



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:45 AM UTC

PDB ID : 2FBP / pdb\_00002fbp  
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.

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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

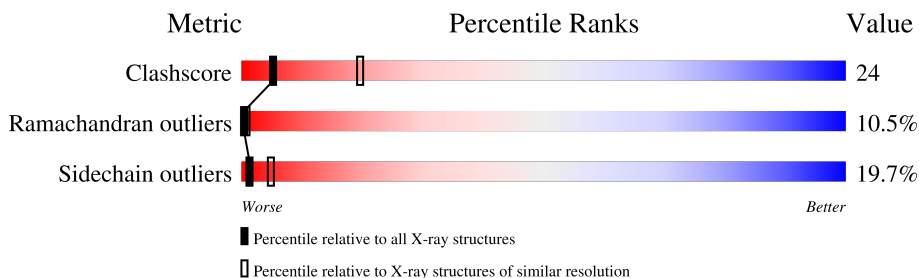
# 1 Overall quality at a glance

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  $\geq 3$ , 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	335	 28% 39% 21% 7% 5%
1	B	335	 23% 36% 23% 13% 5%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5936 atoms, of which 1076 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
			Total	C	H	N	O	S			
1	A	317	2968	1546	538	409	460	15	0	0	1
1	B	317	2968	1546	538	409	460	15	0	0	1

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

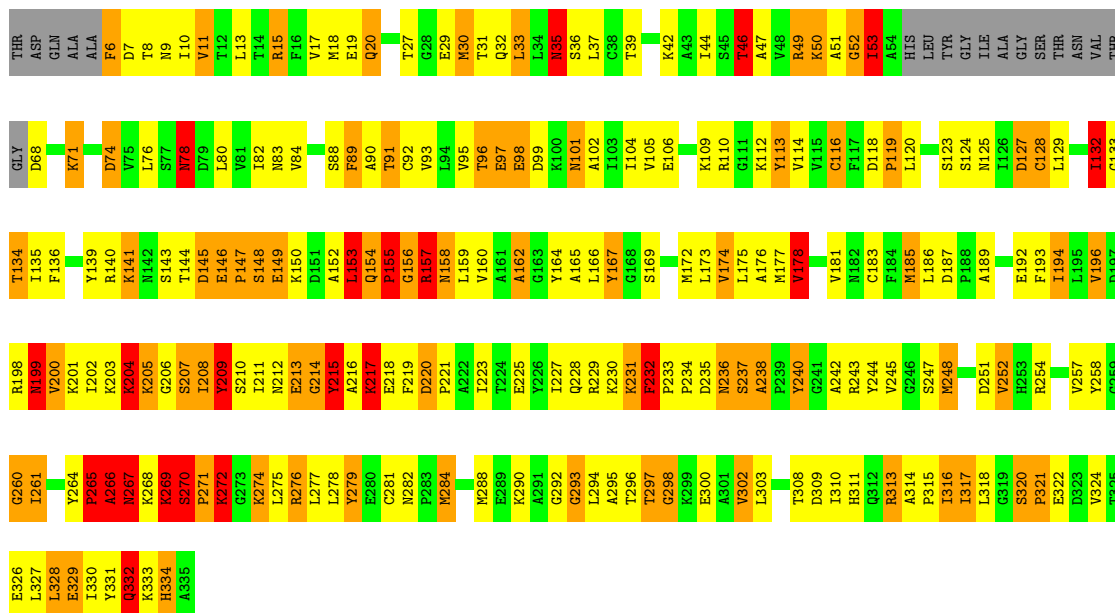
### 3 Residue-property plots

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 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.

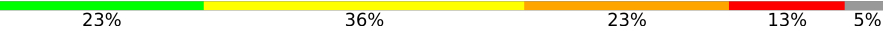
Note EDS was not executed.

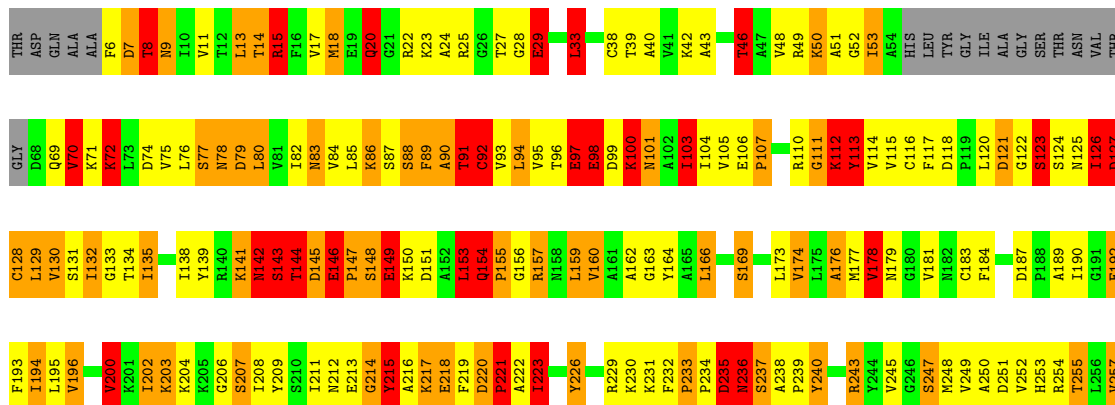
- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A:  28% 39% 21% 7% 5%



- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:  23% 36% 23% 13% 5%





## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	132.30Å 132.30Å 68.00Å 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, $R_{free}$	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	13/2470 (0.5%)	2.54	193/3339 (5.8%)
1	B	1.36	12/2470 (0.5%)	2.48	171/3339 (5.1%)
All	All	1.37	25/4940 (0.5%)	2.51	364/6678 (5.5%)

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	14
1	B	0	11
All	All	0	25

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	ASN	CA-CB	-7.29	1.42	1.53
1	B	124	SER	CA-CB	7.08	1.58	1.53
1	A	53	ILE	C-N	-6.80	1.23	1.33
1	A	82	ILE	CA-CB	-6.56	1.46	1.54
1	B	334	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	53	ILE	C-N	-6.41	1.24	1.33
1	A	274	LYS	CA-CB	6.39	1.63	1.53
1	A	334	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	248	MET	CA-CB	-6.34	1.43	1.53
1	B	311	HIS	CD2-NE2	-6.14	1.31	1.37
1	B	7	ASP	CA-CB	6.04	1.61	1.53
1	B	193	PHE	CA-CB	-5.97	1.45	1.53
1	A	311	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	10	ILE	CA-CB	5.90	1.60	1.53
1	A	36	SER	CA-CB	-5.72	1.44	1.53
1	B	253	HIS	CD2-NE2	-5.58	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	THR	CA-CB	5.58	1.62	1.53
1	A	74	ASP	CA-CB	-5.52	1.44	1.53
1	B	83	ASN	CA-C	-5.40	1.45	1.52
1	A	37	LEU	CA-CB	-5.35	1.45	1.53
1	B	103	ILE	CA-CB	5.31	1.60	1.54
1	B	200	VAL	CA-CB	5.27	1.59	1.54
1	B	144	THR	CA-CB	5.23	1.62	1.53
1	A	156	GLY	CA-C	5.23	1.59	1.51
1	B	121	ASP	CA-CB	5.18	1.62	1.53

