



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 2SBL / pdb_00002sbl
Title : THE THREE-DIMENSIONAL STRUCTURE OF AN ARACHIDONIC
ACID 15-LIPOXYGENASE
Authors : Amzel, L.M.; Boyington, J.C.
Deposited on : 1993-07-22
Resolution : 2.60 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) : **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

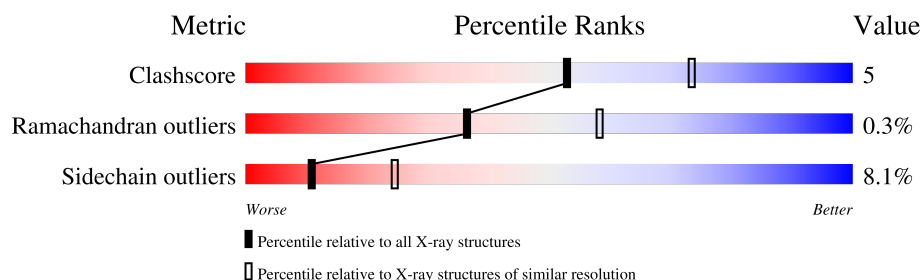
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	839	 71% 22% . .
1	B	839	 71% 21% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12955 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 LIPOXYGENASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	807	Total	C	N	O	S	0	0	0
			6445	4133	1090	1204	18			
1	A	807	Total	C	N	O	S	0	0	0
			6445	4133	1090	1204	18			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	63	Total	O	0	0
			63	63		

D320	G321	Q322	H323	K326	H331	Q334	V335	H340	K341	T342	E344	R348	V354	S369	D372	Q379	K382	T383	T384	A385	D386	S387	L399	L404	L407	D408	Y409	H410	F413	V417	N421	Q422	A430	P453	HIS	SER	ALA	GLY	ASP	LEU					
SER	A461	S464	Q465	V474	W479	N489	H494	Q495	L496	M497	S498	H499	W500	L501	N502	T503	H504	A505	A506	M507	I512	A513	T514	H515	R516	H517	L518	H522	L528	T529	P530	H531	Y532	N535	I538	L541	A542	R543	N548	A549	N550	G551	I552	V564	V570
Y571	W574	I586	K587	A591	I592	K593	D594	P595	S596	H599	G600	V601	R602	I605	Y608	L615	E616	I617	W618	T623	W624	V629	L645	Q646	H647	H657	L660	W665	K668	L669	L672	I682	I685	L689	H690	F695	P699	Y700	G701						
G702	L703	R707	S711	R712	R713	L714	E722	Y723	E724	H730	L735	S747	V750	H757	D760	H771	W772	T773	S774	N787	K788	L789	K790	N800	N801	D802	P803	Q806	R809	L810	G811	L819	S824	T829	G832	I837	S838	I839							

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.50Å 125.60Å 94.70Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12955	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.89	31/6606 (0.5%)	1.56	97/8973 (1.1%)
1	B	0.89	31/6606 (0.5%)	1.56	97/8973 (1.1%)
All	All	0.89	62/13212 (0.5%)	1.56	194/17946 (1.1%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	VAL	CA-CB	7.20	1.63	1.54
1	B	131	VAL	CA-CB	7.17	1.63	1.54
1	B	531	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	757	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	531	HIS	CD2-NE2	-7.04	1.30	1.37
1	B	757	HIS	CD2-NE2	-7.04	1.30	1.37
1	B	647	HIS	CD2-NE2	-6.97	1.30	1.37
1	A	647	HIS	CD2-NE2	-6.96	1.30	1.37
1	B	284	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	284	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	515	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	515	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	730	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	730	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	147	HIS	CD2-NE2	-6.61	1.30	1.37
1	B	522	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	84	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	522	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	84	HIS	CD2-NE2	-6.57	1.30	1.37
1	B	323	HIS	CD2-NE2	-6.50	1.30	1.37
1	B	248	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	323	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	248	HIS	CD2-NE2	-6.43	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	HIS	CD2-NE2	-6.33	1.30	1.37
1	B	410	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	53	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	504	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	629	VAL	CA-CB	6.24	1.57	1.54
1	B	629	VAL	CA-CB	6.21	1.57	1.54
1	A	53	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	504	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	494	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	771	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	494	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	599	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	771	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	331	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	331	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	599	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	657	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	499	HIS	CD2-NE2	-5.82	1.31	1.37
1	B	499	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	657	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	690	HIS	CG-ND1	-5.74	1.31	1.38
1	B	690	HIS	CG-ND1	-5.73	1.31	1.38
1	B	690	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	499	HIS	CG-ND1	-5.72	1.31	1.38
1	A	690	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	499	HIS	CG-ND1	-5.68	1.32	1.38
1	B	410	HIS	CG-ND1	-5.68	1.32	1.38
1	A	410	HIS	CG-ND1	-5.64	1.32	1.38
1	B	517	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	517	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	504	HIS	CG-ND1	-5.35	1.32	1.38
1	A	504	HIS	CG-ND1	-5.34	1.32	1.38
1	B	284	HIS	CG-ND1	-5.30	1.32	1.38
1	A	284	HIS	CG-ND1	-5.27	1.32	1.38
1	A	290	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	290	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	323	HIS	CG-ND1	-5.10	1.32	1.38
1	B	323	HIS	CG-ND1	-5.09	1.32	1.38

