



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2FBP
Title : STRUCTURE REFINEMENT OF FRUCTOSE-1,6-BISPHOSPHATASE AND ITS FRUCTOSE 2,6-BISPHOSPHATE COMPLEX AT 2.8 ANGSTROMS RESOLUTION
Authors : Ke, H.; Thorpe, C.M.; Seaton, B.A.; Marcus, F.; Lipscomb, W.N.
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

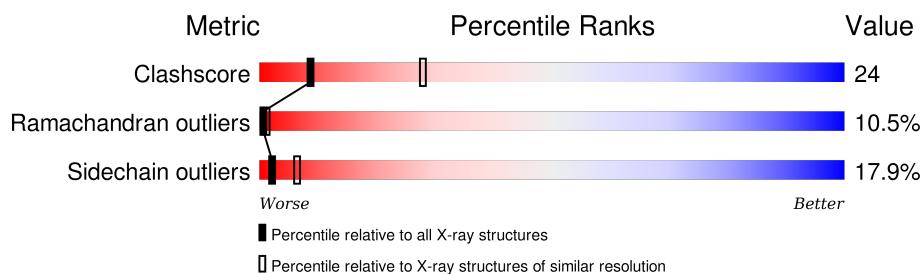
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

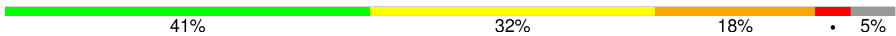
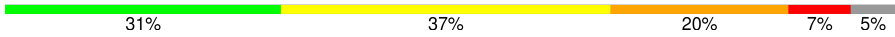
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	

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
1	A	317	Total	C	H	N	O	S	0	0	1
			2968	1546	538	409	460	15			
1	B	317	Total	C	H	N	O	S	0	0	1
			2968	1546	538	409	460	15			

There are 6 discrepancies between the modelled and reference sequences:

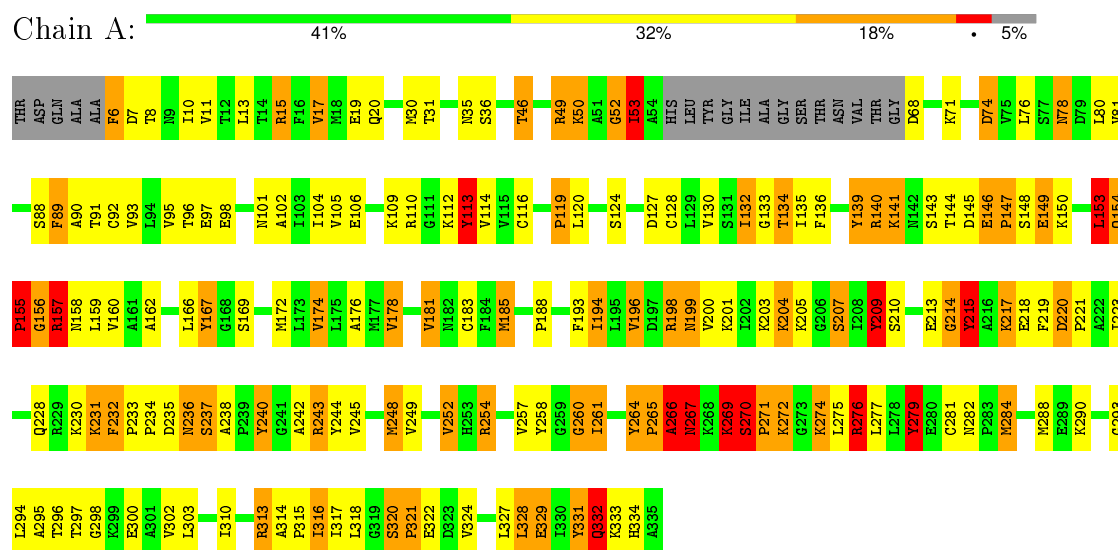
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	CONFLICT	UNP P00636
A	96	THR	SER	CONFLICT	UNP P00636
A	199	ASN	ASP	CONFLICT	UNP P00636
B	20	GLN	GLU	CONFLICT	UNP P00636
B	96	THR	SER	CONFLICT	UNP P00636
B	199	ASN	ASP	CONFLICT	UNP P00636

