Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:45 AM GMT

PDB ID	:	2SBL
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

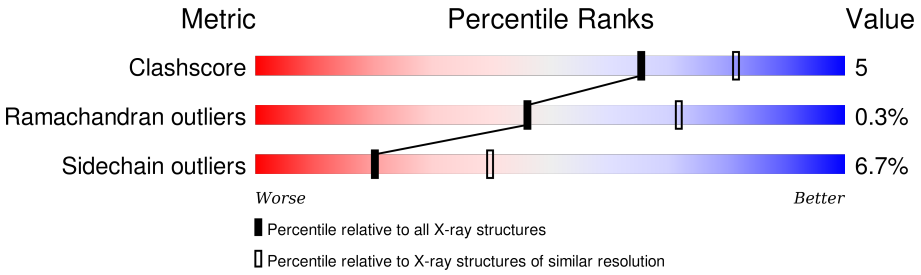
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 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 <=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	839	76% 19%
1	B	839	76% 19%

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 (three-letter code: 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		

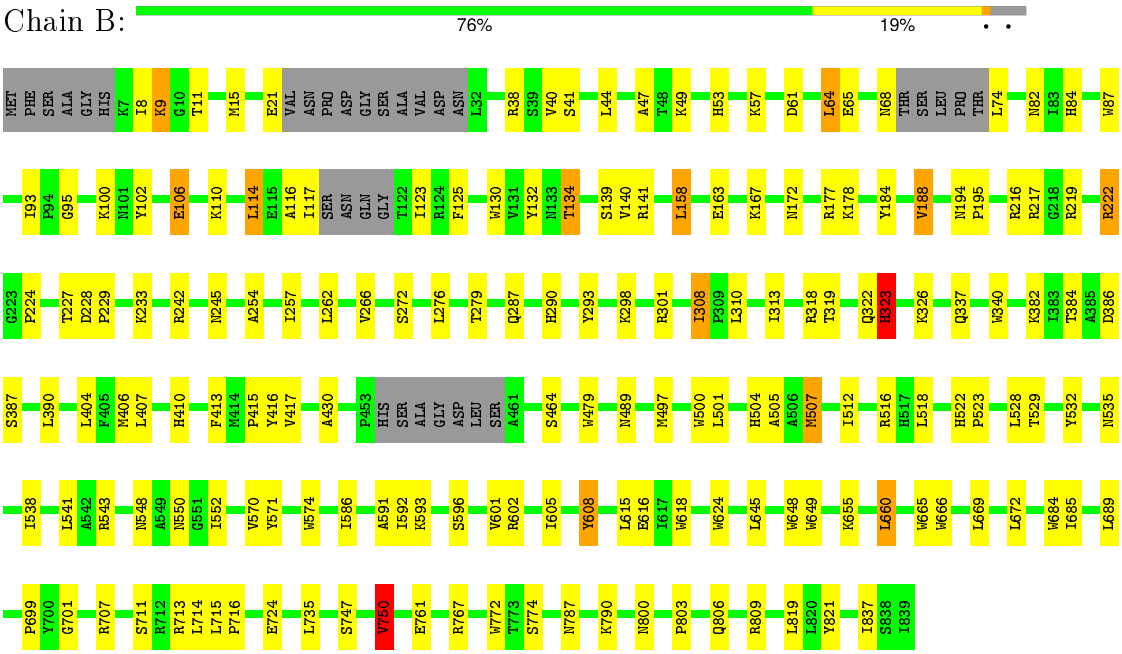
3 Residue-property plots (i)

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.