All (194) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CA-CB-CG	9.77	122.37	112.60
1	B	61	ASP	CA-CB-CG	9.74	122.34	112.60
1	A	605	ILE	N-CA-C	-9.13	93.88	106.85
1	B	605	ILE	N-CA-C	-9.13	93.89	106.85
1	B	188	VAL	N-CA-CB	-9.09	96.28	111.38
1	A	188	VAL	N-CA-CB	-9.07	96.32	111.38
1	B	188	VAL	CB-CA-C	9.06	121.56	111.59
1	A	188	VAL	CB-CA-C	9.04	121.53	111.59
1	B	750	VAL	CB-CA-C	-8.62	100.73	112.02
1	A	750	VAL	CB-CA-C	-8.61	100.74	112.02
1	B	68	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	68	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	A	240	VAL	N-CA-C	-7.49	99.46	108.45
1	B	240	VAL	N-CA-C	-7.48	99.47	108.45
1	B	757	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	A	757	HIS	CB-CG-CD2	-7.13	121.93	131.20
1	A	141	ARG	NE-CZ-NH2	-6.82	113.06	119.20
1	B	194	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	B	141	ARG	NE-CZ-NH2	-6.79	113.09	119.20
1	A	194	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	B	531	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	531	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	B	507	MET	CG-SD-CE	-6.44	86.74	100.90
1	A	507	MET	CG-SD-CE	-6.43	86.75	100.90
1	B	750	VAL	N-CA-CB	6.41	118.78	110.57
1	A	535	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	B	535	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	531	HIS	CA-CB-CG	-6.40	107.40	113.80
1	A	750	VAL	N-CA-CB	6.38	118.74	110.57
1	A	531	HIS	CA-CB-CG	-6.37	107.43	113.80
1	B	334	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	A	245	ASN	CB-CG-ND2	6.29	125.83	116.40
1	B	245	ASN	CB-CG-ND2	6.29	125.83	116.40
1	A	84	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	B	248	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	248	HIS	CB-CG-CD2	-6.27	123.04	131.20
1	A	334	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	B	84	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	A	264	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	B	289	VAL	N-CA-C	-6.05	104.96	110.82
1	B	264	GLN	OE1-CD-NE2	-6.04	116.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	VAL	N-CA-C	-6.03	104.97	110.82
1	B	308	ILE	N-CA-C	6.02	121.89	108.88
1	A	308	ILE	N-CA-C	6.02	121.89	108.88
1	A	53	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	B	53	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	A	267	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	B	267	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	A	829	THR	N-CA-C	5.93	120.58	113.23
1	B	829	THR	N-CA-C	5.92	120.58	113.23
1	B	479	TRP	CG-CD2-CE3	5.92	139.82	133.90
1	B	515	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	479	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	A	713	ARG	CA-CB-CG	5.87	125.85	114.10
1	A	515	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	322	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	B	713	ARG	CA-CB-CG	5.86	125.83	114.10
1	B	322	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	624	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	B	624	TRP	CG-CD2-CE3	5.78	139.68	133.90
1	B	147	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	147	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	51	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	51	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	87	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	B	87	TRP	CG-CD2-CE3	5.71	139.61	133.90
1	B	422	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	B	331	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	422	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	331	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	522	HIS	CA-C-N	5.69	125.16	119.24
1	B	522	HIS	C-N-CA	5.69	125.16	119.24
1	A	522	HIS	CA-C-N	5.69	125.15	119.24
1	A	522	HIS	C-N-CA	5.69	125.15	119.24
1	B	535	ASN	CB-CG-ND2	5.68	124.92	116.40
1	A	535	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	515	HIS	CA-CB-CG	-5.66	108.14	113.80
1	B	465	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	B	335	VAL	N-CA-C	-5.65	107.16	111.62
1	B	730	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	A	335	VAL	N-CA-C	-5.64	107.16	111.62
1	A	500	TRP	CB-CG-CD1	-5.64	118.44	126.90
1	A	290	HIS	CB-CG-CD2	-5.64	123.87	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	465	GLN	OE1-CD-NE2	-5.62	116.97	122.60
1	B	500	TRP	CB-CG-CD1	-5.62	118.47	126.90
1	A	730	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	B	515	HIS	CA-CB-CG	-5.59	108.20	113.80
1	B	245	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	B	474	VAL	CB-CA-C	-5.56	104.75	112.04
1	A	245	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	474	VAL	CB-CA-C	-5.55	104.76	112.04
1	B	287	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	228	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	624	TRP	CB-CG-CD1	-5.53	118.60	126.90
1	A	624	TRP	CB-CG-CD1	-5.53	118.61	126.90