3 Residue-property plots

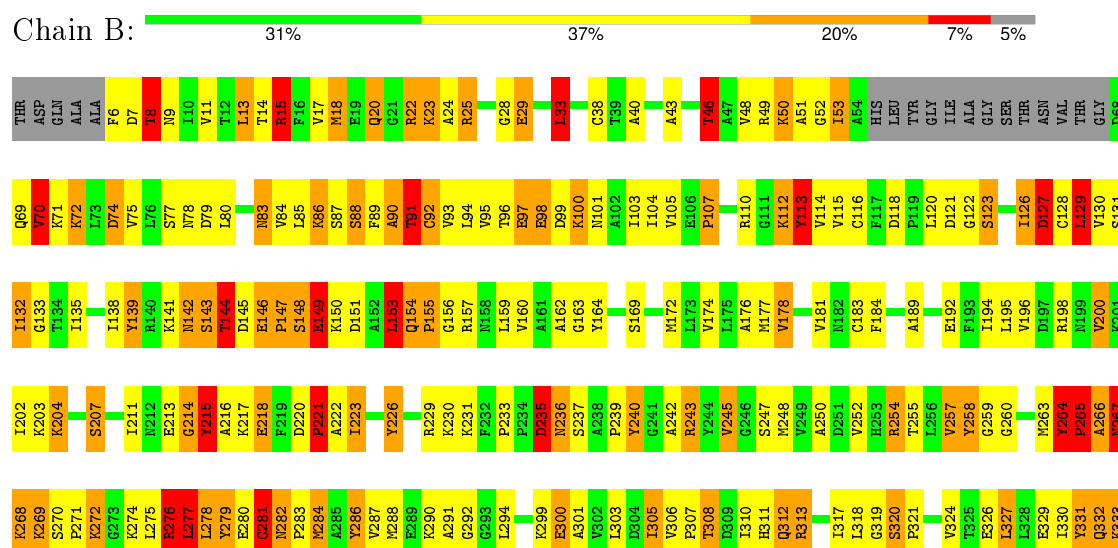
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.30 Å 132.30 Å 68.00 Å 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.	Xtriage
Total number of atoms	5936	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.08	2/2470 (0.1%)	2.07	88/3339 (2.6%)
1	B	1.03	0/2470	2.01	69/3339 (2.1%)
All	All	1.06	2/4940 (0.0%)	2.04	157/6678 (2.4%)

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	14
1	B	0	11
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	SER	CA-CB	-5.76	1.44	1.52
1	A	149	GLU	CB-CG	5.57	1.62	1.52