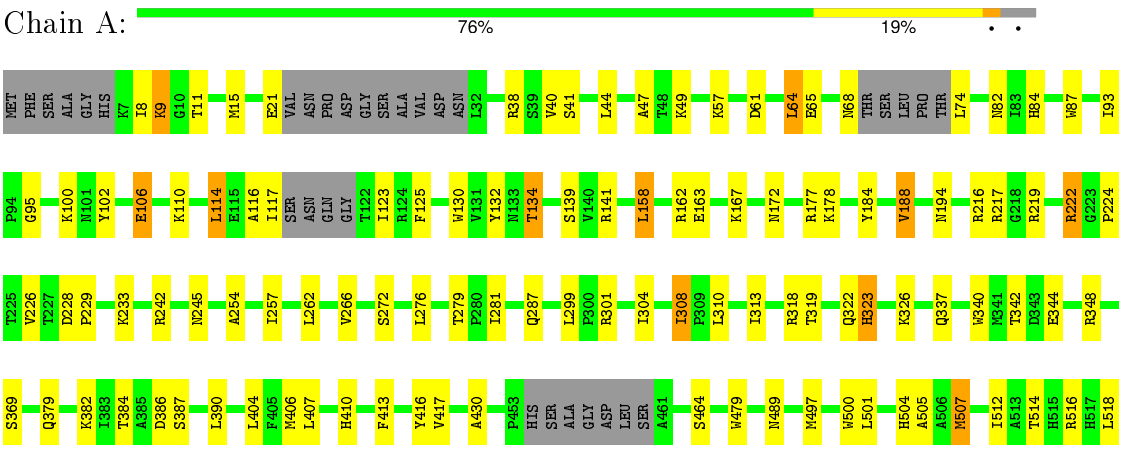
- Molecule 1: LIPOXYGENASE-1

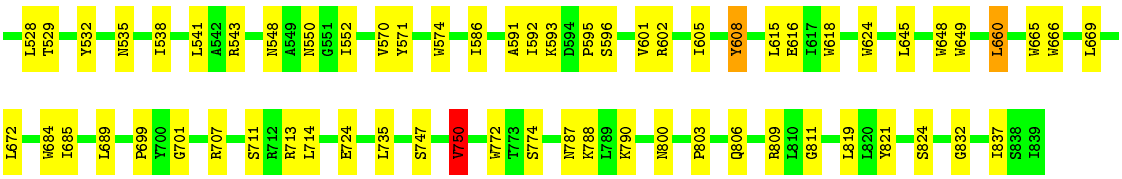
Chain B:



- Molecule 1: LIPOXYGENASE-1

Chain A:




L528
T529
V532
N535
I538
L541
A542
R543
N548
A549
N550
G551
I552
V570
Y571
W574
I586
A591
I592
K593
D594
P595
S596
V601
R602
I605
Y608
L615
E616
I617
W618
W624
L645
W648
W649
L660
W665
W666
L669
L672
W684
I685
L689
P699
Y700
G701
R707
S711
R712
R713
L714
E724
L735
S747
V750
W772
T773
S774
N787
K788
L789
K790
N800
P803
Q806
R809
I810
G811
L819
L820
Y821
S824
G832
I837
S838
I839

4 Data and refinement statistics (i)

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

5.1 Standard geometry

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	0.73	0/6606	1.34	81/8973 (0.9%)
1	B	0.73	0/6606	1.34	80/8973 (0.9%)
All	All	0.73	0/13212	1.34	161/17946 (0.9%)

There are no bond length outliers.