1	A	228	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	287	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	196	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	196	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	194	ASN	CA-C-N	5.52	125.35	119.28
1	B	194	ASN	C-N-CA	5.52	125.35	119.28
1	B	421	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	624	TRP	CE2-CD2-CG	-5.51	100.58	107.20
1	A	489	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	624	TRP	CE2-CD2-CG	-5.50	100.60	107.20
1	A	421	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	B	502	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	194	ASN	CA-C-N	5.49	125.32	119.28
1	A	194	ASN	C-N-CA	5.49	125.32	119.28
1	B	517	HIS	N-CA-C	5.49	121.39	114.31
1	A	517	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A	502	ASN	OD1-CG-ND2	-5.47	117.12	122.60
1	B	517	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	408	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	408	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	194	ASN	CB-CG-ND2	5.46	124.59	116.40
1	B	489	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	372	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	517	HIS	N-CA-C	5.45	121.33	114.31
1	B	618	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	B	372	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	194	ASN	CB-CG-ND2	5.42	124.53	116.40
1	B	665	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	618	TRP	CG-CD2-CE3	5.40	139.30	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	A	760	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	760	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	93	ILE	CA-C-N	5.39	125.15	119.76
1	B	93	ILE	C-N-CA	5.39	125.15	119.76
1	A	665	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	A	93	ILE	CA-C-N	5.38	125.14	119.76
1	A	93	ILE	C-N-CA	5.38	125.14	119.76
1	B	665	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	B	772	TRP	CG-CD2-CE3	5.36	139.26	133.90
1	A	772	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	B	801	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	264	GLN	CG-CD-NE2	5.33	124.40	116.40
1	A	246	LEU	N-CA-C	5.33	117.42	109.59
1	A	264	GLN	CG-CD-NE2	5.32	124.38	116.40
1	A	801	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	B	246	LEU	N-CA-C	5.31	117.40	109.59
1	A	517	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	B	517	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	772	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	B	772	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	B	668	LYS	O-C-N	-5.24	117.11	123.29
1	A	623	THR	CA-CB-OG1	-5.23	101.76	109.60
1	B	495	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	623	THR	CA-CB-OG1	-5.21	101.78	109.60
1	B	340	TRP	CG-CD2-CE3	5.21	139.10	133.90
1	B	61	ASP	N-CA-CB	5.19	117.71	109.71
1	A	668	LYS	O-C-N	-5.19	117.17	123.29
1	A	495	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	340	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	340	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	B	340	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	61	ASP	N-CA-CB	5.17	117.67	109.71
1	A	61	ASP	CB-CA-C	-5.16	102.52	110.26
1	B	61	ASP	CB-CA-C	-5.16	102.52	110.26
1	A	130	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	130	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	B	618	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	87	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	B	87	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	354	VAL	CB-CA-C	-5.12	104.23	112.16
1	A	479	TRP	CB-CG-CD1	-5.12	119.22	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	B	354	VAL	CB-CA-C	-5.10	104.25	112.16
1	B	479	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	A	479	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	A	695	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	310	LEU	CA-C-N	5.09	124.70	119.05
1	B	310	LEU	C-N-CA	5.09	124.70	119.05
1	B	479	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	A	290	HIS	CB-CG-ND1	5.08	130.32	122.70
1	B	500	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	B	695	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	310	LEU	CA-C-N	5.06	124.67	119.05
1	A	310	LEU	C-N-CA	5.06	124.67	119.05
1	A	574	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	574	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	500	TRP	CE2-CD2-CG	-5.05	101.13	107.20
1	B	290	HIS	CB-CG-ND1	5.05	130.28	122.70
1	B	494	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	A	340	TRP	CB-CG-CD1	-5.04	119.34	126.90
1	A	494	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	500	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	B	500	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	A	107	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	340	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	B	489	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	248	HIS	CB-CG-ND1	5.01	130.22	122.70
1	A	320	ASP	N-CA-C	-5.01	107.01	112.72