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	PRO	CA-C-N	-12.81	89.02	117.20
1	A	6	PHE	CA-C-N	-11.95	90.91	117.20
1	A	157	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	A	207	SER	N-CA-CB	-10.82	94.27	110.50
1	A	269	LYS	N-CA-C	-8.89	86.99	111.00
1	B	240	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	B	53	ILE	N-CA-C	-8.64	87.67	111.00
1	A	207	SER	N-CA-C	8.63	134.31	111.00
1	A	30	MET	CG-SD-CE	-8.59	86.45	100.20
1	A	154	GLN	N-CA-C	-8.51	88.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ALA	N-CA-C	8.33	133.50	111.00
1	A	276	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	284	MET	CG-SD-CE	8.28	113.45	100.20
1	B	229	ARG	CA-CB-CG	7.95	130.89	113.40
1	B	83	ASN	N-CA-CB	7.95	124.91	110.60
1	A	207	SER	CA-C-N	-7.60	100.48	117.20
1	A	269	LYS	CA-CB-CG	7.60	130.12	113.40
1	A	266	ALA	N-CA-CB	-7.58	99.48	110.10
1	A	269	LYS	N-CA-CB	7.57	124.22	110.60
1	B	83	ASN	CB-CA-C	-7.57	95.27	110.40
1	B	46	THR	CA-CB-CG2	7.44	122.82	112.40
1	B	46	THR	CA-CB-OG1	-7.42	93.41	109.00
1	A	274	LYS	CA-CB-CG	7.35	129.56	113.40
1	B	235	ASP	CA-C-N	-7.25	101.25	117.20
1	A	329	GLU	CA-CB-CG	7.22	129.29	113.40
1	B	22	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	160	VAL	CG1-CB-CG2	-7.15	99.47	110.90
1	A	139	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	A	198	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	70	VAL	N-CA-C	7.11	130.18	111.00
1	B	267	ASN	N-CA-C	7.10	130.17	111.00
1	A	236	ASN	O-C-N	7.05	133.99	122.70
1	A	52	GLY	N-CA-C	-6.97	95.68	113.10
1	B	8	THR	N-CA-C	6.96	129.79	111.00
1	B	88	SER	N-CA-C	-6.95	92.25	111.00
1	B	207	SER	CA-C-N	-6.89	102.05	117.20
1	B	164	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	B	91	THR	CA-CB-CG2	-6.88	102.77	112.40
1	A	209	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	89	PHE	N-CA-C	-6.77	92.73	111.00
1	B	207	SER	N-CA-CB	-6.74	100.39	110.50
1	B	8	THR	CA-C-N	6.74	132.02	117.20
1	B	207	SER	N-CA-C	6.66	128.99	111.00
1	A	249	VAL	CG1-CB-CG2	-6.62	100.30	110.90
1	A	153	LEU	CA-C-N	-6.58	102.72	117.20
1	B	153	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	A	196	VAL	CA-CB-CG2	-6.50	101.15	110.90
1	A	185	MET	CA-CB-CG	-6.50	102.26	113.30
1	B	130	VAL	CA-C-N	-6.42	103.08	117.20
1	A	235	ASP	N-CA-CB	6.40	122.11	110.60
1	B	74	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	132	ILE	CB-CG1-CD1	-6.37	96.07	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ILE	CB-CA-C	6.34	124.27	111.60
1	B	95	VAL	CA-CB-CG2	-6.33	101.40	110.90
1	B	235	ASP	C-N-CA	6.33	137.54	121.70
1	B	278	LEU	CA-CB-CG	6.31	129.82	115.30
1	B	135	ILE	CA-CB-CG2	-6.31	98.27	110.90
1	B	264	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	68	ASP	CA-C-N	6.25	130.95	117.20
1	B	13	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	254	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	267	ASN	N-CA-C	6.19	127.71	111.00
1	A	88	SER	N-CA-C	-6.18	94.30	111.00
1	B	139	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	B	333	LYS	N-CA-C	-6.16	94.37	111.00
1	A	155	PRO	N-CA-C	6.15	128.10	112.10
1	B	33	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	130	VAL	CG1-CB-CG2	6.12	120.70	110.90
1	B	17	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	A	248	MET	CA-CB-CG	-6.08	102.96	113.30
1	A	220	ASP	N-CA-C	6.04	127.30	111.00
1	A	17	VAL	CG1-CB-CG2	-6.03	101.25	110.90
1	A	81	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	B	299	LYS	N-CA-C	-6.01	94.78	111.00
1	A	207	SER	O-C-N	6.01	132.31	122.70
1	A	274	LYS	CB-CG-CD	6.00	127.20	111.60
1	B	312	GLN	CA-CB-CG	6.00	126.60	113.40