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	B	141	ARG	NE-CZ-NH2	-14.43	113.09	120.30
1	B	141	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	141	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	608	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	B	608	TYR	CB-CG-CD2	-9.33	115.40	121.00
1	A	624	TRP	CD1-CG-CD2	9.24	113.69	106.30
1	B	624	TRP	CD1-CG-CD2	9.22	113.67	106.30
1	A	500	TRP	CD1-CG-CD2	9.13	113.60	106.30
1	B	500	TRP	CD1-CG-CD2	9.12	113.59	106.30
1	B	130	TRP	CD1-CG-CD2	9.10	113.58	106.30
1	A	130	TRP	CD1-CG-CD2	9.07	113.55	106.30
1	A	772	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	B	772	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	B	340	TRP	CD1-CG-CD2	8.68	113.24	106.30
1	A	340	TRP	CD1-CG-CD2	8.67	113.24	106.30
1	B	618	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	618	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	B	574	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	574	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	684	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	B	507	MET	CG-SD-CE	-8.41	86.74	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	507	MET	CG-SD-CE	-8.41	86.75	100.20
1	A	624	TRP	CE2-CD2-CG	-8.39	100.58	107.30
1	B	684	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	B	624	TRP	CE2-CD2-CG	-8.37	100.60	107.30
1	A	665	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	B	665	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	A	665	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	B	665	TRP	CE2-CD2-CG	-8.18	100.76	107.30
1	B	87	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	A	87	TRP	CD1-CG-CD2	8.09	112.78	106.30
1	A	772	TRP	CE2-CD2-CG	-8.02	100.89	107.30
1	B	772	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	340	TRP	CE2-CD2-CG	-7.89	100.98	107.30
1	B	340	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	A	130	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	130	TRP	CE2-CD2-CG	-7.86	101.02	107.30
1	B	618	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	87	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	B	666	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	479	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	B	87	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	666	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	618	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	B	479	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A	479	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	B	479	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	B	500	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	A	574	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	A	500	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	B	574	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	B	649	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	A	649	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	B	648	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	648	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	A	684	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	666	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	B	684	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	B	666	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	648	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	B	648	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	B	649	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	649	TRP	CE2-CD2-CG	-7.35	101.42	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	188	VAL	N-CA-CB	-6.92	96.28	111.50
1	A	188	VAL	N-CA-CB	-6.90	96.32	111.50
1	B	217	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	217	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	B	177	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	177	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	177	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	500	TRP	CB-CG-CD1	-6.59	118.44	127.00
1	B	479	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	B	500	TRP	CB-CG-CD1	-6.57	118.47	127.00
1	A	479	TRP	CG-CD2-CE3	6.54	139.79	133.90
1	B	624	TRP	CB-CG-CD1	-6.46	118.60	127.00
1	A	624	TRP	CG-CD2-CE3	6.46	139.71	133.90
1	A	624	TRP	CB-CG-CD1	-6.46	118.61	127.00
1	B	624	TRP	CG-CD2-CE3	6.42	139.68	133.90
1	A	87	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	B	87	TRP	CG-CD2-CE3	6.34	139.61	133.90
1	A	605	ILE	N-CA-C	-6.34	93.88	111.00
1	B	605	ILE	N-CA-C	-6.34	93.89	111.00
1	A	219	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	618	TRP	CG-CD2-CE3	6.05	139.34	133.90
1	B	38	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	665	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	618	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	665	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	38	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	479	TRP	CB-CG-CD1	-5.98	119.22	127.00
1	B	219	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	479	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	B	772	TRP	CG-CD2-CE3	5.96	139.26	133.90
1	A	772	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	A	340	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	B	340	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	B	340	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	A	340	TRP	CG-CD2-CE3	5.75	139.08	133.90
1	A	665	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	A	608	TYR	CB-CG-CD1	5.66	124.40	121.00
1	A	713	ARG	CA-CB-CG	5.66	125.85	113.40
1	B	665	TRP	CB-CG-CD1	-5.65	119.65	127.00
1	B	713	ARG	CA-CB-CG	5.65	125.83	113.40
1	B	608	TYR	CB-CG-CD1	5.63	124.38	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	750	VAL	CB-CA-C	-5.62	100.73	111.40
1	A	750	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	500	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	B	500	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	B	624	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	624	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	618	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	B	618	TRP	CB-CG-CD1	-5.50	119.85	127.00
1	A	216	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	500	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	B	500	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	B	130	TRP	CG-CD1-NE1	-5.50	104.61	110.10
1	A	130	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	B	216	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	219	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	772	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	A	772	TRP	CB-CG-CD1	-5.44	119.92	127.00
1	B	340	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	340	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	B	390	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	390	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	188	VAL	CB-CA-C	5.34	121.56	111.40
1	A	188	VAL	CB-CA-C	5.33	121.53	111.40
1	A	242	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	242	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	219	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	87	TRP	CB-CG-CD1	-5.28	120.14	127.00
1	A	618	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	B	242	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	618	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	87	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	242	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	574	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	574	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	772	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	B	772	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	B	821	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	A	821	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	B	222	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	648	TRP	CG-CD2-CE3	5.09	138.49	133.90
1	A	222	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	516	ARG	NE-CZ-NH1	5.09	122.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	416	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	A	684	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	B	666	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	B	406	MET	CG-SD-CE	-5.08	92.08	100.20
1	B	648	TRP	CG-CD2-CE3	5.07	138.47	133.90
1	A	416	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	406	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	666	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	A	684	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	B	684	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	B	684	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	A	162	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	516	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:701:GLY:HA2	1:A:707:ARG:HB2	1.88	0.56
1:B:701:GLY:HA2	1:B: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:A:787:ASN:HA	1:A:790:LYS:HE3	1.89	0.54
1:B:787:ASN:HA	1:B: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:A:262:LEU:HD12	1:A:266:VAL:HB	1.93	0.50
1:B:800:ASN:HD22	1:B:809:ARG:HE	1.60	0.50
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:A:272:SER:O	1:A:276:LEU:HG	2.15	0.47
1:A:117:ILE:HG12	1:A:123:ILE:HD11	1.96	0.47
1:A:413:PHE:O	1:A:417:VAL:HG23	2.15	0.47
1:B:184:TYR:HB3	1:B:512:ILE:HG23	1.96	0.47
1:A:382:LYS:HD2	1:A:464:SER:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:HIS:NE2	1:A:281:ILE:CD1	2.77	0.47
1:A:507:MET:HE2	1:A:532:TYR:HE1	1.79	0.47
1:A:571:TYR:CZ	1:A:660:LEU:HD22	2.50	0.47
1:B:413:PHE:O	1:B:417:VAL:HG23	2.15	0.47
1:B:272:SER:O	1:B:276:LEU:HG	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:A:106:GLU:HG2	1:A:132:TYR:CZ	2.51	0.46
1:B:685:ILE:HA	1:B:689:LEU:HB3	1.98	0.46
1:B:571:TYR:CZ	1:B:660:LEU:HD22	2.50	0.46
1:B:195:PRO:HD2	3:B:891:HOH:O	2.14	0.46
1:A:224:PRO:HB2	1:A:229:PRO:HA	1.98	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: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:310:LEU:HB2	1:B:313:ILE:HB	1.98	0.45
1:B:224:PRO:HB2	1:B:229:PRO:HA	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:A:310:LEU:HB2	1:A:313:ILE:HB	1.98	0.45
1:B:100:LYS:NZ	1:B:134:THR:HG21	2.32	0.45
1:B:507:MET:HE2	1:B:532:TYR:HE1	1.81	0.45
1:B:178:LYS:HA	1:B:178:LYS:HD3	1.84	0.45
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:A:163:GLU:O	1:A:167:LYS:HG2	2.18	0.44
1:B:803:PRO:HA	1:B:806:GLN:HG2	2.00	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:A:47:ALA:HB2	1:A:95:GLY:HA3	2.01	0.43
1:B:222:ARG:NH1	1:B:233:LYS:O	2.51	0.43
1:B:504:HIS:CE1	1:B:538:ILE:HD12	2.54	0.43
1:B:68:ASN:HB2	1:B:82:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:NH1	1:A:233:LYS:O	2.51	0.42
1:A:529:THR:HA	1:A:532:TYR:CD2	2.54	0.42
1:A:501:LEU:HA	1:A:505:ALA:HB3	2.01	0.42
1:B:552:ILE:HG21	1:B:750:VAL:HG21	2.00	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:A:68:ASN:HB2	1:A:82:ASN:ND2	2.34	0.42
1:B:501:LEU:HA	1:B:505:ALA:HB3	2.01	0.42
1:A:404:LEU:HA	1:A:404:LEU:HD12	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:HD2	1:A:788:LYS:HA	1.90	0.42
1:B:228:ASP:HA	1:B:229:PRO:HD2	1.82	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:404:LEU:HD12	1:B:404:LEU:HA	1.93	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:592:ILE:HD11	1:B:602:ARG:NH2	2.36	0.41
1:B:298:LYS:HA	1:B:323:HIS:O	2.20	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
1:A:93:ILE:CG2	1:A:117:ILE:HD11	2.51	0.41
1:A:592:ILE:HD11	1:A:602:ARG:NH2	2.36	0.41
1:A:299:LEU:HB2	1:A:304:ILE:HD11	2.03	0.41
1:A:824:SER:HB2	1:A:832:GLY:HA3	2.03	0.41
1:B:497:MET:CG	1:B:570:VAL:HG11	2.51	0.41
1:A:514:THR:HG21	1:A:532:TYR:HE2	1.86	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:B:522:HIS:HA	1:B:523:PRO:HD2	1.92	0.40
1:B:49:LYS:HD2	1:B:57:LYS:HE3	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	46	72
1	B	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	46	72
All	All	1594/1678 (95%)	1528 (96%)	62 (4%)	4 (0%)	46	72