All (364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	SER	N-CA-C	16.89	134.31	109.14
1	B	207	SER	N-CA-C	14.27	128.99	108.86
1	A	282	ASN	OD1-CG-ND2	-13.37	109.23	122.60
1	B	6	PHE	CA-CB-CG	11.30	125.10	113.80
1	A	269	LYS	N-CA-C	-11.18	86.99	110.80
1	B	232	PHE	CA-CB-CG	-11.16	102.64	113.80
1	B	88	SER	N-CA-C	-11.11	92.25	109.25
1	B	333	LYS	N-CA-C	-10.88	94.37	109.71
1	B	46	THR	CA-CB-OG1	-10.79	93.41	109.60
1	B	278	LEU	N-CA-C	10.79	125.71	112.54
1	A	220	ASP	CA-CB-CG	10.75	123.35	112.60
1	A	207	SER	N-CA-CB	-10.71	94.27	111.62
1	A	266	ALA	N-CA-C	10.65	133.50	110.80
1	A	89	PHE	N-CA-C	-10.29	92.73	108.67
1	A	10	ILE	CB-CA-C	10.25	124.27	111.25
1	A	236	ASN	CA-CB-CG	-10.21	102.39	112.60
1	B	83	ASN	N-CA-CB	10.06	124.91	110.12
1	B	70	VAL	N-CA-C	10.02	130.18	109.34
1	A	98	GLU	N-CA-C	9.93	121.87	111.14
1	A	154	GLN	N-CA-C	-9.86	88.02	109.81
1	B	9	ASN	CA-CB-CG	9.86	122.45	112.60
1	A	88	SER	N-CA-C	-9.72	94.30	109.76
1	A	220	ASP	O-C-N	-9.45	110.45	121.32
1	A	6	PHE	CA-CB-CG	9.45	123.25	113.80
1	B	97	GLU	N-CA-C	-9.40	100.72	110.97
1	A	10	ILE	N-CA-CB	-9.39	99.76	111.31
1	B	235	ASP	CA-C-N	9.35	137.54	122.67
1	B	235	ASP	C-N-CA	9.35	137.54	122.67
1	B	83	ASN	CB-CA-C	-9.35	95.27	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ASN	N-CA-C	9.10	130.17	110.80
1	B	255	THR	N-CA-C	-9.08	101.78	113.12
1	B	325	THR	CA-C-O	-9.02	111.34	120.82
1	A	274	LYS	N-CA-C	-9.02	100.87	112.23
1	B	202	ILE	N-CA-C	8.95	121.47	108.58
1	A	236	ASN	O-C-N	8.92	133.99	123.02
1	B	8	THR	N-CA-C	8.91	129.79	110.80
1	A	145	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	83	ASN	CA-CB-CG	-8.71	103.89	112.60
1	B	196	VAL	N-CA-C	-8.52	105.00	111.90
1	A	7	ASP	N-CA-C	-8.51	96.06	109.50
1	A	132	ILE	CB-CG1-CD1	-8.44	96.07	113.80
1	B	121	ASP	CA-CB-CG	8.42	121.02	112.60
1	A	329	GLU	N-CA-C	-8.41	101.02	111.11
1	B	229	ARG	CA-CB-CG	8.40	130.89	114.10
1	B	219	PHE	CA-CB-CG	8.36	122.16	113.80
1	B	53	ILE	N-CA-C	-8.33	87.67	111.00
1	B	113	TYR	N-CA-C	8.32	122.65	109.50
1	B	142	ASN	CA-CB-CG	8.31	120.91	112.60
1	A	236	ASN	N-CA-C	8.31	121.97	109.25
1	A	272	LYS	N-CA-C	-8.31	98.19	110.48
1	B	299	LYS	N-CA-C	-8.30	94.78	108.48
1	B	317	ILE	N-CA-C	-8.21	96.65	108.48
1	A	174	VAL	N-CA-C	-8.17	95.95	107.80
1	A	269	LYS	N-CA-CB	8.12	124.22	110.49
1	B	312	GLN	N-CA-C	8.07	121.55	108.63
1	A	235	ASP	N-CA-CB	8.05	122.11	109.71
1	A	207	SER	CA-C-N	8.03	134.27	122.71
1	A	207	SER	C-N-CA	8.03	134.27	122.71
1	A	269	LYS	CA-CB-CG	8.01	130.12	114.10
1	A	267	ASN	N-CA-C	7.94	127.71	110.80
1	A	220	ASP	N-CA-C	7.92	127.30	109.81
1	B	160	VAL	O-C-N	7.88	129.95	121.83
1	A	308	THR	N-CA-C	-7.87	105.65	114.62
1	B	33	LEU	N-CA-C	-7.85	102.31	111.03
1	B	239	PRO	N-CA-C	7.85	123.50	111.57
1	A	199	ASN	CA-CB-CG	-7.78	104.83	112.60
1	B	125	ASN	N-CA-C	-7.77	100.48	112.99
1	A	9	ASN	N-CA-C	-7.75	97.99	109.62
1	A	8	THR	N-CA-CB	-7.73	99.28	110.65
1	A	274	LYS	CA-CB-CG	7.73	129.56	114.10
1	A	110	ARG	N-CA-C	7.72	120.72	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLU	CA-CB-CG	7.60	129.29	114.10
1	A	155	PRO	N-CA-C	7.59	128.10	112.47
1	A	78	ASN	CA-CB-CG	7.58	120.18	112.60
1	A	264	TYR	N-CA-C	-7.56	95.01	108.55
1	A	270	SER	O-C-N	-7.56	112.63	121.32
1	B	179	ASN	N-CA-C	7.51	122.51	112.30
1	A	18	MET	CA-C-O	-7.48	113.00	120.70
1	A	207	SER	O-C-N	7.42	132.31	122.96
1	A	52	GLY	N-CA-C	-7.38	95.68	113.18
1	A	118	ASP	N-CA-C	-7.37	98.14	109.64
1	B	141	LYS	N-CA-C	7.36	120.24	111.33
1	A	206	GLY	CA-C-N	-7.35	110.60	122.36
1	A	206	GLY	C-N-CA	-7.35	110.60	122.36
1	B	277	LEU	N-CA-C	7.31	126.38	110.80
1	B	7	ASP	N-CA-C	7.31	123.01	109.56
1	A	205	LYS	N-CA-C	-7.30	97.63	108.79
1	A	252	VAL	O-C-N	-7.29	114.32	121.90
1	B	206	GLY	CA-C-N	-7.26	110.84	122.53
1	B	206	GLY	C-N-CA	-7.26	110.84	122.53
1	B	78	ASN	N-CA-C	-7.26	103.36	111.28
1	B	46	THR	CA-CB-CG2	7.25	122.82	110.50
1	B	135	ILE	CA-CB-CG2	-7.19	98.27	110.50
1	B	239	PRO	O-C-N	-7.19	114.37	123.14
1	A	141	LYS	CG-CD-CE	-7.17	94.80	111.30
1	B	299	LYS	CA-C-O	-7.17	114.59	119.68
1	A	282	ASN	CB-CG-ND2	7.16	127.14	116.40
1	B	39	THR	CA-CB-OG1	-7.16	98.87	109.60
1	A	272	LYS	O-C-N	7.10	130.98	122.96
1	A	326	GLU	N-CA-C	-7.07	103.50	111.07
1	B	320	SER	CA-CB-OG	6.99	125.08	111.10
1	A	298	GLY	N-CA-C	-6.98	105.69	115.32
1	A	271	PRO	N-CA-C	-6.96	98.12	112.47
1	B	145	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	132	ILE	CA-C-O	-6.94	114.15	121.44
1	B	331	TYR	N-CA-C	6.94	119.44	111.11
1	A	96	THR	CA-C-O	-6.93	113.00	121.11
1	A	274	LYS	CB-CG-CD	6.91	127.20	111.30
1	B	271	PRO	CA-C-O	6.85	126.65	121.38
1	A	128	CYS	N-CA-C	-6.83	104.94	113.20
1	B	265	PRO	CA-C-N	6.79	134.51	121.54
1	B	265	PRO	C-N-CA	6.79	134.51	121.54
1	B	200	VAL	N-CA-C	6.79	119.21	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	GLN	OE1-CD-NE2	-6.78	115.82	122.60
1	B	22	ARG	N-CA-C	-6.78	105.16	113.50
1	A	9	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	A	52	GLY	CA-C-N	6.74	133.83	121.70
1	A	52	GLY	C-N-CA	6.74	133.83	121.70
1	B	118	ASP	N-CA-C	-6.74	96.56	108.69
1	B	190	ILE	N-CA-C	6.71	118.60	112.43
1	A	330	ILE	N-CA-C	6.71	117.46	110.62
1	A	124	SER	N-CA-C	6.61	118.50	109.11
1	A	164	TYR	CA-C-O	-6.61	114.16	121.23