There are no chirality outliers.

There are no planarity outliers.

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	6445	0	6397	66	2
1	B	6445	0	6397	69	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	63	0	0	5	0
All	All	12955	0	12794	129	2

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 5.

All (129) 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:767:ARG:NE	3:B:902:HOH:O	2.02	0.91
1:B:655:LYS:HG2	1:A:226:VAL:HG11	1.55	0.89
1:A:507:MET:HE1	1:A:682:ILE:HG23	1.67	0.76
1:B:507:MET:HE1	1:B:682:ILE:HG23	1.67	0.76
1:B:538:ILE:HD11	1:B:837:ILE:HG22	1.77	0.66
1:A:538:ILE:HD11	1:A:837:ILE:HG22	1.77	0.66
1:B:53:HIS:CD2	1:A:281:ILE:CD1	2.83	0.62
1:B:140:VAL:HG11	1:A:276:LEU:HD21	1.82	0.61
1:B:308:ILE:HG21	1:B:319:THR:HG21	1.83	0.61
1:A:308:ILE:HG21	1:A:319:THR:HG21	1.83	0.61
1:B:701:GLY:HA2	1:B:707:ARG:HB2	1.88	0.56
1:A:701:GLY:HA2	1:A:707:ARG:HB2	1.88	0.56
1:A:9:LYS:HD2	1:A:84:HIS:NE2	2.22	0.55
1:B:767:ARG:CZ	3:B:902:HOH:O	2.47	0.55
1:B:9:LYS:HD2	1:B:84:HIS:NE2	2.22	0.55
1:B:787:ASN:HA	1:B:790:LYS:HE3	1.89	0.54
1:A:787:ASN:HA	1:A:790:LYS:HE3	1.89	0.54
1:B:301:ARG:HG2	1:B:322:GLN:O	2.08	0.54
1:A:106:GLU:HG2	1:A:132:TYR:CE2	2.43	0.54
1:A:301:ARG:HG2	1:A:322:GLN:O	2.08	0.53
1:B:106:GLU:HG2	1:B:132:TYR:CE2	2.43	0.53
1:A:543:ARG:O	1:A:548:ASN:HB3	2.09	0.53
1:B:543:ARG:O	1:B:548:ASN:HB3	2.09	0.53
1:B:40:VAL:HB	1:B:64:LEU:HD22	1.92	0.52
1:A:40:VAL:HB	1:A:64:LEU:HD22	1.92	0.52
1:B:53:HIS:NE2	1:A:281:ILE:HD12	2.26	0.51
1:A:15:MET:SD	1:A:110:LYS:HE3	2.52	0.50
1:B:53:HIS:CD2	1:A:281:ILE:HD12	2.46	0.50
1:B:800:ASN:HD22	1:B:809:ARG:HE	1.60	0.50
1:A:262:LEU:HD12	1:A:266:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:MET:SD	1:B:110:LYS:HE3	2.52	0.50
1:A:800:ASN:HD22	1:A:809:ARG:HE	1.60	0.50
1:B:262:LEU:HD12	1:B:266:VAL:HB	1.93	0.49
1:B:767:ARG:NH2	3:B:902:HOH:O	2.46	0.49
1:B:116:ALA:HB3	1:B:123:ILE:HD12	1.95	0.49
1:B:117:ILE:HG12	1:B:123:ILE:HD11	1.96	0.48
1:A:116:ALA:HB3	1:A:123:ILE:HD12	1.95	0.48
1:B:410:HIS:HA	1:B:430:ALA:HB1	1.96	0.47
