11	1.89	0.55
1:B:235:ASP:CG	1:B:236:ASN:H	2.15	0.55
1:A:269:LYS:O	1:A:272:LYS:HA	2.07	0.55
1:B:231:LYS:O	1:B:239:PRO:HB3	2.07	0.55
1:B:233:PRO:HG3	1:B:239:PRO:HD3	1.88	0.55
1:A:40:ALA:HA	1:A:80:LEU:HD22	1.89	0.54
1:A:145:ASP:CG	1:A:147:PRO:HA	2.32	0.54
1:A:92:CYS:HA	1:A:105:VAL:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:CYS:HA	1:B:105:VAL:HB	1.90	0.54
1:B:309:ASP:O	1:B:312:GLN:HB2	2.08	0.54
1:A:223:ILE:CD1	1:A:265:PRO:HG2	2.38	0.54
1:B:12:THR:HG22	1:B:192:GLU:HG2	1.90	0.53
1:A:181:VAL:HG21	1:A:291:ALA:HB2	1.91	0.53
1:A:71:LYS:H	1:A:71:LYS:HD2	1.73	0.53
1:A:267:ASN:OD1	1:A:268:LYS:NZ	2.39	0.52
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.08	0.52
1:B:248:MET:HE2	1:B:284:MET:HG3	1.92	0.52
1:B:89:PHE:HD2	1:B:109:LYS:HA	1.75	0.52
1:A:132:ILE:HG13	1:A:167:TYR:HB2	1.91	0.52
1:B:205:LYS:HZ1	1:B:322:GLU:HB3	1.75	0.52
1:B:186:LEU:O	1:B:188:PRO:HD3	2.10	0.52
1:B:91:THR:O	1:B:110:ARG:HA	2.11	0.51
1:A:96:THR:HG22	1:A:98:GLU:N	2.27	0.50
1:A:129:LEU:HD12	1:B:166:LEU:HD12	1.94	0.49
1:A:215:TYR:CD1	1:A:216:ALA:N	2.80	0.49
1:B:211:ILE:HD13	1:B:227:ILE:HD11	1.93	0.49
1:B:157:ARG:O	1:B:157:ARG:HG3	2.12	0.49
1:A:254:ARG:HA	1:B:128:CYS:HB2	1.95	0.49
1:B:104:ILE:HG21	1:B:149:GLU:OE2	2.11	0.49
1:A:244:TYR:HE2	1:B:243:ARG:NH1	2.11	0.48
1:A:94:LEU:HB2	1:A:103:ILE:HG13	1.95	0.48
1:A:96:THR:HG22	1:A:97:GLU:N	2.28	0.48
1:A:40:ALA:HB2	1:A:84:VAL:HG11	1.95	0.48
1:B:206:GLY:HA3	1:B:260:GLY:N	2.28	0.48
1:B:269:LYS:HD3	1:B:274:LYS:HB2	1.95	0.48