1	B	282	ASN	CB-CG-ND2	6.61	126.31	116.40
1	B	267	ASN	CA-C-O	-6.60	111.08	120.51
1	A	8	THR	CB-CA-C	6.59	120.62	109.55
1	B	270	SER	N-CA-C	6.57	120.91	110.73
1	A	30	MET	CG-SD-CE	-6.57	86.45	100.90
1	A	153	LEU	CB-CA-C	-6.56	101.99	111.70
1	A	98	GLU	O-C-N	-6.56	115.01	122.09
1	A	251	ASP	CA-CB-CG	-6.55	106.05	112.60
1	B	192	GLU	N-CA-C	6.55	119.28	108.99
1	B	125	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	207	SER	N-CA-CB	-6.54	100.39	111.31
1	A	225	GLU	N-CA-C	-6.54	103.84	110.97
1	A	46	THR	CA-CB-OG1	-6.53	99.81	109.60
1	A	313	ARG	N-CA-C	-6.52	99.95	110.32
1	A	266	ALA	N-CA-CB	-6.51	99.48	110.49
1	B	278	LEU	N-CA-CB	-6.51	99.58	110.39
1	A	282	ASN	CA-C-N	6.50	126.00	119.24
1	A	282	ASN	C-N-CA	6.50	126.00	119.24
1	A	247	SER	CA-CB-OG	-6.48	98.14	111.10
1	A	227	ILE	N-CA-C	-6.45	104.23	110.42
1	A	149	GLU	CB-CG-CD	6.44	123.54	112.60
1	B	221	PRO	N-CA-C	6.44	125.73	112.47
1	A	11	VAL	N-CA-C	6.43	113.09	106.21
1	B	111	GLY	O-C-N	-6.42	116.49	123.29
1	B	8	THR	O-C-N	-6.41	114.06	122.59
1	A	308	THR	CB-CA-C	6.41	117.80	109.28
1	A	134	THR	CA-C-O	-6.40	113.44	120.36
1	A	116	CYS	N-CA-C	-6.40	98.97	109.40
1	A	20	GLN	O-C-N	-6.39	115.34	122.12
1	B	92	CYS	N-CA-C	-6.39	104.18	112.68
1	A	156	GLY	O-C-N	-6.37	114.42	122.70
1	A	36	SER	N-CA-C	-6.35	104.28	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	ILE	CA-C-O	6.34	126.92	120.96
1	B	247	SER	N-CA-C	-6.33	99.51	109.50
1	A	200	VAL	N-CA-C	6.31	122.47	109.34
1	A	235	ASP	N-CA-C	-6.29	100.35	109.59
1	B	312	GLN	CA-CB-CG	6.25	126.60	114.10
1	A	213	GLU	N-CA-C	6.22	119.97	112.38
1	A	33	LEU	N-CA-C	-6.22	104.42	111.14
1	B	207	SER	CA-C-O	6.20	128.28	121.40
1	B	148	SER	O-C-N	6.20	130.83	122.59
1	A	127	ASP	CA-C-O	6.19	126.80	119.06
1	B	106	GLU	N-CA-C	6.19	118.62	110.08
1	B	98	GLU	N-CA-C	6.18	123.97	110.80
1	B	130	VAL	O-C-N	6.18	130.24	122.52
1	B	15	ARG	N-CA-C	-6.16	104.99	113.18
1	A	209	TYR	N-CA-C	-6.16	99.16	109.07
1	B	86	LYS	O-C-N	-6.14	114.43	122.59
1	B	130	VAL	N-CA-C	-6.12	103.38	110.05
1	A	97	GLU	O-C-N	6.12	128.45	122.09
1	A	192	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	74	ASP	CB-CA-C	-6.09	101.32	110.88
1	A	292	GLY	CA-C-N	6.06	129.87	121.26
1	A	292	GLY	C-N-CA	6.06	129.87	121.26
1	B	169	SER	N-CA-C	-6.06	104.00	111.33
1	A	20	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	15	ARG	CB-CG-CD	-6.05	97.38	111.30
1	A	332	GLN	CA-CB-CG	6.05	126.20	114.10
1	B	94	LEU	O-C-N	-6.04	115.55	123.16
1	A	129	LEU	N-CA-C	6.04	119.97	112.24
1	B	14	THR	N-CA-C	6.04	120.12	112.87
1	A	165	ALA	N-CA-C	-6.03	99.08	108.90
1	A	175	LEU	O-C-N	-6.02	116.14	123.30
1	A	51	ALA	N-CA-C	-5.99	100.23	109.76
1	A	309	ASP	O-C-N	-5.99	115.60	123.21
1	A	46	THR	N-CA-C	-5.99	104.13	112.45
1	B	101	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	214	GLY	N-CA-C	-5.98	99.02	113.18
1	B	123	SER	N-CA-C	5.96	123.50	110.80
1	A	158	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	B	177	MET	CB-CG-SD	-5.96	94.83	112.70
1	B	153	LEU	N-CA-C	-5.95	100.70	109.62
1	B	240	TYR	O-C-N	-5.94	115.63	122.93
1	A	185	MET	CA-CB-CG	-5.92	102.26	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	SER	N-CA-C	-5.92	98.19	110.80
1	B	282	ASN	CA-C-O	-5.92	112.06	120.16
1	B	82	ILE	CA-C-O	-5.91	113.39	120.78
1	A	215	TYR	CA-CB-CG	5.91	124.53	113.90
1	A	106	GLU	CA-CB-CG	5.89	125.88	114.10
1	B	79	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	68	ASP	CA-C-O	-5.87	110.83	120.80
1	A	99	ASP	N-CA-C	5.84	118.74	110.50
1	B	142	ASN	N-CA-C	5.83	123.22	110.80
1	B	220	ASP	CA-C-N	5.83	127.12	119.84
1	B	220	ASP	C-N-CA	5.83	127.12	119.84
1	B	282	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	202	ILE	CA-C-N	-5.82	114.52	123.14
1	A	202	ILE	C-N-CA	-5.82	114.52	123.14
1	A	238	ALA	N-CA-C	5.82	122.67	109.81
1	A	284	MET	N-CA-CB	-5.81	101.56	110.16
1	A	194	ILE	N-CA-CB	-5.81	99.06	111.37
1	B	215	TYR	N-CA-C	5.80	123.16	110.80
1	B	255	THR	CB-CA-C	5.80	119.13	109.56
1	A	215	TYR	N-CA-C	5.78	118.05	111.11
1	A	46	THR	CA-CB-CG2	5.78	120.32	110.50
1	B	101	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	212	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	208	ILE	O-C-N	-5.75	116.67	123.05
1	A	101	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	236	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	271	PRO	CA-C-O	5.71	131.00	120.60
1	A	44	ILE	N-CA-C	-5.71	104.95	110.72
1	B	187	ASP	CA-C-O	5.71	125.72	119.32
1	B	284	MET	CG-SD-CE	5.70	113.45	100.90
1	A	9	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	7	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	39	THR	N-CA-C	5.68	118.20	111.33
1	B	235	ASP	O-C-N	5.68	130.14	122.59
1	A	91	THR	N-CA-CB	-5.67	101.68	111.55
1	A	101	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	160	VAL	N-CA-C	-5.66	105.07	113.39
1	B	235	ASP	CA-C-O	5.66	128.60	120.51
1	B	190	ILE	CB-CA-C	-5.65	104.75	111.65
1	A	207	SER	CA-CB-OG	5.65	122.40	111.10
1	B	154	GLN	N-CA-C	5.65	122.29	109.81
1	A	264	TYR	O-C-N	5.62	125.16	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	GLU	O-C-N	-5.62	114.86	121.32
1	A	178	VAL	N-CA-C	5.60	118.90	111.17
1	B	89	PHE	N-CA-C	-5.60	98.59	108.23
