



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:19 AM UTC

PDB ID : 2HF0 / pdb_00002hf0
Title : Bifidobacterium longum bile salt hydrolase
Authors : Suresh, C.G.; Kumar, R.S.; Brannigan, J.A.
Deposited on : 2006-06-22
Resolution : 2.30 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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

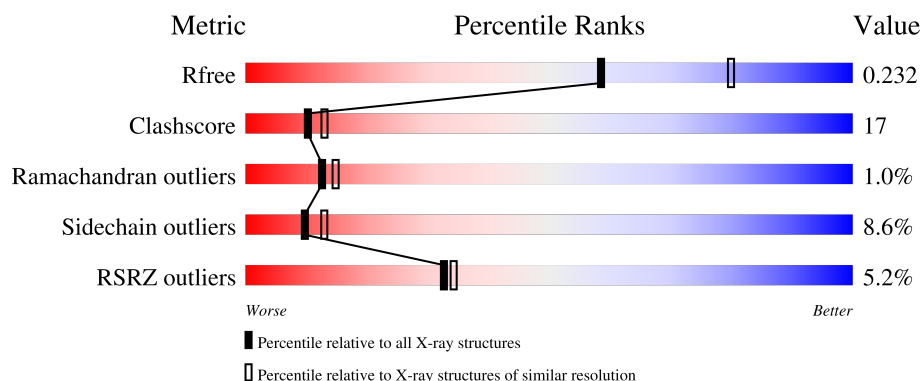
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	316	
1	B	316	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5177 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bile salt hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	15	0	0
			2463	1547	417	482	17			
1	B	316	Total	C	N	O	S	14	0	0
			2463	1547	417	482	17			

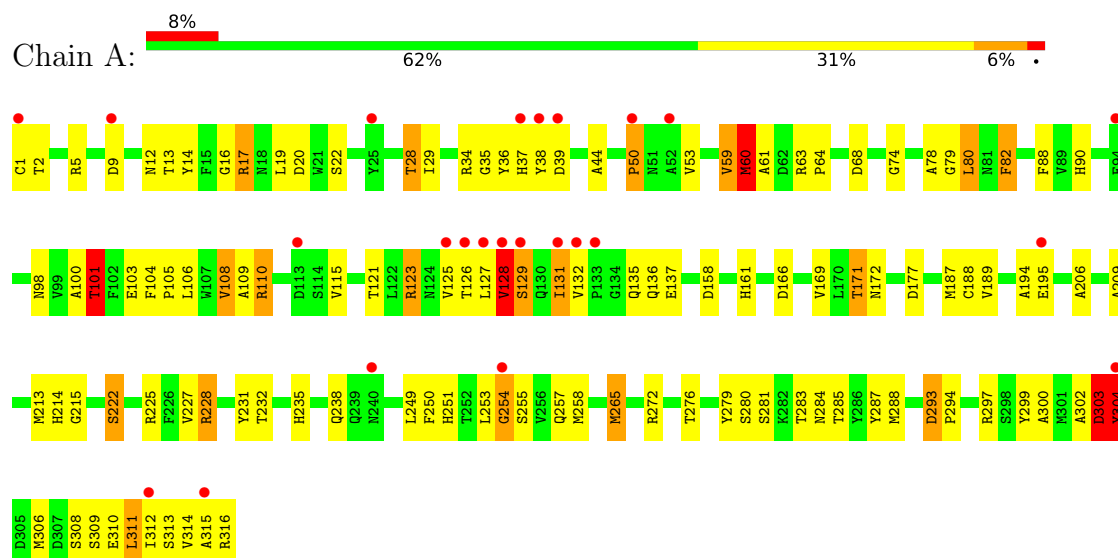
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	120	Total	O	0	0
			120	120		
2	B	131	Total	O	0	0
			131	131		