1:A:231:LYS:O	1:A:233:PRO:HD3	2.14	0.48
1:B:86:LYS:HA	1:B:91:THR:CG2	2.43	0.48
1:B:185:MET:O	1:B:193:PHE:HA	2.13	0.48
1:B:125:ASN:HB3	1:B:130:VAL:HG11	1.95	0.47
1:B:266:ALA:HB1	1:B:269:LYS:HB2	1.96	0.47
1:A:48:VAL:HG11	1:A:132:ILE:HD11	1.97	0.47
1:B:48:VAL:HG22	1:B:73:LEU:HD21	1.95	0.47
1:B:141:LYS:HE2	1:B:148:SER:HB3	1.97	0.47
1:A:268:LYS:HD3	1:A:268:LYS:HA	1.60	0.47
1:B:157:ARG:HD3	1:B:303:LEU:HD13	1.97	0.47
1:B:294:LEU:O	1:B:318:LEU:HA	2.15	0.47
1:B:233:PRO:HA	1:B:234:PRO:HD3	1.82	0.47
1:A:93:VAL:HB	1:A:114:VAL:HG22	1.96	0.47
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLN:HB2	1:B:307:PRO:HB2	1.97	0.47
1:B:203:LYS:HG2	1:B:205:LYS:O	2.15	0.47
1:A:288:MET:HE3	1:A:318:LEU:HD13	1.95	0.46
1:A:296:THR:HG22	1:A:298:GLY:H	1.80	0.46
1:B:267:ASN:HA	1:B:272:LYS:NZ	2.30	0.46
1:B:100:LYS:O	1:B:310:ILE:HD11	2.15	0.46
1:B:133:GLY:HA3	1:B:165:ALA:O	2.16	0.46
1:B:122:GLY:HA3	1:B:132:ILE:HG22	1.97	0.46
1:B:268:LYS:HA	1:B:268:LYS:HD2	1.67	0.46
1:A:29:GLU:HG2	1:A:90:ALA:HA	1.97	0.46
1:A:297:THR:HB	1:A:300:GLU:O	2.16	0.46
1:B:88:SER:O	1:B:90:ALA:N	2.49	0.46
1:B:297:THR:HG22	1:B:315:PRO:HG2	1.97	0.46
1:A:172:MET:HE1	1:A:183:CYS:HB3	1.98	0.46
1:A:120:LEU:HD23	1:A:123:SER:HB3	1.98	0.45
1:A:214:GLY:O	1:A:216:ALA:N	2.49	0.45
1:A:77:SER:O	1:A:81:VAL:HG23	2.17	0.45
1:B:110:ARG:HH12	1:B:147:PRO:HB3	1.82	0.45
1:B:95:VAL:HG22	1:B:153:LEU:HD12	1.99	0.45
1:B:279:TYR:O	1:B:283:PRO:HD2	2.17	0.45
1:A:124:SER:O	1:A:125:ASN:HB2	2.16	0.44