1	A	42	LYS	O-C-N	-5.60	116.20	122.03
1	B	164	TYR	N-CA-C	5.59	115.94	108.23
1	A	334	HIS	CA-CB-CG	-5.57	108.23	113.80
1	B	236	ASN	CB-CG-ND2	5.57	124.76	116.40
1	B	333	LYS	CA-CB-CG	5.57	125.24	114.10
1	A	248	MET	CA-CB-CG	-5.57	102.96	114.10
1	B	249	VAL	CB-CA-C	-5.56	104.74	112.02
1	A	211	ILE	O-C-N	-5.55	118.14	122.97
1	B	178	VAL	N-CA-CB	-5.54	102.08	111.23
1	A	29	GLU	CA-CB-CG	-5.53	103.03	114.10
1	B	277	LEU	CA-C-N	5.52	129.94	120.72
1	B	277	LEU	C-N-CA	5.52	129.94	120.72
1	A	35	ASN	CA-CB-CG	-5.51	107.08	112.60
1	A	6	PHE	CA-C-N	5.51	131.21	122.62
1	A	6	PHE	C-N-CA	5.51	131.21	122.62
1	B	159	LEU	CA-C-O	5.50	126.96	120.69
1	B	18	MET	CB-CG-SD	-5.49	96.22	112.70
1	A	15	ARG	CA-CB-CG	5.49	125.08	114.10
1	A	187	ASP	CA-C-N	5.48	125.57	119.87
1	A	187	ASP	C-N-CA	5.48	125.57	119.87
1	A	232	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	117	PHE	N-CA-C	5.47	118.33	108.48
1	B	237	SER	CA-C-O	-5.44	114.66	120.92
1	A	313	ARG	CA-CB-CG	5.44	124.98	114.10
1	A	155	PRO	N-CD-CG	5.44	111.36	103.20
1	A	196	VAL	CA-CB-CG2	-5.44	101.15	110.40
1	A	269	LYS	CB-CA-C	-5.43	99.61	110.42
1	B	134	THR	CA-CB-OG1	-5.43	101.45	109.60
1	B	13	LEU	CA-C-N	5.43	131.09	120.99
1	B	13	LEU	C-N-CA	5.43	131.09	120.99
1	B	112	LYS	N-CA-C	5.42	122.35	110.80
1	A	248	MET	CB-CG-SD	-5.41	96.46	112.70
1	A	332	GLN	CB-CG-CD	5.41	121.80	112.60
1	A	204	LYS	N-CA-C	5.39	122.28	110.80
1	B	149	GLU	N-CA-CB	-5.39	101.39	110.49
1	A	260	GLY	N-CA-C	5.38	125.94	113.18
1	B	13	LEU	CD1-CG-CD2	-5.38	98.96	110.80
1	B	20	GLN	N-CA-CB	5.38	118.58	110.30
1	B	143	SER	CA-C-N	5.37	131.80	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	SER	C-N-CA	5.37	131.80	121.54
1	B	209	TYR	O-C-N	-5.37	117.26	123.33
1	B	251	ASP	O-C-N	-5.37	116.03	122.15
1	A	162	ALA	N-CA-C	-5.36	100.77	108.60
1	B	135	ILE	CA-CB-CG1	5.36	119.51	110.40
1	B	208	ILE	N-CA-CB	-5.36	102.57	112.43
1	A	32	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	268	LYS	N-CA-C	-5.34	101.94	109.96
1	B	39	THR	OG1-CB-CG2	5.34	119.99	109.30
1	A	157	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	A	124	SER	CA-C-O	5.33	129.26	121.86
1	A	50	LYS	CA-CB-CG	5.32	124.75	114.10
1	A	97	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	302	VAL	CB-CA-C	-5.32	105.16	111.81
1	A	27	THR	N-CA-C	5.32	119.87	113.17
1	A	235	ASP	CA-C-O	5.31	126.74	120.58
1	A	265	PRO	CA-C-N	5.31	131.69	121.54
1	A	265	PRO	C-N-CA	5.31	131.69	121.54
1	A	296	THR	CA-C-N	5.31	130.43	121.14
1	A	296	THR	C-N-CA	5.31	130.43	121.14
1	A	297	THR	CA-CB-OG1	-5.31	101.64	109.60
1	B	100	LYS	O-C-N	5.31	128.21	122.11
1	B	126	ILE	CB-CA-C	-5.31	105.13	112.24
1	B	95	VAL	CA-CB-CG2	-5.29	101.40	110.40
1	B	27	THR	O-C-N	5.29	129.60	123.41
1	A	53	ILE	N-CA-C	-5.28	96.22	111.00
1	A	106	GLU	CA-C-N	5.28	125.59	119.47
1	A	106	GLU	C-N-CA	5.28	125.59	119.47
1	B	296	THR	N-CA-C	5.27	117.49	108.90
1	A	252	VAL	N-CA-CB	-5.26	103.83	110.57
1	B	80	LEU	N-CA-CB	-5.26	102.38	110.01
1	A	36	SER	CA-CB-OG	-5.25	100.60	111.10
1	B	100	LYS	N-CA-C	5.25	120.03	111.37
1	B	88	SER	O-C-N	-5.24	116.57	123.02
1	A	293	GLY	O-C-N	-5.23	118.73	123.54
1	B	72	LYS	N-CA-C	5.22	121.92	110.80
1	B	233	PRO	N-CA-C	-5.22	104.33	110.70
1	B	29	GLU	CB-CG-CD	5.21	121.46	112.60
1	B	271	PRO	N-CA-C	-5.20	104.54	113.12
1	B	220	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	216	ALA	N-CA-C	-5.18	105.12	111.75
1	B	234	PRO	N-CA-C	-5.17	101.81	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLN	N-CA-C	5.17	118.75	112.23
1	B	6	PHE	N-CA-C	-5.17	96.53	111.00
1	B	194	ILE	N-CA-CB	-5.17	102.40	111.39
1	A	229	ARG	N-CA-C	-5.17	105.83	111.82
1	A	271	PRO	O-C-N	5.16	129.60	122.64
1	A	189	ALA	N-CA-C	-5.16	106.25	112.54
1	A	160	VAL	CG1-CB-CG2	-5.15	99.47	110.80
1	B	91	THR	CA-CB-OG1	5.15	117.33	109.60
1	B	79	ASP	CA-C-O	5.14	126.22	120.82
1	B	157	ARG	CA-CB-CG	5.13	124.37	114.10
1	B	302	VAL	N-CA-C	5.13	118.25	111.17
1	B	268	LYS	CA-C-O	-5.13	113.17	120.51
1	B	148	SER	CA-C-N	5.13	131.34	121.54
1	B	148	SER	C-N-CA	5.13	131.34	121.54
1	B	272	LYS	N-CA-C	5.13	121.72	110.80
1	A	6	PHE	O-C-N	5.12	131.19	123.00
1	B	174	VAL	N-CA-C	-5.11	101.05	108.36
1	B	176	ALA	CA-C-O	5.11	125.94	120.32
1	B	212	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	17	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	A	278	LEU	N-CA-C	5.08	117.48	111.33
1	B	128	CYS	CA-C-N	5.08	131.24	121.54
1	B	128	CYS	C-N-CA	5.08	131.24	121.54
1	A	83	ASN	O-C-N	5.07	127.36	122.09
1	B	274	LYS	CA-CB-CG	5.07	124.25	114.10
1	A	173	LEU	N-CA-C	-5.07	100.16	108.41
1	B	238	ALA	CA-C-N	5.06	125.27	120.31
1	B	238	ALA	C-N-CA	5.06	125.27	120.31
1	B	166	LEU	N-CA-CB	-5.06	102.16	110.21
1	A	212	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	164	TYR	CB-CA-C	-5.06	101.21	110.62
1	A	207	SER	CA-C-O	5.06	127.17	121.51
1	A	152	ALA	CA-C-N	5.05	130.17	123.20
1	A	152	ALA	C-N-CA	5.05	130.17	123.20
1	A	217	LYS	CA-C-O	-5.04	115.21	120.55
1	B	173	LEU	N-CA-C	-5.03	100.21	108.41
1	B	229	ARG	N-CA-C	-5.02	107.16	113.28
1	A	101	ASN	CB-CG-ND2	5.02	123.92	116.40
1	B	97	GLU	CA-CB-CG	5.02	124.13	114.10
1	A	123	SER	CA-C-N	-5.00	116.09	122.79
1	A	123	SER	C-N-CA	-5.00	116.09	122.79