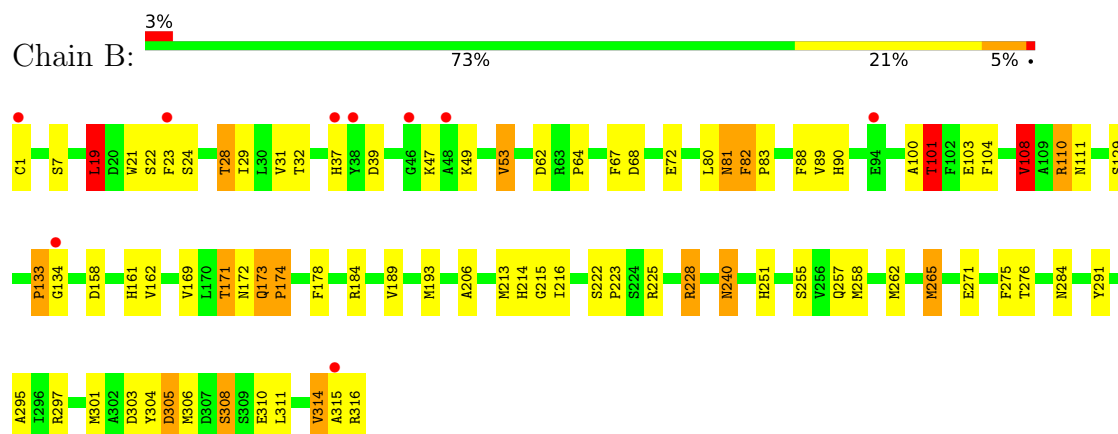
3 Residue-property plots [i](#)

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 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.

• Molecule 1: Bile salt hydrolase



• Molecule 1: Bile salt hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.98Å 123.98Å 219.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.30) 99.5 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.228 0.194 , 0.232	Depositor DCC
R_{free} test set	2364 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5177	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	2.07	33/2528 (1.3%)	1.42	22/3437 (0.6%)
1	B	1.54	18/2528 (0.7%)	1.23	7/3437 (0.2%)
All	All	1.83	51/5056 (1.0%)	1.33	29/6874 (0.4%)