1:B:166:LEU:CD2	1:B:249:VAL:HG12	2.46	0.44
1:A:212:ASN:HB2	1:A:244:TYR:CZ	2.51	0.44
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.98	0.44
1:A:157:ARG:NH1	1:A:157:ARG:O	2.50	0.44
1:A:226:TYR:HB2	1:A:330:ILE:HD12	1.99	0.44
1:A:49:ARG:HD2	1:B:49:ARG:NH1	2.32	0.44
1:B:157:ARG:HB2	1:B:303:LEU:HB3	2.00	0.44
1:B:29:GLU:OE1	1:B:112:LYS:NZ	2.51	0.44
1:A:108:GLU:HG2	1:A:109:LYS:HG3	1.99	0.44
1:A:17:VAL:HG11	1:A:34:LEU:HD12	2.00	0.44
1:A:222:ALA:HB1	1:A:330:ILE:HG22	2.00	0.43
1:A:119:PRO:HA	1:A:134:THR:HG23	1.99	0.43
1:A:275:LEU:HD13	1:A:316:ILE:HG22	2.00	0.43
1:B:264:TYR:CE2	1:B:266:ALA:HB2	2.53	0.43
1:A:80:LEU:O	1:A:80:LEU:HD23	2.18	0.43
1:A:332:GLN:HG3	1:A:333:LYS:HG3	2.00	0.43
1:B:200:VAL:O	1:B:201:LYS:NZ	2.52	0.43
1:B:96:THR:HG22	1:B:98:GLU:H	1.79	0.43
1:B:218:GLU:H	1:B:218:GLU:CD	2.27	0.43
1:B:290:LYS:HD3	1:B:290:LYS:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:CYS:SG	1:B:258:TYR:HE2	2.42	0.43
1:B:164:TYR:OH	1:B:174:VAL:HG21	2.19	0.43
1:A:138:ILE:HB	1:A:161:ALA:HB3	2.01	0.43
1:A:164:TYR:CD1	1:A:249:VAL:HG13	2.54	0.43
1:B:12:THR:CG2	1:B:192:GLU:HG2	2.48	0.43
1:A:126:ILE:HG21	1:A:132:ILE:HD13	2.01	0.43
1:B:327:LEU:O	1:B:330:ILE:HB	2.19	0.43
1:B:222:ALA:HB3	1:B:331:TYR:CE1	2.54	0.42
1:B:97:GLU:CD	1:B:276:ARG:HH22	2.27	0.42
1:B:266:ALA:CB	1:B:269:LYS:HB2	2.50	0.42
1:A:71:LYS:HG2	1:A:72:LYS:H	1.85	0.41
1:B:203:LYS:HE2	1:B:205:LYS:O	2.20	0.41
1:A:216:ALA:O	1:A:220:ASP:N	2.53	0.41