1:A:184:TYR:HB3	1:A:512:ILE:HG23	1.96	0.47
1:B:761:GLU:HG2	3:B:899:HOH:O	2.14	0.47
1:B:184:TYR:HB3	1:B:512:ILE:HG23	1.96	0.47
1:A:117:ILE:HG12	1:A:123:ILE:HD11	1.96	0.47
1:A:272:SER:O	1:A:276:LEU:HG	2.15	0.47
1:A:382:LYS:HD2	1:A:464:SER:HB2	1.97	0.47
1:A:413:PHE:O	1:A:417:VAL:HG23	2.15	0.47
1:B:53:HIS:NE2	1:A:281:ILE:CD1	2.77	0.47
1:A:571:TYR:CZ	1:A:660:LEU:HD22	2.50	0.47
1:B:272:SER:O	1:B:276:LEU:HG	2.15	0.47
1:B:413:PHE:O	1:B:417:VAL:HG23	2.15	0.47
1:A:410:HIS:HA	1:A:430:ALA:HB1	1.96	0.47
1:A:114:LEU:HD22	1:A:125:PHE:HE1	1.81	0.46
1:A:685:ILE:HA	1:A:689:LEU:HB3	1.98	0.46
1:B:318:ARG:HB2	1:B:326:LYS:CG	2.46	0.46
1:B:571:TYR:CZ	1:B:660:LEU:HD22	2.50	0.46
1:B:685:ILE:HA	1:B:689:LEU:HB3	1.98	0.46
1:A:106:GLU:HG2	1:A:132:TYR:CZ	2.51	0.46
1:B:195:PRO:HD2	3:B:891:HOH:O	2.14	0.46
1:B:114:LEU:HD22	1:B:125:PHE:HE1	1.80	0.46
1:B:382:LYS:HD2	1:B:464:SER:HB2	1.97	0.46
1:A:224:PRO:HB2	1:A:229:PRO:HA	1.98	0.46
1:A:100:LYS:NZ	1:A:134:THR:HG21	2.32	0.45
1:A:586:ILE:HD13	1:A:593:LYS:HG2	1.98	0.45
1:B:106:GLU:HG2	1:B:132:TYR:CZ	2.51	0.45
1:B:586:ILE:HD13	1:B:593:LYS:HG2	1.98	0.45
1:B:224:PRO:HB2	1:B:229:PRO:HA	1.98	0.45
1:B:310:LEU:HB2	1:B:313:ILE:HB	1.98	0.45
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.82	0.45
1:A:318:ARG:HB2	1:A:326:LYS:CG	2.46	0.45
1:B:100:LYS:NZ	1:B:134:THR:HG21	2.32	0.45
1:B:178:LYS:HA	1:B:178:LYS:HD3	1.84	0.45
1:A:310:LEU:HB2	1:A:313:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HA	1:B:158:LEU:HD13	2.00	0.44
1:A:47:ALA:HA	1:A:158:LEU:HD13	2.00	0.44
1:A:65:GLU:HB2	1:A:82:ASN:O	2.18	0.44
1:B:803:PRO:HA	1:B:806:GLN:HG2	2.00	0.44
1:A:163:GLU:O	1:A:167:LYS:HG2	2.18	0.44
1:B:65:GLU:HB2	1:B:82:ASN:O	2.17	0.43
1:A:504:HIS:CE1	1:A:538:ILE:HD12	2.54	0.43
1:B:645:LEU:HG	1:B:669:LEU:HD23	2.01	0.43
1:B:163:GLU:O	1:B:167:LYS:HG2	2.18	0.43
1:B:222:ARG:NH1	1:B:233:LYS:O	2.51	0.43
1:A:47:ALA:HB2	1:A:95:GLY:HA3	2.01	0.43
1:B:68:ASN:HB2	1:B:82:ASN:ND2	2.34	0.43
1:B:504:HIS:CE1	1:B:538:ILE:HD12	2.54	0.43
1:A:222:ARG:NH1	1:A:233:LYS:O	2.51	0.42