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	1	1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	VAL	CA-CB	-41.18	1.06	1.54
1	A	128	VAL	CA-C	28.18	1.83	1.52
1	A	127	LEU	C-N	27.45	1.66	1.33
1	A	128	VAL	C-O	24.29	1.50	1.24
1	B	315	ALA	C-N	-12.82	1.15	1.33
1	A	127	LEU	CA-CB	-12.67	1.34	1.52
1	A	315	ALA	C-N	-10.26	1.19	1.33
1	A	127	LEU	C-O	9.29	1.35	1.23
1	B	162	VAL	CA-CB	-8.74	1.43	1.54
1	A	128	VAL	N-CA	8.24	1.56	1.46
1	A	228	ARG	CD-NE	-8.15	1.34	1.46
1	A	127	LEU	N-CA	8.12	1.57	1.46
1	B	228	ARG	CD-NE	-7.55	1.35	1.46
1	A	250	PHE	N-CA	-6.88	1.37	1.46
1	B	89	VAL	CA-CB	6.75	1.60	1.54
1	A	60	MET	CA-CB	-6.61	1.44	1.53
1	B	215	GLY	C-O	-6.60	1.15	1.24
1	A	227	VAL	C-O	-6.46	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	VAL	CB-CG2	6.36	1.73	1.52
1	A	188	CYS	C-O	-6.34	1.15	1.24
1	A	177	ASP	CG-OD2	6.28	1.37	1.25
1	A	59	VAL	CA-CB	6.26	1.61	1.54
1	B	64	PRO	CA-C	6.24	1.58	1.52
1	B	295	ALA	CA-CB	6.14	1.63	1.53
1	A	209	ALA	CA-C	6.04	1.60	1.52
1	A	265	MET	SD-CE	-6.03	1.64	1.79
1	B	184	ARG	N-CA	-6.01	1.38	1.46
1	B	276	THR	N-CA	-5.97	1.39	1.46
1	A	232	THR	C-O	-5.90	1.17	1.24
1	A	126	THR	CA-C	5.76	1.59	1.52
1	B	108	VAL	CA-CB	5.71	1.61	1.54
1	A	82	PHE	C-O	5.69	1.31	1.24
1	B	265	MET	SD-CE	-5.67	1.65	1.79
1	B	258	MET	SD-CE	-5.64	1.65	1.79
1	A	285	THR	CA-C	5.52	1.59	1.52
1	A	222	SER	C-O	-5.51	1.19	1.24
1	B	262	MET	N-CA	5.49	1.53	1.46
1	A	109	ALA	CA-C	5.45	1.60	1.52
1	A	126	THR	CA-CB	5.37	1.60	1.53
1	B	133	PRO	C-O	5.33	1.29	1.23
1	A	166	ASP	C-O	-5.33	1.17	1.24
1	A	115	VAL	CA-CB	5.32	1.61	1.54
1	B	53	VAL	CA-CB	5.26	1.62	1.54
1	A	214	HIS	C-O	-5.24	1.17	1.23
1	B	19	LEU	N-CA	-5.22	1.39	1.46
1	B	310	GLU	CA-C	5.21	1.58	1.52
1	A	187	MET	CA-C	5.20	1.59	1.52
1	A	215	GLY	C-O	-5.19	1.16	1.24
1	B	88	PHE	N-CA	5.12	1.52	1.45
1	A	280	SER	CA-C	5.09	1.58	1.52
1	A	299	TYR	CA-C	-5.07	1.48	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH2	-12.10	108.31	119.20
1	A	78	ALA	CA-C-N	-10.52	112.16	122.36
1	A	78	ALA	C-N-CA	-10.52	112.16	122.36
1	A	253	LEU	CA-C-N	-10.39	107.28	122.46
1	A	253	LEU	C-N-CA	-10.39	107.28	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	NE-CZ-NH2	-9.90	110.28	119.20
1	A	128	VAL	O-C-N	-9.15	112.69	122.67
1	A	303	ASP	CA-C-N	8.13	136.34	121.70
1	A	303	ASP	C-N-CA	8.13	136.34	121.70
1	A	228	ARG	NE-CZ-NH1	7.97	129.47	121.50
1	A	228	ARG	CD-NE-CZ	7.48	134.87	124.40
1	A	250	PHE	O-C-N	-7.28	113.85	122.15
1	B	101	THR	N-CA-CB	-7.12	99.32	109.94
1	A	137	GLU	N-CA-CB	6.72	119.84	109.97
1	A	310	GLU	N-CA-C	6.65	119.83	109.52
1	A	101	THR	OG1-CB-CG2	6.46	122.22	109.30
1	B	228	ARG	CD-NE-CZ	5.96	132.75	124.40
1	B	314	VAL	CB-CA-C	5.80	119.25	111.19
1	A	50	PRO	N-CA-C	5.80	120.18	111.14
1	A	303	ASP	O-C-N	-5.71	115.00	122.59
1	B	101	THR	CB-CA-C	5.57	119.72	110.81
1	A	293	ASP	CA-C-N	5.51	125.60	119.87
1	A	293	ASP	C-N-CA	5.51	125.60	119.87
1	A	82	PHE	CA-C-N	-5.47	114.14	119.78
1	A	82	PHE	C-N-CA	-5.47	114.14	119.78
1	A	128	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	A	304	TYR	CB-CA-C	5.12	119.83	110.10
1	B	108	VAL	N-CA-CB	5.12	116.54	110.55
1	B	108	VAL	N-CA-C	5.07	115.28	110.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	304	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	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	2463	0	2290	96	0
1	B	2463	0	2290	68	0
2	A	120	0	0	7	0
2	B	131	0	0	4	0
All	All	5177	0	4580	161	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 17.