1:B:294:LEU:HB3	1:B:324:VAL:HG11	2.02	0.41
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.85	0.41
1:A:264:TYR:HB3	1:A:275:LEU:HD11	2.03	0.41
1:A:323:ASP:O	1:A:326:GLU:HB3	2.21	0.41
1:B:149:GLU:H	1:B:149:GLU:CD	2.28	0.41
1:B:153:LEU:HD23	1:B:153:LEU:C	2.46	0.41
1:B:267:ASN:HA	1:B:272:LYS:HZ2	1.84	0.41
1:A:276:ARG:HH22	2:A:336:FDP:H11	1.85	0.41
1:B:272:LYS:HB3	1:B:272:LYS:HZ3	1.86	0.41
1:A:29:GLU:O	1:A:33:LEU:HB2	2.21	0.41
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.21	0.41
1:A:135:ILE:HG23	1:A:164:TYR:HB3	2.04	0.41
1:B:138:ILE:HD12	1:B:161:ALA:O	2.21	0.41
1:A:205:LYS:HG3	1:A:322:GLU:HB3	2.03	0.40
1:B:270:SER:C	1:B:272:LYS:N	2.79	0.40
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.54	0.40
1:B:141:LYS:HG2	1:B:152:ALA:HB1	2.03	0.40
1:A:187:ASP:OD2	1:B:50:LYS:NZ	2.53	0.40
1:A:226:TYR:OH	1:A:230:LYS:NZ	2.51	0.40
1:A:299:LYS:HE3	1:A:299:LYS:HA	2.02	0.40
1:A:263:MET:HB2	1:A:317:ILE:HG12	2.04	0.40
1:B:295:ALA:HA	1:B:317:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/335 (93%)	260 (83%)	33 (11%)	19 (6%)	1	3
1	B	312/335 (93%)	253 (81%)	38 (12%)	21 (7%)	1	3
All	All	624/670 (93%)	513 (82%)	71 (11%)	40 (6%)	1	3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	123	SER
1	A	125	ASN
1	A	147	PRO
1	A	207	SER
1	A	215	TYR
1	A	221	PRO
1	A	224	THR
1	A	266	ALA
1	A	267	ASN
1	A	269	LYS
1	B	8	THR
1	B	131	SER
1	B	144	THR
1	B	150	LYS
1	B	221	PRO
1	B	266	ALA
1	B	267	ASN
1	B	272	LYS
1	A	265	PRO
1	A	274	LYS
1	B	24	ALA
1	B	157	ARG
