



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2IUJ
Title : Crystal Structure of Soybean Lipxygenase-B
Authors : Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on : 2006-06-05
Resolution : 2.40 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

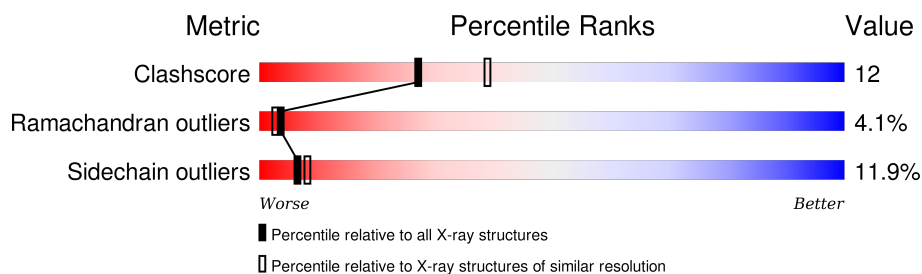
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	853	 60% 29% 7% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6799 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 L-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6692	4307	1110	1262	13			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is water.

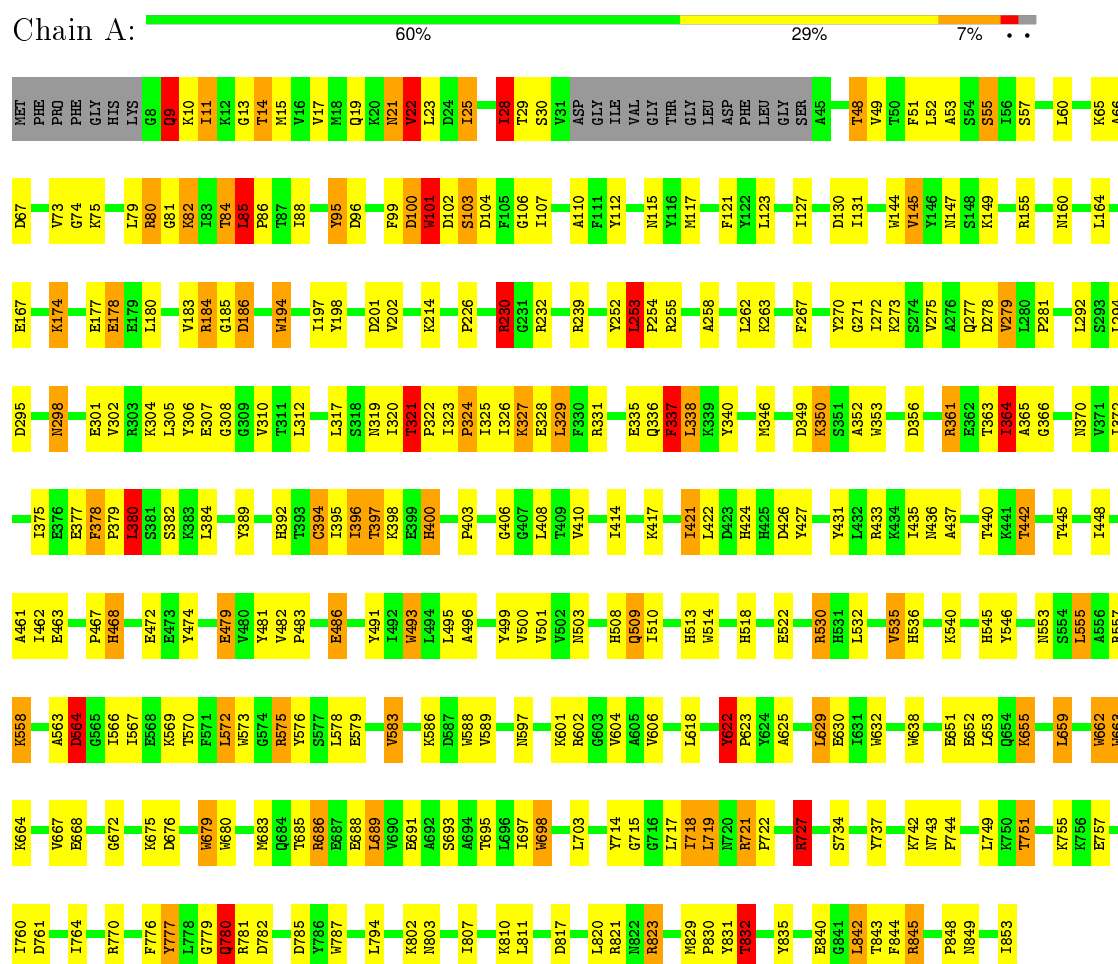
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

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: LIPOXYGENASE L-5



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.99 Å 105.31 Å 105.92 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	89.5 (15.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.050 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	0.80	0/6866	1.58	117/9322 (1.3%)