1	A	181	VAL	CG1-CB-CG2	-5.99	101.31	110.90
1	B	248	MET	CG-SD-CE	-5.98	90.63	100.20
1	A	243	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	A	264	TYR	N-CA-C	-5.92	95.01	111.00
1	A	313	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	215	TYR	CA-CB-CG	5.86	124.53	113.40
1	B	177	MET	CB-CG-SD	-5.86	94.83	112.40
1	B	196	VAL	CG1-CB-CG2	-5.84	101.55	110.90
1	A	332	GLN	CA-CB-CG	5.82	126.20	113.40
1	A	8	THR	N-CA-CB	-5.80	99.28	110.30
1	A	270	SER	N-CA-CB	-5.80	101.81	110.50
1	A	140	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	15	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	257	VAL	CG1-CB-CG2	-5.73	101.72	110.90
1	A	141	LYS	CG-CD-CE	-5.70	94.80	111.90
1	B	277	LEU	N-CA-C	5.70	126.38	111.00
1	A	106	GLU	CA-CB-CG	5.67	125.88	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	THR	CA-CB-CG2	5.66	120.32	112.40
1	B	214	GLY	N-CA-C	-5.63	99.02	113.10
1	A	220	ASP	O-C-N	-5.60	110.45	121.10
1	A	272	LYS	CA-C-N	-5.60	105.01	116.20
1	A	174	VAL	N-CA-C	-5.58	95.95	111.00
1	A	110	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	279	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	7	ASP	N-CA-C	-5.54	96.06	111.00
1	A	282	ASN	OD1-CG-ND2	-5.51	109.23	121.90
1	A	220	ASP	CA-C-N	5.51	132.52	117.10
1	A	296	THR	CA-C-N	-5.51	105.09	117.20
1	A	53	ILE	N-CA-C	-5.48	96.22	111.00
1	A	15	ARG	CB-CG-CD	-5.47	97.38	111.60
1	B	242	ALA	CB-CA-C	-5.46	101.92	110.10
1	B	278	LEU	N-CA-C	5.45	125.71	111.00
1	A	155	PRO	N-CD-CG	5.44	111.36	103.20
1	A	236	ASN	CA-C-N	-5.43	105.24	117.20
1	B	278	LEU	N-CA-CB	-5.41	99.58	110.40
1	B	8	THR	O-C-N	-5.40	114.06	122.70
1	A	269	LYS	CB-CA-C	-5.39	99.61	110.40
1	B	18	MET	CB-CG-SD	-5.39	96.22	112.40
1	B	333	LYS	CA-CB-CG	5.38	125.24	113.40
1	A	271	PRO	N-CA-C	-5.38	98.12	112.10
1	A	155	PRO	CA-C-N	5.38	126.95	116.20
1	B	6	PHE	N-CA-C	-5.36	96.53	111.00
1	B	118	ASP	N-CA-C	-5.35	96.56	111.00
1	B	276	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	248	MET	CB-CG-SD	-5.31	96.46	112.40
1	B	317	ILE	N-CA-C	-5.31	96.65	111.00
1	A	15	ARG	CA-CB-CG	5.31	125.08	113.40
1	A	6	PHE	O-C-N	5.31	131.19	122.70
1	A	313	ARG	CA-CB-CG	5.27	124.98	113.40
1	B	172	MET	CA-CB-CG	-5.27	104.35	113.30
1	B	299	LYS	CA-C-N	5.26	128.78	117.20
1	A	284	MET	CA-CB-CG	-5.26	104.36	113.30
1	B	7	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	254	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	235	ASP	CA-C-N	-5.24	105.67	117.20
1	B	221	PRO	N-CA-C	5.24	125.73	112.10
1	A	252	VAL	O-C-N	-5.24	114.32	122.70
1	B	240	TYR	CA-C-N	5.23	126.67	116.20
1	B	129	LEU	CB-CG-CD1	-5.21	102.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	PRO	O-C-N	-5.21	114.37	122.70
1	A	53	ILE	CG1-CB-CG2	-5.20	99.97	111.40
1	A	124	SER	CA-C-N	-5.19	105.78	117.20
1	A	156	GLY	O-C-N	-5.18	114.42	122.70
1	B	86	LYS	O-C-N	-5.17	114.43	122.70
1	B	164	TYR	CG-CD2-CE2	-5.17	117.16	121.30
1	B	164	TYR	CD1-CG-CD2	5.17	123.58	117.90
1	A	50	LYS	CA-CB-CG	5.16	124.75	113.40
1	B	320	SER	CA-CB-OG	5.14	125.08	111.20
1	A	260	GLY	N-CA-C	5.14	125.94	113.10
1	B	265	PRO	C-N-CA	5.12	134.51	121.70
1	B	149	GLU	N-CA-CB	-5.12	101.39	110.60
1	A	194	ILE	N-CA-CB	-5.10	99.06	110.80
1	B	148	SER	O-C-N	5.08	130.83	122.70
1	A	134	THR	CA-C-N	5.07	128.36	117.20
1	B	245	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	A	207	SER	C-N-CA	5.03	134.27	121.70
1	A	113	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	284	MET	N-CA-CB	-5.02	101.56	110.60
1	B	113	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	A	236	ASN	CA-CB-CG	-5.01	102.39	113.40