1	B	223	ILE
1	B	235	ASP

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Mol	Chain	Res	Type
1	A	49	ARG
1	A	234	PRO
1	A	236	ASN
1	A	271	PRO
1	B	130	VAL
1	B	147	PRO
1	B	148	SER
1	B	149	GLU
1	B	72	LYS
1	B	154	GLN
1	A	146	GLU
1	B	280	GLU
1	B	265	PRO
1	A	270	SER
1	B	155	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	266/278 (96%)	224 (84%)	42 (16%)	2	9
1	B	266/278 (96%)	203 (76%)	63 (24%)	1	3
All	All	532/556 (96%)	427 (80%)	105 (20%)	1	5

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	15	ARG
1	A	19	GLU
1	A	25	ARG
1	A	27	THR
1	A	35	ASN
1	A	42	LYS
1	A	50	LYS

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Mol	Chain	Res	Type
1	A	71	LYS
1	A	73	LEU
1	A	74	ASP
1	A	84	VAL
1	A	101	ASN
1	A	103	ILE
1	A	130	VAL
1	A	144	THR
1	A	145	ASP
1	A	147	PRO
1	A	157	ARG
1	A	174	VAL
1	A	186	LEU
1	A	200	VAL
1	A	201	LYS
1	A	203	LYS
1	A	211	ILE
1	A	215	TYR
1	A	224	THR
1	A	228	GLN
1	A	230	LYS
1	A	232	PHE
1	A	236	ASN
1	A	270	SER
1	A	275	LEU
1	A	276	ARG
1	A	280	GLU
1	A	296	THR
1	A	299	LYS
1	A	300	GLU
1	A	302	VAL
1	A	306	VAL
1	A	313	ARG
1	A	322	GLU
1	B	10	ILE
1	B	14	THR
1	B	15	ARG
1	B	20	GLN
1	B	23	LYS
1	B	25	ARG
1	B	27	THR
1	B	31	THR

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	42	LYS
1	B	46	THR
1	B	69	GLN
1	B	71	LYS
1	B	72	LYS
1	B	93	VAL
1	B	95	VAL
1	B	97	GLU
1	B	101	ASN
1	B	103	ILE
1	B	104	ILE
1	B	106	GLU
1	B	112	LYS
1	B	115	VAL
1	B	121	ASP
1	B	123	SER
1	B	124	SER
1	B	127	ASP
1	B	131	SER
1	B	141	LYS
1	B	144	THR