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	167	TYR	Sidechain
1	A	193	PHE	Sidechain
1	A	209	TYR	Sidechain
1	A	215	TYR	Sidechain
1	A	219	PHE	Sidechain
1	A	240	TYR	Sidechain
1	A	244	TYR	Sidechain
1	A	270	SER	Peptide
1	A	271	PRO	Mainchain
1	A	279	TYR	Sidechain
1	A	331	TYR	Sidechain
1	A	6	PHE	Mainchain,Sidechain
1	B	113	TYR	Sidechain
1	B	143	SER	Mainchain
1	B	146	GLU	Peptide
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	258	TYR	Sidechain
1	B	264	TYR	Sidechain
1	B	270	SER	Peptide
1	B	286	TYR	Sidechain
1	B	331	TYR	Sidechain
1	B	52	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	2430	538	2486	110	0
1	B	2430	538	2486	151	0
All	All	4860	1076	4972	240	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 24.

All (240) 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:B:252:VAL:HG11	1:B:284:MET:SD	2.10	0.91
1:A:270:SER:HA	1:A:272:LYS:HG3	1.53	0.90
1:B:115:VAL:HG12	1:B:138:ILE:HG12	1.53	0.90
1:B:277:LEU:HA	1:B:281:CYS:SG	2.13	0.89
1:B:271:PRO:HB2	1:B:313:ARG:HG2	1.57	0.85
1:A:232:PHE:HD2	1:B:218:GLU:HB3	1.44	0.82
1:A:288:MET:HG3	1:A:318:LEU:HD13	1.61	0.82
1:A:157:ARG:HB3	1:A:303:LEU:HB3	1.64	0.79
1:B:13:LEU:HD23	1:B:38:CYS:SG	2.23	0.79
1:A:316:ILE:HD13	1:A:318:LEU:HD23	1.69	0.75
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.25	0.75
1:B:29:GLU:HB3	1:B:113:TYR:HE2	1.54	0.73
1:A:267:ASN:HA	1:A:272:LYS:HD3	1.71	0.72
1:A:172:MET:HE1	1:A:185:MET:SD	2.29	0.71
1:B:162:ALA:HB3	1:B:286:TYR:HD2	1.56	0.70
1:B:265:PRO:O	1:B:272:LYS:HB3	1.91	0.70
1:A:71:LYS:HD3	1:A:74:ASP:HB2	1.73	0.70
1:B:222:ALA:HB3	1:B:331:TYR:CE1	2.27	0.69
1:A:15:ARG:O	1:A:19:GLU:HG2	1.93	0.69
1:A:78:ASN:HB2	1:A:119:PRO:HG2	1.74	0.68
1:B:267:ASN:HA	1:B:272:LYS:HE3	1.75	0.68
1:A:159:LEU:HD13	1:A:162:ALA:HB2	1.74	0.68
1:B:235:ASP:HB3	1:B:237:SER:H	1.59	0.67
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.58	0.67
1:B:141:LYS:HE2	1:B:148:SER:HA	1.76	0.67
1:A:297:THR:HB	1:A:300:GLU:H	1.60	0.66
1:B:294:LEU:HB3	1:B:324:VAL:HG11	1.75	0.66
1:A:135:ILE:HG12	1:A:284:MET:HE1	1.78	0.66
1:B:252:VAL:HG21	1:B:284:MET:CG	2.26	0.65
1:B:332:GLN:NE2	1:B:333:LYS:H	1.95	0.65
1:B:91:THR:O	1:B:110:ARG:HA	1.98	0.64
1:A:89:PHE:HA	1:A:109:LYS:O	1.96	0.64
1:B:280:GLU:O	1:B:283:PRO:HD2	1.98	0.63
1:B:207:SER:HB2	1:B:240:TYR:CE2	2.34	0.63
1:A:209:TYR:HA	1:A:261:ILE:HG23	1.81	0.63
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.81	0.63
1:A:13:LEU:O	1:A:17:VAL:HG23	1.99	0.63
1:A:230:LYS:HE2	1:A:240:TYR:CZ	2.34	0.62
1:B:292:GLY:O	1:B:321:PRO:HG3	1.99	0.62
1:B:85:LEU:HD13	1:B:115:VAL:HG21	1.79	0.62
1:A:329:GLU:O	1:A:332:GLN:HB3	2.00	0.62
1:B:269:LYS:H	1:B:269:LYS:HD3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD23	1:B:129:LEU:HD12	1.81	0.61
1:A:231:LYS:NZ	1:B:213:GLU:HB3	2.14	0.61
1:B:267:ASN:HA	1:B:272:LYS:CE	2.30	0.61
1:A:30:MET:HE3	1:A:177:MET:HE3	1.83	0.61
1:B:310:ILE:HG13	1:B:311:HIS:ND1	2.16	0.61
1:A:332:GLN:OE1	1:A:333:LYS:HB2	2.01	0.60
1:B:91:THR:HB	1:B:105:VAL:HG21	1.83	0.60
1:A:50:LYS:NZ	1:B:189:ALA:HB2	2.16	0.60
1:A:231:LYS:HE3	1:B:217:LYS:HG2	1.82	0.59
1:A:120:LEU:HD11	1:A:132:ILE:HD12	1.85	0.59
1:B:100:LYS:H	1:B:100:LYS:HD3	1.65	0.59
1:B:160:VAL:O	1:B:178:VAL:HG23	2.02	0.59
1:A:276:ARG:HG2	1:A:279:TYR:CZ	2.38	0.59
1:A:49:ARG:HH22	1:A:167:TYR:HB3	1.67	0.58
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.03	0.58
1:A:298:GLY:HA2	1:A:328:LEU:HD21	1.85	0.58
1:B:252:VAL:HG21	1:B:284:MET:SD	2.43	0.58
1:B:100:LYS:O	1:B:310:ILE:HD11	2.03	0.58
1:B:99:ASP:HA	1:B:100:LYS:HZ2	1.68	0.58
1:B:204:LYS:O	1:B:320:SER:HB2	2.04	0.58
1:B:153:LEU:HD12	1:B:278:LEU:HD11	1.85	0.57
1:B:248:MET:HE2	1:B:284:MET:HG2	1.87	0.57
1:A:205:LYS:HB2	1:A:322:GLU:HB2	1.87	0.57
1:B:20:GLN:HE21	1:B:20:GLN:N	2.03	0.57
1:A:169:SER:O	1:B:49:ARG:HG3	2.05	0.56
1:B:86:LYS:HG2	1:B:94:LEU:HD11	1.87	0.56
1:B:213:GLU:O	1:B:217:LYS:HB2	2.05	0.56
1:B:97:GLU:HA	1:B:279:TYR:CZ	2.40	0.56
1:B:163:GLY:HA2	1:B:287:VAL:HG21	1.86	0.56
1:A:52:GLY:O	1:A:53:ILE:HG13	2.05	0.56
1:B:96:THR:HG22	1:B:97:GLU:N	2.20	0.56
1:A:93:VAL:HG13	1:A:102:ALA:HB1	1.88	0.56
1:A:150:LYS:O	1:A:153:LEU:HD12	2.06	0.56
1:B:330:ILE:O	1:B:334:HIS:HB2	2.06	0.55
1:A:207:SER:HB3	1:A:240:TYR:CZ	2.41	0.55
1:B:72:LYS:O	1:B:75:VAL:HG12	2.06	0.55
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.88	0.55
1:B:92:CYS:SG	1:B:141:LYS:HB2	2.46	0.55
1:B:332:GLN:NE2	1:B:333:LYS:N	2.55	0.55
1:B:13:LEU:CD2	1:B:38:CYS:SG	2.94	0.54
1:B:327:LEU:O	1:B:330:ILE:HB	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HB2	1:B:103:ILE:HG23	1.88	0.54
1:A:50:LYS:HZ1	1:B:189:ALA:HB2	1.73	0.54
1:A:133:GLY:HA2	1:A:167:TYR:CD2	2.44	0.53
1:B:93:VAL:HG23	1:B:104:ILE:HA	1.90	0.53
1:A:146:GLU:H	1:A:147:PRO:HA	1.74	0.53
1:A:320:SER:O	1:A:324:VAL:HG23	2.08	0.53
1:A:293:GLY:HA2	1:A:321:PRO:HD3	1.90	0.53
1:B:153:LEU:CD1	1:B:278:LEU:HD11	2.38	0.53
1:B:50:LYS:HD2	1:B:53:ILE:HD12	1.90	0.52
1:B:122:GLY:HA3	1:B:132:ILE:HG22	1.92	0.52
1:A:11:VAL:HA	1:A:15:ARG:HD3	1.91	0.52
1:A:199:ASN:O	1:A:201:LYS:NZ	2.43	0.52
1:A:146:GLU:H	1:A:147:PRO:CA	2.20	0.52
1:A:276:ARG:HG2	1:A:279:TYR:OH	2.10	0.52
1:B:288:MET:HG3	1:B:318:LEU:HD13	1.91	0.52
1:A:248:MET:HE3	1:A:275:LEU:HD13	1.92	0.52
1:B:40:ALA:O	1:B:43:ALA:HB3	2.09	0.51
1:B:89:PHE:N	1:B:89:PHE:CD1	2.77	0.51
1:B:154:GLN:HA	1:B:307:PRO:HG2	1.93	0.51
1:A:95:VAL:HG13	1:A:310:ILE:HD12	1.92	0.51
1:B:131:SER:HB2	1:B:250:ALA:HB2	1.93	0.51
1:A:210:SER:HB2	1:A:254:ARG:HH22	1.74	0.51
1:B:277:LEU:O	1:B:282:ASN:N	2.44	0.50
1:A:233:PRO:HG2	1:A:237:SER:O	2.11	0.50
1:A:213:GLU:O	1:A:217:LYS:HB2	2.11	0.50
1:A:91:THR:HG23	1:A:105:VAL:HG21	1.94	0.49
1:A:92:CYS:HA	1:A:105:VAL:HB	1.93	0.49
1:B:252:VAL:HG21	1:B:284:MET:HG2	1.94	0.49
1:A:185:MET:HE1	1:B:51:ALA:O	2.12	0.49