1:B:552:ILE:HG21	1:B:750:VAL:HG21	2.00	0.42
1:A:501:LEU:HA	1:A:505:ALA:HB3	2.01	0.42
1:A:529:THR:HA	1:A:532:TYR:CD2	2.54	0.42
1:A:178:LYS:HA	1:A:178:LYS:HD3	1.84	0.42
1:A:645:LEU:HG	1:A:669:LEU:HD23	2.01	0.42
1:B:47:ALA:HB2	1:B:95:GLY:HA3	2.01	0.42
1:A:803:PRO:HA	1:A:806:GLN:HG2	2.00	0.42
1:A:552:ILE:HG21	1:A:750:VAL:HG21	2.00	0.42
1:B:501:LEU:HA	1:B:505:ALA:HB3	2.01	0.42
1:A:68:ASN:HB2	1:A:82:ASN:ND2	2.34	0.42
1:A:404:LEU:HD12	1:A:404:LEU:HA	1.93	0.42
1:B:529:THR:HA	1:B:532:TYR:CD2	2.54	0.42
1:A:301:ARG:HE	1:A:322:GLN:HE21	1.68	0.42
1:A:591:ALA:HB1	1:A:601:VAL:HG22	2.02	0.42
1:A:788:LYS:HA	1:A:788:LYS:HD2	1.90	0.42
1:B:228:ASP:HA	1:B:229:PRO:HD2	1.82	0.41
1:B:404:LEU:HD12	1:B:404:LEU:HA	1.93	0.41
1:B:591:ALA:HB1	1:B:601:VAL:HG22	2.02	0.41
1:A:49:LYS:HD2	1:A:57:LYS:HE3	2.01	0.41
1:B:100:LYS:HE3	1:B:102:TYR:OH	2.20	0.41
1:B:254:ALA:O	1:B:257:ILE:HG12	2.20	0.41
1:B:298:LYS:HA	1:B:323:HIS:O	2.20	0.41
1:B:592:ILE:HD11	1:B:602:ARG:NH2	2.36	0.41
1:A:254:ALA:O	1:A:257:ILE:HG12	2.20	0.41
1:B:715:LEU:HA	1:B:716:PRO:HD3	1.82	0.41
1:A:497:MET:CG	1:A:570:VAL:HG11	2.51	0.41
1:B:301:ARG:HE	1:B:322:GLN:HE21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:CG2	1:A:117:ILE:HD11	2.51	0.41
1:B:497:MET:CG	1:B:570:VAL:HG11	2.51	0.41
1:A:299:LEU:HB2	1:A:304:ILE:HD11	2.03	0.41
1:A:592:ILE:HD11	1:A:602:ARG:NH2	2.36	0.41
1:A:824:SER:HB2	1:A:832:GLY:HA3	2.03	0.41
1:B:318:ARG:HB2	1:B:326:LYS:HG3	2.03	0.41
1:A:318:ARG:HB2	1:A:326:LYS:HG3	2.03	0.41
1:A:514:THR:HG21	1:A:532:TYR:HE2	1.86	0.41
1:B:49:LYS:HD2	1:B:57:LYS:HE3	2.02	0.40
1:B:522:HIS:HA	1:B:523:PRO:HD2	1.92	0.40
1:B:195:PRO:HB2	1:B:227:THR:OG1	2.21	0.40
1:A:100:LYS:HE3	1:A:102:TYR:OH	2.20	0.40
1:A:342:THR:HB	1:A:344:GLU:OE1	2.22	0.40
1:B:290:HIS:HA	1:B:293:TYR:CE2	2.56	0.40
1:B:93:ILE:CG2	1:B:117:ILE:HD11	2.51	0.40
1:A:369:SER:HB3	1:A:379:GLN:O	2.22	0.40
1:A:348:ARG:HD3	1:A:811:GLY:HA3	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:PRO:O	1:A:595:PRO:CG[4_546]	1.91	0.29
1:B:415:PRO:CB	1:A:595:PRO:CB[4_546]	2.02	0.18