1	B	145	ASP
1	B	147	PRO
1	B	148	SER
1	B	151	ASP
1	B	153	LEU
1	B	154	GLN
1	B	158	ASN
1	B	166	LEU
1	B	182	ASN
1	B	192	GLU
1	B	196	VAL
1	B	198	ARG
1	B	200	VAL
1	B	204	LYS
1	B	207	SER
1	B	215	TYR
1	B	217	LYS
1	B	218	GLU
1	B	230	LYS
1	B	236	ASN

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Mol	Chain	Res	Type
1	B	237	SER
1	B	263	MET
1	B	265	PRO
1	B	268	LYS
1	B	272	LYS
1	B	279	TYR
1	B	283	PRO
1	B	289	GLU
1	B	297	THR
1	B	316	ILE
1	B	320	SER
1	B	325	THR
1	B	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	FDP	B	336	-	19,20,20	0.73	0	29,32,32	1.08	2 (6%)
2	FDP	A	336	-	19,20,20	0.66	0	29,32,32	1.09	2 (6%)

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	FDP	B	336	-	-	3/12/34/34	0/1/1/1
2	FDP	A	336	-	-	6/12/34/34	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	FDP	C1-C2-C3	-2.57	107.27	114.83
2	A	336	FDP	C1-C2-C3	-2.42	107.73	114.83
2	A	336	FDP	O5P-P2-O6	2.13	112.22	106.67
2	B	336	FDP	O5P-P2-O6	2.07	112.06	106.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

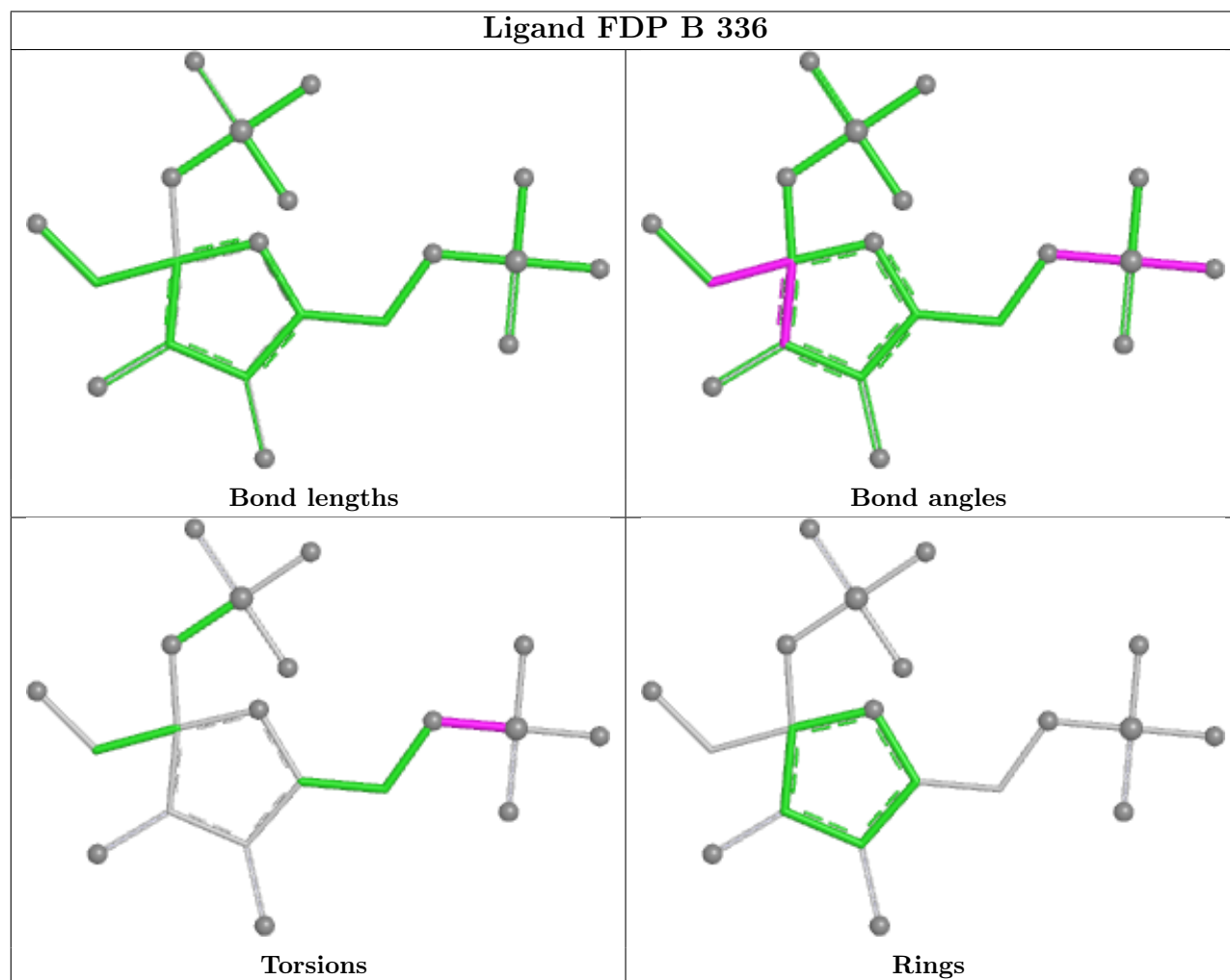
Mol	Chain	Res	Type	Atoms
2	A	336	FDP	O1-C1-C2-O5
2	A	336	FDP	C6-O6-P2-O5P
2	A	336	FDP	C6-O6-P2-O6P
2	B	336	FDP	C6-O6-P2-O4P
2	B	336	FDP	C6-O6-P2-O5P
2	B	336	FDP	C6-O6-P2-O6P
2	A	336	FDP	O1-C1-C2-O2
2	A	336	FDP	O1-C1-C2-C3
2	A	336	FDP	C6-O6-P2-O4P

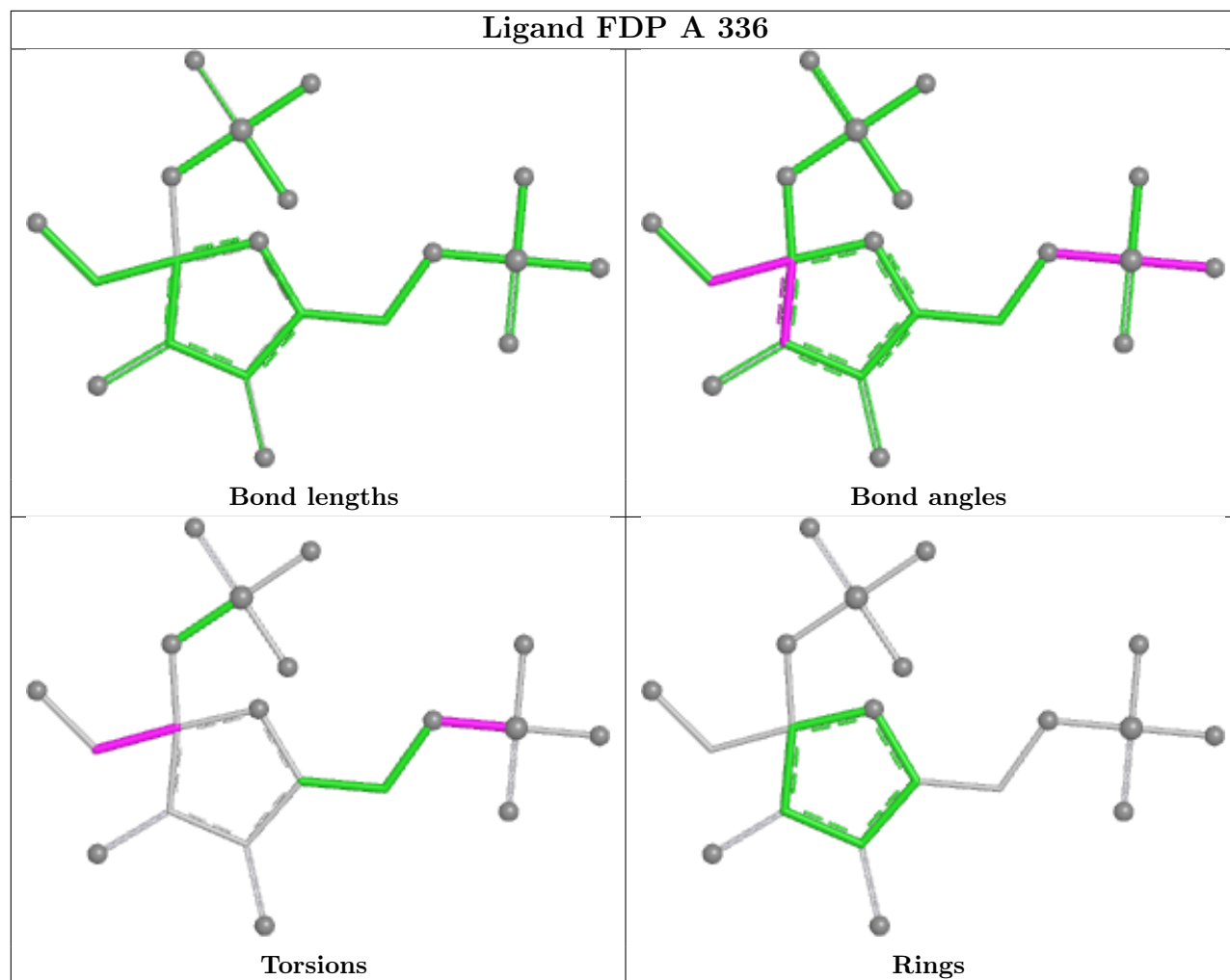
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	336	FDP	2	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.