All (161) 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:128:VAL:CA	1:A:128:VAL:C	1.83	1.49
1:A:171:THR:CG2	1:A:172:ASN:H	1.52	1.21
1:B:171:THR:CG2	1:B:172:ASN:H	1.56	1.17
1:A:171:THR:HG22	1:A:172:ASN:H	1.07	1.15
1:B:171:THR:HG22	1:B:172:ASN:H	1.24	0.98
1:A:171:THR:HG22	1:A:172:ASN:N	1.73	0.93
1:B:171:THR:HG23	1:B:172:ASN:H	1.33	0.91
1:A:171:THR:CG2	1:A:172:ASN:N	2.21	0.90
1:B:72:GLU:HB3	1:B:301:MET:HE1	1.54	0.90
1:B:171:THR:CG2	1:B:172:ASN:N	2.26	0.87
1:A:101:THR:HG21	2:A:346:HOH:O	1.75	0.86
1:B:171:THR:HG22	1:B:172:ASN:N	1.83	0.86
1:B:22:SER:HB3	1:B:265:MET:HE3	1.58	0.86
1:B:22:SER:N	1:B:265:MET:HE1	1.91	0.85
1:A:254:GLY:HA2	1:A:257:GLN:HB3	1.57	0.84
1:A:171:THR:HG23	1:A:172:ASN:H	1.42	0.83
1:A:79:GLY:C	1:A:80:LEU:HD23	2.05	0.81
1:A:35:GLY:HA3	1:A:308:SER:O	1.79	0.81
1:B:101:THR:HG21	2:B:371:HOH:O	1.80	0.81
1:A:22:SER:HB3	1:A:265:MET:CE	2.12	0.80
1:A:128:VAL:C	1:A:128:VAL:CB	2.47	0.79
1:B:214:HIS:HD2	2:B:358:HOH:O	1.65	0.79
1:B:171:THR:HG21	1:B:222:SER:O	1.82	0.79
1:A:172:ASN:HD22	1:A:225:ARG:HH22	1.34	0.76
1:A:231:TYR:O	1:A:235:HIS:HD2	1.70	0.75
1:B:72:GLU:CB	1:B:301:MET:HE1	2.20	0.71
1:A:35:GLY:CA	1:A:308:SER:O	2.38	0.71
1:B:304:TYR:HB2	1:B:306:MET:HE3	1.74	0.69
1:A:251:HIS:HD2	1:B:257:GLN:OE1	1.75	0.69
1:A:171:THR:HG23	1:A:172:ASN:N	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ALA:HB3	1:A:206:ALA:HB2	1.76	0.67
1:B:47:LYS:HB2	1:B:111:ASN:HD22	1.61	0.66
1:B:172:ASN:HD22	1:B:225:ARG:HH22	1.43	0.65
1:A:80:LEU:HD23	1:A:80:LEU:N	2.10	0.65
1:B:90:HIS:HD2	1:B:129:SER:O	1.79	0.65
1:A:123:ARG:HG2	1:A:123:ARG:NH1	2.10	0.64
1:A:110:ARG:NH1	2:A:401:HOH:O	2.31	0.64
1:B:47:LYS:H	1:B:111:ASN:ND2	1.96	0.63
1:B:240:ASN:ND2	1:B:240:ASN:H	1.96	0.63
1:A:39:ASP:CG	2:A:335:HOH:O	2.41	0.63
1:A:16:GLY:HA3	1:A:249:LEU:HD11	1.81	0.62
1:A:22:SER:CB	1:A:265:MET:CE	2.77	0.62
1:B:240:ASN:H	1:B:240:ASN:HD22	1.46	0.62
1:A:22:SER:CB	1:A:265:MET:HE1	2.30	0.62
1:B:228:ARG:HD2	1:B:255:SER:O	2.00	0.62
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.63	0.61
1:A:36:TYR:CD1	1:A:311:LEU:HD13	2.35	0.61
1:B:31:VAL:HG11	1:B:306:MET:HE1	1.81	0.61
1:B:240:ASN:HD22	1:B:240:ASN:N	1.99	0.61
1:B:171:THR:CG2	1:B:222:SER:OG	2.48	0.61
1:A:158:ASP:OD1	1:A:161:HIS:HE1	1.82	0.61
1:A:231:TYR:O	1:A:235:HIS:CD2	2.53	0.61
1:B:158:ASP:OD1	1:B:161:HIS:HE1	1.84	0.60
1:A:101:THR:HG23	2:A:384:HOH:O	2.02	0.60
1:B:265:MET:HE2	1:B:271:GLU:CB	2.31	0.60
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.15	0.59