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	Sidechain,Mainchain
1	B	113	TYR	Sidechain
1	B	143	SER	Mainchain
1	B	146	GLU	Peptide

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Mol	Chain	Res	Type	Group
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 ⓘ

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	103	0
1	B	2430	538	2486	148	0
All	All	4860	1076	4972	232	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 (232) 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:B:115:VAL:HG12	1:B:138:ILE:HG12	1.53	0.90
1:A:270:SER:HA	1:A:272:LYS:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:294:LEU:HB3	1:B:324:VAL:HG11	1.75	0.66
1:A:297:THR:HB	1:A:300:GLU:H	1.60	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:B:114:VAL:HB	1:B:139:TYR:HB2	1.81	0.63
1:A:209:TYR:HA	1:A:261:ILE:HG23	1.81	0.63
1:A:13:LEU:O	1:A:17:VAL:HG23	1.99	0.63
1:B:292:GLY:O	1:B:321:PRO:HG3	1.99	0.62
1:A:230:LYS:HE2	1:A:240:TYR:CZ	2.34	0.62
1:B:85:LEU:HD13	1:B:115:VAL:HG21	1.79	0.62
1:B:269:LYS:H	1:B:269:LYS:HD3	1.64	0.62
1:A:329:GLU:O	1:A:332:GLN:HB3	2.00	0.62
1:A:231:LYS:NZ	1:B:213:GLU:HB3	2.14	0.61
1:A:166:LEU:HD23	1:B:129:LEU:HD12	1.81	0.61
1:B:267:ASN:HA	1:B:272:LYS:CE	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG21	1:B:284:MET:SD	2.43	0.58
1:A:298:GLY:HA2	1:A:328:LEU:HD21	1.85	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:288:MET:HE1	1:B:319:GLY:HA2	1.86	0.57
1:A:205:LYS:HB2	1:A:322:GLU:HB2	1.87	0.57
1:B:96:THR:HG22	1:B:97:GLU:N	2.20	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: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:A:231:LYS:HZ2	1:B:213:GLU:HB3	1.69	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
1:B:94:LEU:HB2	1:B:103:ILE:HG23	1.88	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:320:SER:O	1:A:324:VAL:HG23	2.08	0.53
1:A:146:GLU:H	1:A:147:PRO:HA	1.74	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:122:GLY:HA3	1:B:132:ILE:HG22	1.92	0.52
1:B:50:LYS:HD2	1:B:53:ILE:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:252:VAL:HG21	1:B:284:MET:HG2	1.94	0.49
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:A:204:LYS:HG2	1:A:322:GLU:HG3	1.94	0.49
1:B:252:VAL:CG1	1:B:284:MET:SD	2.95	0.49
1:A:178:VAL:O	1:A:290:LYS:NZ	2.46	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:B:74:ASP:HB3	1:B:123:SER:HB2	1.95	0.48
1:A:141:LYS:HE3	1:A:148:SER:HB3	1.95	0.48
1:A:270:SER:O	1:A:272:LYS:NZ	2.42	0.48
1:B:33:LEU:HD11	1:B:138:ILE:HG21	1.95	0.48
1:A:210:SER:HA	1:A:243:ARG:O	2.14	0.48
1:A:31:THR:O	1:A:35:ASN:HB2	2.13	0.48
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: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:221:PRO:HG2	1:B:331:TYR:OH	2.14	0.47
1:A:104:ILE:HD12	1:A:149:GLU:HA	1.97	0.47
1:B:294:LEU:CB	1:B:324:VAL:HG11	2.42	0.46
1:B:99:ASP:CA	1:B:100:LYS:HZ2	2.27	0.46
1:A:50:LYS:HZ3	1:B:189:ALA:HB2	1.80	0.46
1:B:46:THR:O	1:B:49:ARG:N	2.48	0.46
1:B:13:LEU:HA	1:B:184:PHE:CE2	2.50	0.46
1:A:96:THR:HG22	1:A:97:GLU:N	2.30	0.46