1:A:204:LYS:HG2	1:A:322:GLU:HG3	1.94	0.49
1:A:178:VAL:O	1:A:290:LYS:NZ	2.46	0.49
1:B:252:VAL:CG1	1:B:284:MET:SD	2.95	0.49
1:B:276:ARG:HA	1:B:313:ARG:HA	1.94	0.49
1:B:74:ASP:HB3	1:B:123:SER:CB	2.42	0.49
1:B:176:ALA:HB3	1:B:287:VAL:HG22	1.93	0.48
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.13	0.48
1:A:141:LYS:HE3	1:A:148:SER:HB3	1.95	0.48
1:B:74:ASP:HB3	1:B:123:SER:HB2	1.95	0.48
1:B:33:LEU:HD11	1:B:138:ILE:HG21	1.95	0.48
1:A:31:THR:O	1:A:35:ASN:HB2	2.13	0.48
1:A:210:SER:HA	1:A:243:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLY:HA3	1:B:303:LEU:O	2.14	0.48
1:B:100:LYS:HG2	1:B:101:ASN:OD1	2.14	0.48
1:B:120:LEU:HA	1:B:133:GLY:O	2.14	0.48
1:B:174:VAL:HG22	1:B:183:CYS:SG	2.54	0.48
1:B:254:ARG:O	1:B:254:ARG:HG2	2.14	0.47
1:A:172:MET:HE2	1:B:129:LEU:HD11	1.96	0.47
1:B:92:CYS:SG	1:B:113:TYR:N	2.88	0.47
1:B:29:GLU:HB3	1:B:113:TYR:CE2	2.43	0.47
1:B:92:CYS:SG	1:B:111:GLY:O	2.62	0.47
1:B:221:PRO:HG2	1:B:331:TYR:OH	2.14	0.47
1:A:231:LYS:HZ1	1:B:213:GLU:HB3	1.80	0.47
1:A:104:ILE:HD12	1:A:149:GLU:HA	1.97	0.47
1:B:46:THR:O	1:B:49:ARG:N	2.48	0.46
1:B:99:ASP:CA	1:B:100:LYS:HZ2	2.27	0.46
1:B:294:LEU:CB	1:B:324:VAL:HG11	2.42	0.46
1:A:96:THR:HG22	1:A:97:GLU:N	2.30	0.46
1:B:13:LEU:HA	1:B:184:PHE:CE2	2.50	0.46
1:B:211:ILE:HD12	1:B:263:MET:HG3	1.97	0.46
1:A:294:LEU:HD12	1:A:321:PRO:HA	1.97	0.46
1:B:15:ARG:O	1:B:18:MET:HB3	2.16	0.46
1:A:135:ILE:HG22	1:A:136:PHE:N	2.31	0.46
1:A:230:LYS:HE2	1:A:240:TYR:CE2	2.51	0.46
1:B:267:ASN:HA	1:B:272:LYS:NZ	2.30	0.46
1:A:116:CYS:SG	1:A:153:LEU:HD22	2.57	0.45
1:B:126:ILE:O	1:B:129:LEU:N	2.49	0.45
1:B:77:SER:O	1:B:80:LEU:HB3	2.16	0.45
1:B:207:SER:HB3	1:B:260:GLY:HA2	1.98	0.45
1:B:300:GLU:HB2	1:B:305:ILE:HD11	1.99	0.45
1:A:257:VAL:HG23	1:A:258:TYR:CD2	2.51	0.45
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.75	0.45
1:B:86:LYS:CG	1:B:94:LEU:HD11	2.46	0.45
1:B:20:GLN:HE21	1:B:20:GLN:H	1.63	0.45
1:B:96:THR:HG22	1:B:98:GLU:H	1.82	0.45
1:B:235:ASP:CG	1:B:236:ASN:H	2.24	0.45
1:B:286:TYR:O	1:B:290:LYS:HG2	2.17	0.45
1:A:155:PRO:HB3	1:A:158:ASN:HB2	1.99	0.45
1:B:154:GLN:H	1:B:155:PRO:HD3	1.81	0.45
1:B:264:TYR:HE1	1:B:266:ALA:HB2	1.81	0.45
1:B:223:ILE:O	1:B:226:TYR:HB3	2.17	0.44
1:B:233:PRO:O	1:B:235:ASP:N	2.50	0.44
1:A:218:GLU:OE2	1:B:231:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:HD1	1:A:139:TYR:O	2.00	0.44
1:B:202:ILE:HG22	1:B:291:ALA:O	2.17	0.44
1:A:176:ALA:HB2	1:A:181:VAL:HG22	1.99	0.44
1:A:166:LEU:HD21	1:B:129:LEU:HB2	1.99	0.44
1:A:258:TYR:HE2	1:B:128:CYS:SG	2.40	0.44
1:B:96:THR:HG21	1:B:98:GLU:HB2	1.99	0.44
1:A:153:LEU:HD13	1:A:310:ILE:HG21	1.99	0.44
1:B:9:ASN:O	1:B:11:VAL:HG23	2.18	0.44
1:B:181:VAL:HB	1:B:200:VAL:HG13	1.99	0.43
1:A:252:VAL:HG11	1:A:284:MET:CG	2.48	0.43
1:B:88:SER:O	1:B:90:ALA:N	2.51	0.43
1:A:328:LEU:HD22	1:A:328:LEU:HA	1.60	0.43
1:A:245:VAL:HG22	1:B:245:VAL:HG22	2.00	0.43
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.52	0.43
1:A:128:CYS:HB3	1:B:258:TYR:CE2	2.54	0.43
1:B:288:MET:HE2	1:B:319:GLY:N	2.32	0.43
1:B:40:ALA:HB2	1:B:84:VAL:HG11	2.01	0.43
1:A:141:LYS:NZ	1:A:143:SER:O	2.52	0.42
1:B:214:GLY:O	1:B:216:ALA:N	2.52	0.42
1:B:116:CYS:HB3	1:B:279:TYR:HB3	2.01	0.42
1:B:126:ILE:HD13	1:B:132:ILE:CD1	2.49	0.42
1:B:301:ALA:O	1:B:305:ILE:HD12	2.20	0.42
1:A:267:ASN:HA	1:A:272:LYS:HG2	2.00	0.42
1:B:163:GLY:HA2	1:B:287:VAL:CG2	2.49	0.42
1:B:216:ALA:O	1:B:220:ASP:N	2.52	0.42
1:B:96:THR:HG22	1:B:98:GLU:N	2.34	0.42
1:A:295:ALA:O	1:A:302:VAL:HG23	2.20	0.42
1:A:317:ILE:HG21	1:A:327:LEU:HD23	2.02	0.42
1:B:20:GLN:N	1:B:20:GLN:NE2	2.67	0.42
1:A:265:PRO:HB3	1:A:317:ILE:HD11	2.01	0.42
1:A:223:ILE:HD13	1:A:327:LEU:HD21	2.01	0.42
1:A:277:LEU:HD13	1:A:314:ALA:CB	2.49	0.42
1:B:154:GLN:O	1:B:306:VAL:HG13	2.20	0.42
1:A:267:ASN:HA	1:A:272:LYS:CD	2.46	0.42
1:B:107:PRO:HA	1:B:110:ARG:HD2	2.02	0.41
1:B:294:LEU:HB2	1:B:324:VAL:HG21	2.02	0.41
1:B:112:LYS:O	1:B:141:LYS:N	2.52	0.41
1:B:149:GLU:CD	1:B:149:GLU:H	2.28	0.41
1:B:204:LYS:C	1:B:320:SER:HB2	2.44	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.76	0.41
1:A:231:LYS:HZ2	1:B:213:GLU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:NZ	1:B:101:ASN:OD1	2.45	0.41
1:A:214:GLY:O	1:A:217:LYS:N	2.53	0.41
1:B:132:ILE:HD13	1:B:132:ILE:HG21	1.70	0.41
1:A:33:LEU:C	1:A:33:LEU:HD23	2.46	0.41
1:B:48:VAL:O	1:B:51:ALA:HB2	2.20	0.41
1:A:203:LYS:O	1:A:205:LYS:N	2.53	0.41
1:A:203:LYS:NZ	1:A:258:TYR:O	2.45	0.41
1:A:231:LYS:HD2	1:B:213:GLU:O	2.21	0.41
1:A:270:SER:O	1:A:272:LYS:NZ	2.42	0.41
1:B:243:ARG:HH11	1:B:243:ARG:HD3	1.75	0.41
1:B:326:GLU:O	1:B:330:ILE:HG12	2.21	0.41
1:B:269:LYS:HD3	1:B:269:LYS:N	2.34	0.41
1:B:306:VAL:HA	1:B:307:PRO:HD2	1.81	0.41
1:A:49:ARG:NH2	1:A:167:TYR:HB3	2.35	0.41
1:A:119:PRO:HA	1:A:134:THR:HG23	2.02	0.41
1:A:153:LEU:HD13	1:A:310:ILE:CG2	2.50	0.41
1:A:215:TYR:CE1	1:A:266:ALA:HB1	2.56	0.41
1:B:149:GLU:O	1:B:151:ASP:N	2.54	0.41
1:B:255:THR:O	1:B:259:GLY:HA2	2.21	0.41
1:B:275:LEU:HA	1:B:280:GLU:OE1	2.21	0.41
1:A:258:TYR:HE2	1:B:128:CYS:HB3	1.86	0.41
1:A:209:TYR:OH	1:A:242:ALA:HB2	2.21	0.40
1:A:242:ALA:O	1:A:243:ARG:HG2	2.22	0.40
1:A:272:LYS:HB2	1:A:315:PRO:HG3	2.02	0.40
1:B:217:LYS:HA	1:B:220:ASP:OD2	2.22	0.40
1:A:275:LEU:HB3	1:A:281:CYS:SG	2.61	0.40
1:B:100:LYS:H	1:B:100:LYS:CD	2.34	0.40
1:A:46:THR:O	1:A:47:ALA:C	2.64	0.40
1:A:232:PHE:CD2	1:B:218:GLU:HB3	2.36	0.40
1:A:258:TYR:HE2	1:B:128:CYS:CB	2.34	0.40
1:B:142:ASN:O	1:B:144:THR:N	2.54	0.40
1:A:258:TYR:CZ	1:B:127:ASP:HB2	2.57	0.40
1:B:89:PHE:N	1:B:89:PHE:HD1	2.19	0.40
1:B:308:THR:N	1:B:312:GLN:OE1	2.54	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	313/335 (93%)	258 (82%)	31 (10%)	24 (8%)	1	2
1	B	313/335 (93%)	221 (71%)	50 (16%)	42 (13%)	0	0
All	All	626/670 (93%)	479 (76%)	81 (13%)	66 (10%)	0	1