1:A:225:ARG:NE	1:A:258:MET:HE2	2.17	0.59
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.65	0.59
1:A:284:ASN:ND2	2:A:366:HOH:O	2.35	0.59
1:A:303:ASP:H	1:A:304:TYR:HA	1.68	0.59
1:A:251:HIS:HE1	1:B:291:TYR:O	1.86	0.57
1:A:228:ARG:HD2	1:A:255:SER:O	2.04	0.57
1:A:104:PHE:O	1:A:108:VAL:HG13	2.05	0.56
1:B:171:THR:HG23	1:B:172:ASN:N	2.05	0.56
1:B:32:THR:HG22	1:B:110:ARG:HH12	1.71	0.56
1:B:265:MET:HE2	1:B:271:GLU:CA	2.37	0.55
1:B:265:MET:HE2	1:B:271:GLU:HA	1.89	0.55
1:A:79:GLY:C	1:A:80:LEU:CD2	2.80	0.54
1:B:28:THR:CG2	1:B:29:ILE:O	2.56	0.54
1:B:240:ASN:ND2	1:B:240:ASN:N	2.54	0.54
1:A:50:PRO:HB3	1:A:110:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:HB2	1:A:129:SER:HB2	1.90	0.53
1:B:62:ASP:CG	1:B:62:ASP:O	2.51	0.53
1:A:128:VAL:C	1:A:128:VAL:N	2.66	0.53
1:B:21:TRP:C	1:B:265:MET:HE1	2.32	0.53
1:A:254:GLY:HA2	1:A:257:GLN:CB	2.34	0.52
1:A:257:GLN:NE2	1:B:251:HIS:ND1	2.58	0.52
1:A:12:ASN:ND2	2:A:435:HOH:O	2.36	0.51
1:A:36:TYR:O	1:A:110:ARG:NH2	2.42	0.51
1:A:39:ASP:O	1:A:63:ARG:NH2	2.44	0.50
1:A:128:VAL:C	1:A:128:VAL:HB	2.33	0.50
1:A:171:THR:CG2	1:A:222:SER:OG	2.58	0.50
1:A:172:ASN:ND2	1:A:225:ARG:HH22	2.04	0.50
1:B:284:ASN:ND2	2:B:417:HOH:O	2.44	0.50
1:B:22:SER:CB	1:B:265:MET:HE3	2.37	0.50
1:A:279:TYR:OH	1:A:284:ASN:ND2	2.44	0.50
1:B:37:HIS:NE2	1:B:39:ASP:OD1	2.39	0.49
1:B:189:VAL:HG13	1:B:213:MET:HA	1.94	0.49
1:A:2:THR:O	1:A:17:ARG:HA	2.13	0.49
1:A:34:ARG:HG3	1:A:306:MET:O	2.12	0.49
1:A:90:HIS:NE2	1:A:131:ILE:HD11	2.27	0.49
1:B:67:PHE:N	1:B:67:PHE:CD1	2.79	0.49
1:B:90:HIS:CD2	1:B:129:SER:O	2.62	0.49
1:A:132:VAL:HB	1:A:135:GLN:HB2	1.94	0.49
1:B:1:CYS:N	1:B:172:ASN:HD21	2.11	0.48
1:B:173:GLN:NE2	1:B:173:GLN:H	2.11	0.48
1:A:90:HIS:CD2	1:A:131:ILE:CD1	2.96	0.48
1:A:22:SER:N	1:A:265:MET:HE1	2.29	0.48
1:A:283:THR:O	1:A:284:ASN:C	2.56	0.48
1:A:22:SER:H	1:A:265:MET:HE1	1.78	0.48
1:B:173:GLN:H	1:B:173:GLN:HE21	1.62	0.48
1:A:80:LEU:N	1:A:80:LEU:CD2	2.76	0.48
1:B:110:ARG:NH1	2:B:388:HOH:O	2.46	0.48
1:A:37:HIS:CD2	1:A:39:ASP:OD1	2.67	0.47
1:B:22:SER:HB3	1:B:265:MET:CE	2.38	0.47
1:A:158:ASP:OD1	1:A:161:HIS:CE1	2.66	0.47
1:A:171:THR:HG21	1:A:222:SER:O	2.12	0.47
1:A:254:GLY:CA	1:A:257:GLN:HB3	2.38	0.47
1:B:104:PHE:O	1:B:108:VAL:HG13	2.14	0.47
1:A:1:CYS:N	1:A:172:ASN:HD21	2.12	0.46
1:A:60:MET:O	1:A:61:ALA:HB3	2.14	0.46
1:A:287:TYR:HA	1:A:297:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:OH	1:A:103:GLU:OE1	2.26	0.46
1:B:265:MET:HE2	1:B:271:GLU:HB2	1.96	0.46