1:B:211:ILE:HD12	1:B:263:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:126:ILE:O	1:B:129:LEU:N	2.49	0.45
1:A:116:CYS:SG	1:A:153:LEU:HD22	2.57	0.45
1:B:207:SER:HB3	1:B:260:GLY:HA2	1.98	0.45
1:B:77:SER:O	1:B:80:LEU:HB3	2.16	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:A:172:MET:CE	1:A:185:MET:SD	3.05	0.45
1:B:86:LYS:CG	1:B:94:LEU:HD11	2.46	0.45
1:B:96:THR:HG22	1:B:98:GLU:H	1.82	0.45
1:B:20:GLN:HE21	1:B:20:GLN:H	1.63	0.45
1:B:286:TYR:O	1:B:290:LYS:HG2	2.17	0.45
1:B:154:GLN:H	1:B:155:PRO:HD3	1.81	0.45
1:A:155:PRO:HB3	1:A:158:ASN:HB2	1.99	0.45
1:B:264:TYR:HE1	1:B:266:ALA:HB2	1.81	0.45
1:B:233:PRO:O	1:B:235:ASP:N	2.50	0.44
1:B:223:ILE:O	1:B:226:TYR:HB3	2.17	0.44
1:B:288:MET:HE1	1:B:319:GLY:CA	2.47	0.44
1:A:218:GLU:OE2	1:B:231:LYS:HB3	2.17	0.44
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:B:88:SER:O	1:B:90:ALA:N	2.51	0.43
1:A:252:VAL:HG11	1:A:284:MET:CG	2.48	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:HA	1:B:85:LEU:HD23	1.52	0.43
1:A:128:CYS:HB3	1:B:258:TYR:CE2	2.54	0.43
1:B:40:ALA:HB2	1:B:84:VAL:HG11	2.01	0.43
1:B:214:GLY:O	1:B:216:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	1:A:143:SER:O	2.52	0.42
1:B:126:ILE:HD13	1:B:132:ILE:CD1	2.49	0.42
1:B:116:CYS:HB3	1:B:279:TYR:HB3	2.01	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:216:ALA:O	1:B:220:ASP:N	2.52	0.42
1:B:163:GLY:HA2	1:B:287:VAL:CG2	2.49	0.42
1:B:96:THR:HG22	1:B:98:GLU:N	2.34	0.42
1:B:20:GLN:NE2	1:B:20:GLN:N	2.67	0.42
1:B:23:LYS:O	1:B:23:LYS:NZ	2.47	0.42
1:A:317:ILE:HG21	1:A:327:LEU:HD23	2.02	0.42
1:A:295:ALA:O	1:A:302:VAL:HG23	2.20	0.42
1:A:265:PRO:HB3	1:A:317:ILE:HD11	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:223:ILE:HD13	1:A:327:LEU:HD21	2.01	0.42
1:A:267:ASN:HA	1:A:272:LYS:CD	2.46	0.42
1:B:294:LEU:HB2	1:B:324:VAL:HG21	2.02	0.41
1:B:107:PRO:HA	1:B:110:ARG:HD2	2.02	0.41
1:A:50:LYS:HZ1	1:B:189:ALA:HB2	1.84	0.41
1:B:112:LYS:O	1:B:141:LYS:N	2.52	0.41
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.76	0.41
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:B:48:VAL:O	1:B:51:ALA:HB2	2.20	0.41
1:A:231:LYS:HD2	1:B:213:GLU:O	2.21	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:B:326:GLU:O	1:B:330:ILE:HG12	2.21	0.41
1:B:243:ARG:HH11	1:B:243:ARG:HD3	1.75	0.41
1:B:277:LEU:HA	1:B:281:CYS:HG	1.84	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:119:PRO:HA	1:A:134:THR:HG23	2.02	0.41
1:B:275:LEU:HA	1:B:280:GLU:OE1	2.21	0.41
1:A:49:ARG:NH2	1:A:167:TYR:HB3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:100:LYS:CD	1:B:100:LYS:H	2.34	0.40
1:A:275:LEU:HB3	1:A:281:CYS:SG	2.61	0.40
1:A:232:PHE:CD2	1:B:218:GLU:HB3	2.36	0.40
1:B:235:ASP:CG	1:B:236:ASN:H	2.24	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 [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	313/335 (93%)	258 (82%)	31 (10%)	24 (8%)	1	2
1	B	313/335 (93%)	221 (71%)	50 (16%)	42 (13%)	0	1
All	All	626/670 (93%)	479 (76%)	81 (13%)	66 (10%)	1	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	227 (85%)	39 (15%)	4	11
1	B	266/278 (96%)	210 (79%)	56 (21%)	1	4
All	All	532/556 (96%)	437 (82%)	95 (18%)	2	6