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	146	GLU
1	A	155	PRO
1	A	200	VAL
1	A	204	LYS
1	A	220	ASP
1	A	237	SER
1	A	260	GLY
1	A	266	ALA
1	A	267	ASN
1	B	8	THR
1	B	24	ALA
1	B	29	GLU
1	B	70	VAL
1	B	72	LYS
1	B	123	SER
1	B	129	LEU
1	B	142	ASN
1	B	144	THR
1	B	147	PRO
1	B	149	GLU
1	B	150	LYS
1	B	178	VAL
1	B	221	PRO
1	B	265	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	266	ALA
1	B	267	ASN
1	B	272	LYS
1	B	277	LEU
1	A	90	ALA
1	A	144	THR
1	A	154	GLN
1	A	238	ALA
1	A	321	PRO
1	A	334	HIS
1	B	127	ASP
1	B	145	ASP
1	B	203	LYS
1	B	215	TYR
1	B	235	ASP
1	B	274	LYS
1	B	334	HIS
1	A	221	PRO
1	B	98	GLU
1	B	157	ARG
1	B	268	LYS
1	B	281	CYS
1	A	147	PRO
1	A	269	LYS
1	B	25	ARG
1	B	90	ALA
1	B	143	SER
1	B	154	GLN
1	B	71	LYS
1	B	107	PRO
1	B	257	VAL
1	A	214	GLY
1	B	121	ASP
1	B	146	GLU
1	A	156	GLY
1	A	234	PRO
1	A	119	PRO
1	A	265	PRO
1	B	28	GLY
1	B	155	PRO
1	B	223	ILE