1:B:305:ASP:O	1:B:308:SER:HB3	2.15	0.46
1:B:304:TYR:CB	1:B:306:MET:HE3	2.43	0.46
1:B:1:CYS:HB3	1:B:80:LEU:HD22	1.98	0.46
1:A:17:ARG:CD	1:A:17:ARG:C	2.89	0.45
1:A:1:CYS:H2	1:A:172:ASN:HD21	1.64	0.45
1:A:254:GLY:C	1:A:257:GLN:H	2.25	0.45
1:A:302:ALA:O	1:A:303:ASP:OD1	2.34	0.45
1:A:28:THR:HG21	1:A:313:SER:OG	2.16	0.45
1:A:300:ALA:O	1:A:303:ASP:HB2	2.16	0.45
1:A:64:PRO:HG2	1:A:106:LEU:HD22	1.98	0.44
1:A:172:ASN:HB2	1:A:222:SER:HB2	1.98	0.44
1:B:133:PRO:HA	1:B:134:GLY:HA2	1.70	0.44
1:A:13:THR:HB	1:A:281:SER:HB3	2.00	0.44
1:B:172:ASN:ND2	1:B:225:ARG:HH22	2.14	0.44
1:A:100:ALA:O	1:A:103:GLU:HG2	2.18	0.43
1:A:90:HIS:CD2	1:A:131:ILE:HD12	2.52	0.43
1:A:74:GLY:HA2	1:A:279:TYR:OH	2.18	0.43
1:A:35:GLY:C	1:A:309:SER:HA	2.43	0.43
1:A:104:PHE:HB3	1:A:105:PRO:HD3	2.01	0.43
1:B:19:LEU:HD22	1:B:275:PHE:CE2	2.54	0.43
1:A:44:ALA:HB2	1:A:98:ASN:O	2.18	0.43
1:B:284:ASN:HB3	1:B:301:MET:HE2	2.00	0.43
1:A:189:VAL:HG13	1:A:213:MET:HA	2.01	0.43
1:B:28:THR:HG23	1:B:29:ILE:O	2.18	0.42
1:B:23:PHE:HD2	1:B:24:SER:O	2.03	0.42
1:B:178:PHE:CD2	1:B:178:PHE:C	2.96	0.42
1:A:28:THR:HG23	1:A:29:ILE:O	2.19	0.42
1:A:59:VAL:O	1:A:59:VAL:HG23	2.20	0.42
1:A:293:ASP:HA	1:A:294:PRO:HD2	1.94	0.42
1:B:37:HIS:HE2	1:B:39:ASP:CG	2.25	0.42
1:A:5:ARG:HA	1:A:14:TYR:O	2.20	0.42
1:A:20:ASP:HA	1:A:272:ARG:O	2.20	0.42
1:A:276:THR:O	1:A:288:MET:HA	2.19	0.42
1:B:82:PHE:N	1:B:83:PRO:CD	2.82	0.42
1:B:174:PRO:HG2	1:B:178:PHE:CG	2.55	0.42
1:A:28:THR:CG2	1:A:29:ILE:O	2.68	0.41
1:A:90:HIS:CD2	1:A:131:ILE:HD11	2.54	0.41
1:A:35:GLY:N	1:A:308:SER:O	2.54	0.41
1:B:67:PHE:N	1:B:67:PHE:HD1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:CE	1:B:206:ALA:HB3	2.50	0.41
1:A:121:THR:O	1:A:125:VAL:HG23	2.19	0.41
1:B:81:ASN:HD22	1:B:81:ASN:HA	1.70	0.41
1:B:100:ALA:O	1:B:103:GLU:HG2	2.21	0.41
1:A:257:GLN:NE2	2:A:378:HOH:O	2.54	0.40
1:B:189:VAL:HG11	1:B:216:ILE:HG12	2.03	0.40
1:B:222:SER:HB3	1:B:223:PRO:HD3	2.02	0.40
1:A:90:HIS:HD2	1:A:129:SER:O	2.04	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	314/316 (99%)	297 (95%)	14 (4%)	3 (1%)	12	15
1	B	314/316 (99%)	302 (96%)	9 (3%)	3 (1%)	12	15
All	All	628/632 (99%)	599 (95%)	23 (4%)	6 (1%)	12	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	TYR
1	A	303	ASP
1	B	303	ASP
1	A	82	PHE
1	B	82	PHE
1	B	174	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	238 (90%)	25 (10%)	8	10
1	B	263/263 (100%)	243 (92%)	20 (8%)	12	16
All	All	526/526 (100%)	481 (91%)	45 (9%)	10	13