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	46	THR
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	74	ASP
1	A	76	LEU
1	A	78	ASN
1	A	80	LEU
1	A	98	GLU
1	A	101	ASN
1	A	112	LYS
1	A	127	ASP
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	188	PRO
1	A	194	ILE
1	A	196	VAL
1	A	198	ARG
1	A	199	ASN
1	A	217	LYS
1	A	228	GLN
1	A	231	LYS
1	A	232	PHE
1	A	236	ASN
1	A	248	MET
1	A	261	ILE
1	A	264	TYR
1	A	269	LYS
1	A	274	LYS
1	A	276	ARG
1	A	313	ARG
1	A	316	ILE
1	A	320	SER
1	A	328	LEU
1	A	331	TYR
1	A	332	GLN
1	B	8	THR
1	B	14	THR
1	B	15	ARG
1	B	20	GLN
1	B	22	ARG
1	B	23	LYS

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Mol	Chain	Res	Type
1	B	25	ARG
1	B	33	LEU
1	B	46	THR
1	B	50	LYS
1	B	69	GLN
1	B	70	VAL
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	112	LYS
1	B	126	ILE
1	B	127	ASP
1	B	132	ILE
1	B	144	THR
1	B	147	PRO
1	B	153	LEU
1	B	159	LEU
1	B	169	SER
1	B	192	GLU
1	B	194	ILE
1	B	195	LEU
1	B	198	ARG
1	B	200	VAL
1	B	204	LYS
1	B	215	TYR
1	B	218	GLU
1	B	230	LYS
1	B	235	ASP
1	B	236	ASN
1	B	243	ARG
1	B	247	SER
1	B	264	TYR
1	B	268	LYS
1	B	269	LYS
1	B	276	ARG
1	B	279	TYR
1	B	281	CYS
1	B	282	ASN

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Mol	Chain	Res	Type
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
1	B	334	HIS

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

Mol	Chain	Res	Type
1	A	282	ASN
1	A	311	HIS
1	B	282	ASN
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 carbohydrates 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 ⓘ

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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