### 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%)	223 (84%)	43 (16%)	2	8
1	B	266/278 (96%)	204 (77%)	62 (23%)	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	20	GLN
1	A	35	ASN
1	A	46	THR
1	A	49	ARG
1	A	71	LYS
1	A	76	LEU
1	A	78	ASN
1	A	80	LEU
1	A	84	VAL
1	A	98	GLU
1	A	101	ASN
1	A	112	LYS
1	A	125	ASN
1	A	127	ASP
1	A	132	ILE
1	A	140	ARG
1	A	145	ASP
1	A	153	LEU
1	A	155	PRO
1	A	157	ARG
1	A	178	VAL
1	A	186	LEU
1	A	194	ILE
1	A	196	VAL
1	A	198	ARG
1	A	199	ASN
1	A	208	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	217	LYS
1	A	228	GLN
1	A	231	LYS
1	A	232	PHE
1	A	236	ASN
1	A	261	ILE
1	A	269	LYS
1	A	272	LYS
1	A	274	LYS
1	A	276	ARG
1	A	313	ARG
1	A	316	ILE
1	A	317	ILE
1	A	320	SER
1	A	328	LEU
1	A	332	GLN
1	B	7	ASP
1	B	8	THR
1	B	14	THR
1	B	15	ARG
1	B	20	GLN
1	B	23	LYS
1	B	33	LEU
1	B	42	LYS
1	B	46	THR
1	B	50	LYS
1	B	69	GLN
1	B	70	VAL
1	B	76	LEU
1	B	77	SER
1	B	79	ASP
1	B	83	ASN
1	B	87	SER
1	B	91	THR
1	B	92	CYS
1	B	97	GLU
1	B	100	LYS
1	B	103	ILE
1	B	112	LYS
1	B	126	ILE
1	B	127	ASP
1	B	130	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	132	ILE
1	B	135	ILE
1	B	144	THR
1	B	147	PRO
1	B	153	LEU
1	B	159	LEU
1	B	166	LEU
1	B	169	SER
1	B	192	GLU
1	B	194	ILE
1	B	195	LEU
1	B	196	VAL
1	B	200	VAL
1	B	203	LYS
1	B	215	TYR
1	B	217	LYS
1	B	218	GLU
1	B	223	ILE
1	B	230	LYS
1	B	235	ASP
1	B	236	ASN
1	B	243	ARG
1	B	247	SER
1	B	257	VAL
1	B	269	LYS
1	B	276	ARG
1	B	279	TYR
1	B	281	CYS
1	B	282	ASN
1	B	300	GLU
1	B	305	ILE
1	B	308	THR
1	B	313	ARG
1	B	327	LEU
1	B	329	GLU
1	B	332	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	142	ASN
1	A	282	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	311	HIS
1	B	332	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.