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

Mol	Chain	Res	Type
1	A	9	ASP
1	A	17	ARG
1	A	19	LEU
1	A	28	THR
1	A	53	VAL
1	A	60	MET
1	A	68	ASP
1	A	80	LEU
1	A	101	THR
1	A	108	VAL
1	A	110	ARG
1	A	123	ARG
1	A	128	VAL
1	A	129	SER
1	A	131	ILE
1	A	136	GLN
1	A	169	VAL
1	A	171	THR
1	A	195	GLU
1	A	238	GLN
1	A	304	TYR
1	A	311	LEU
1	A	312	ILE
1	A	314	VAL
1	A	316	ARG
1	B	7	SER
1	B	19	LEU

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Mol	Chain	Res	Type
1	B	28	THR
1	B	49	LYS
1	B	53	VAL
1	B	68	ASP
1	B	81	ASN
1	B	101	THR
1	B	108	VAL
1	B	110	ARG
1	B	169	VAL
1	B	171	THR
1	B	173	GLN
1	B	240	ASN
1	B	297	ARG
1	B	305	ASP
1	B	308	SER
1	B	311	LEU
1	B	314	VAL
1	B	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	18	ASN
1	A	37	HIS
1	A	81	ASN
1	A	90	HIS
1	A	135	GLN
1	A	136	GLN
1	A	161	HIS
1	A	172	ASN
1	A	235	HIS
1	A	238	GLN
1	A	245	ASN
1	A	251	HIS
1	A	257	GLN
1	A	284	ASN
1	B	18	ASN
1	B	81	ASN
1	B	90	HIS
1	B	111	ASN
1	B	161	HIS

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Mol	Chain	Res	Type
1	B	172	ASN
1	B	173	GLN
1	B	240	ASN
1	B	245	ASN
1	B	257	GLN
1	B	284	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	127:LEU	C	128:VAL	N	1.66
1	A	315:ALA	C	316:ARG	N	1.19
1	B	315:ALA	C	316:ARG	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/316 (99%)	0.63	24 (7%) 20 21	23, 39, 57, 104	1 (0%)
1	B	315/316 (99%)	0.16	9 (2%) 53 56	22, 35, 53, 61	1 (0%)
All	All	630/632 (99%)	0.39	33 (5%) 33 34	22, 36, 55, 104	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	VAL	8.6
1	A	127	LEU	8.2
1	A	129	SER	7.7
1	A	126	THR	5.2
1	A	50	PRO	3.8
1	A	37	HIS	3.3
1	A	125	VAL	3.3
1	B	38	TYR	3.1
1	A	254	GLY	3.1
1	A	315	ALA	3.0
1	A	52	ALA	2.9
1	B	48	ALA	2.9
1	A	240	ASN	2.8
1	A	38	TYR	2.7
1	A	132	VAL	2.6
1	A	94	GLU	2.6
1	B	23	PHE	2.6
1	A	1	CYS	2.5
1	B	315	ALA	2.5
1	B	134	GLY	2.4
1	A	113	ASP	2.3
1	B	37	HIS	2.3
1	B	94	GLU	2.3
1	A	195	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	131	ILE	2.3
1	B	1	CYS	2.2
1	A	39	ASP	2.1
1	A	9	ASP	2.1
1	A	304	TYR	2.1
1	A	312	ILE	2.1
1	A	25	TYR	2.1
1	A	133	PRO	2.1
1	B	46	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.