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 (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	705/730 (97%)	658 (93%)	47 (7%)	20 40
1	B	705/730 (97%)	658 (93%)	47 (7%)	20 40
All	All	1410/1460 (97%)	1316 (93%)	94 (7%)	20 40

All (94) 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	134	THR
1	B	139	SER
1	B	158	LEU
1	B	172	ASN
1	B	188	VAL
1	B	194	ASN
1	B	245	ASN
1	B	279	THR
1	B	287	GLN
1	B	323	HIS
1	B	337	GLN
1	B	384	THR
1	B	386	ASP
1	B	387	SER
1	B	407	LEU
1	B	489	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	518	LEU
1	B	528	LEU
1	B	535	ASN
1	B	541	LEU
1	B	550	ASN
1	B	596	SER
1	B	608	TYR
1	B	615	LEU
1	B	616	GLU
1	B	660	LEU
1	B	672	LEU
1	B	699	PRO
1	B	711	SER
1	B	714	LEU
1	B	724	GLU
1	B	735	LEU
1	B	747	SER
1	B	750	VAL
1	B	774	SER
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	134	THR
1	A	139	SER
1	A	158	LEU
1	A	172	ASN
1	A	188	VAL
1	A	194	ASN
1	A	245	ASN
1	A	279	THR
1	A	287	GLN
1	A	323	HIS
1	A	337	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	THR
1	A	386	ASP
1	A	387	SER
1	A	407	LEU
1	A	489	ASN
1	A	518	LEU
1	A	528	LEU
1	A	535	ASN
1	A	541	LEU
1	A	550	ASN
1	A	596	SER
1	A	608	TYR
1	A	615	LEU
1	A	616	GLU
1	A	660	LEU
1	A	672	LEU
1	A	699	PRO
1	A	711	SER
1	A	714	LEU
1	A	724	GLU
1	A	735	LEU
1	A	747	SER
1	A	750	VAL
1	A	774	SER
1	A	819	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	287	GLN
1	B	322	GLN
1	B	787	ASN
1	B	800	ASN
1	A	287	GLN
1	A	322	GLN
1	A	515	HIS
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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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.