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	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	36 58
1	B	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	36 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1594/1678 (95%)	1528 (96%)	62 (4%)	4 (0%)	36 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	HIS
1	A	323	HIS
1	B	308	ILE
1	A	308	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	705/730 (97%)	648 (92%)	57 (8%)	11 24
1	B	705/730 (97%)	648 (92%)	57 (8%)	11 24
All	All	1410/1460 (97%)	1296 (92%)	114 (8%)	11 24

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ILE
1	B	9	LYS
1	B	11	THR
1	B	21	GLU
1	B	41	SER
1	B	44	LEU
1	B	61	ASP
1	B	64	LEU
1	B	74	LEU
1	B	106	GLU
1	B	114	LEU
1	B	131	VAL
1	B	134	THR
1	B	139	SER

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	172	ASN
1	B	188	VAL
1	B	242	ARG
1	B	245	ASN
1	B	256	GLU
1	B	279	THR
1	B	287	GLN
1	B	292	LEU
1	B	299	LEU
1	B	323	HIS
1	B	384	THR
1	B	386	ASP
1	B	387	SER
1	B	399	LEU
1	B	407	LEU
1	B	474	VAL
1	B	518	LEU
1	B	528	LEU
1	B	541	LEU
1	B	550	ASN
1	B	564	VAL
1	B	587	LYS
1	B	592	ILE
1	B	596	SER
1	B	608	TYR
1	B	615	LEU
1	B	616	GLU
1	B	660	LEU
1	B	669	LEU
1	B	672	LEU
1	B	699	PRO
1	B	703	LEU
1	B	711	SER
1	B	714	LEU
1	B	722	GLU
1	B	724	GLU
1	B	735	LEU
1	B	747	SER
1	B	750	VAL
1	B	774	SER
1	B	789	LEU

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Mol	Chain	Res	Type
1	B	819	LEU
1	A	8	ILE
1	A	9	LYS
1	A	11	THR
1	A	21	GLU
1	A	41	SER
1	A	44	LEU
1	A	61	ASP
1	A	64	LEU
1	A	74	LEU
1	A	106	GLU
1	A	114	LEU
1	A	131	VAL
1	A	134	THR
1	A	139	SER
1	A	158	LEU
1	A	172	ASN
1	A	188	VAL
1	A	242	ARG
1	A	245	ASN
1	A	256	GLU
1	A	279	THR
1	A	287	GLN
1	A	292	LEU
1	A	299	LEU
1	A	323	HIS
1	A	384	THR
1	A	386	ASP
1	A	387	SER
1	A	399	LEU
1	A	407	LEU
1	A	474	VAL
1	A	518	LEU
1	A	528	LEU
1	A	541	LEU
1	A	550	ASN
1	A	564	VAL
1	A	587	LYS
1	A	592	ILE
1	A	596	SER
1	A	608	TYR
1	A	615	LEU

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Mol	Chain	Res	Type
1	A	616	GLU
1	A	660	LEU
1	A	669	LEU
1	A	672	LEU
1	A	699	PRO
1	A	703	LEU
1	A	711	SER
1	A	714	LEU
1	A	722	GLU
1	A	724	GLU
1	A	735	LEU
1	A	747	SER
1	A	750	VAL
1	A	774	SER
1	A	789	LEU
1	A	819	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	230	ASN
1	B	287	GLN
1	B	322	GLN
1	B	537	ASN
1	B	787	ASN
1	B	800	ASN
1	A	33	ASN
1	A	230	ASN
1	A	287	GLN
1	A	322	GLN
1	A	537	ASN
1	A	787	ASN
1	A	800	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.