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	3

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	TRP	CD1-CG-CD2	10.94	115.05	106.30
1	A	602	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	144	TRP	CE2-CD2-CG	-8.97	100.12	107.30
1	A	353	TRP	CD1-CG-CD2	8.93	113.44	106.30
1	A	602	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	680	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	A	101	TRP	CD1-CG-CD2	8.73	113.28	106.30
1	A	679	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	A	727	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	101	TRP	CE2-CD2-CG	-8.38	100.59	107.30
1	A	186	ASP	N-CA-C	8.30	133.41	111.00
1	A	679	TRP	CE2-CD2-CG	-8.21	100.74	107.30
1	A	632	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	A	632	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	A	680	TRP	CE2-CD2-CG	-8.19	100.75	107.30
1	A	638	TRP	CE2-CD2-CG	-8.12	100.80	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	TRP	CE2-CD2-CG	-8.01	100.90	107.30
1	A	663	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	493	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	A	663	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	546	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	A	787	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	353	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	638	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	638	TRP	CG-CD2-CE3	7.57	140.71	133.90
1	A	787	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	A	686	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	588	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	A	15	MET	CG-SD-CE	-7.47	88.25	100.20
1	A	184	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	588	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	835	TYR	CB-CG-CD2	-7.44	116.53	121.00
1	A	514	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	514	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	638	TRP	CB-CG-CD1	-7.34	117.45	127.00
1	A	573	TRP	CD1-CG-CD2	7.31	112.14	106.30
1	A	493	TRP	CG-CD2-CE3	7.26	140.43	133.90
1	A	530	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	573	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	698	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	A	144	TRP	CG-CD2-CE3	7.13	140.32	133.90
1	A	698	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	662	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	194	TRP	CD1-CG-CD2	7.04	111.94	106.30
1	A	662	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	194	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	253	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	239	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	101	TRP	CG-CD2-CE3	6.54	139.79	133.90
1	A	832	THR	CA-CB-CG2	6.51	121.52	112.40
1	A	184	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	821	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	842	LEU	CA-CB-CG	6.36	129.94	115.30
1	A	493	TRP	CB-CG-CD1	-6.35	118.74	127.00
1	A	255	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	397	THR	CA-C-N	-6.32	103.30	117.20
1	A	782	ASP	CA-CB-CG	6.32	127.31	113.40
1	A	632	TRP	CG-CD2-CE3	6.26	139.53	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	TRP	CG-CD1-NE1	-6.25	103.84	110.10
1	A	74	GLY	CA-C-N	-6.21	103.54	117.20
1	A	145	VAL	CG1-CB-CG2	-6.20	100.98	110.90
1	A	680	TRP	CG-CD2-CE3	6.18	139.47	133.90
1	A	832	THR	N-CA-CB	-6.17	98.57	110.30
1	A	230	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	576	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	A	514	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	679	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	A	683	MET	CG-SD-CE	5.90	109.63	100.20
1	A	144	TRP	CB-CG-CD1	-5.87	119.38	127.00
1	A	557	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	467	PRO	N-CA-C	5.83	127.27	112.10
1	A	777	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	79	LEU	CA-C-N	-5.72	104.61	117.20
1	A	679	TRP	CB-CG-CD1	-5.71	119.58	127.00
1	A	575	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	408	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	823	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	22	VAL	N-CA-CB	-5.53	99.33	111.50
1	A	622	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	394	CYS	CA-C-N	-5.52	105.06	117.20
1	A	364	ILE	N-CA-CB	-5.51	98.13	110.80
1	A	755	LYS	CB-CG-CD	-5.50	97.31	111.60
1	A	329	LEU	N-CA-C	-5.45	96.28	111.00
1	A	632	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	A	426	ASP	N-CA-C	5.44	125.68	111.00
1	A	178	GLU	CA-CB-CG	5.43	125.35	113.40
1	A	663	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A	337	PHE	C-N-CA	5.38	135.16	121.70
1	A	340	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	421	ILE	CB-CA-C	-5.38	100.84	111.60
1	A	680	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	A	514	TRP	CB-CG-CD1	-5.33	120.06	127.00
1	A	239	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	782	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	845	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	101	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	A	535	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	A	252	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	74	GLY	O-C-N	5.21	131.03	122.70
1	A	530	ARG	NE-CZ-NH1	5.19	122.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	66	ALA	N-CA-C	5.17	124.96	111.00
1	A	49	VAL	N-CA-C	5.17	124.95	111.00
1	A	306	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	A	95	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	279	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	A	780	GLN	N-CA-C	5.12	124.81	111.00
1	A	396	ILE	N-CA-C	-5.09	97.26	111.00
1	A	9	GLN	N-CA-C	5.08	124.72	111.00
1	A	112	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	787	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	A	49	VAL	N-CA-CB	-5.03	100.44	111.50
1	A	262	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	659	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	588	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	A	448	ILE	CA-C-N	-5.01	106.17	117.20
1	A	787	TRP	CB-CG-CD1	-5.00	120.49	127.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	THR	Peptide
1	A	378	PHE	Peptide
1	A	85	LEU	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	6692	0	6601	160	0
2	A	1	0	0	0	0
3	A	106	0	0	2	0
All	All	6799	0	6601	160	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 12.

All (160) 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:718:ILE:H	1:A:718:ILE:HD13	1.31	0.92
1:A:253:LEU:HD21	1:A:258:ALA:HB2	1.53	0.90
1:A:82:LYS:HG3	1:A:95:TYR:HE2	1.37	0.87
1:A:653:LEU:HD13	1:A:686:ARG:HG3	1.66	0.78
1:A:653:LEU:HD11	1:A:689:LEU:HD12	1.67	0.77
1:A:328:GLU:HA	1:A:331:ARG:HA	1.65	0.77
1:A:394:CYS:SG	1:A:396:ILE:HG12	2.28	0.74
1:A:11:ILE:HG13	1:A:99:PHE:HB2	1.69	0.73
1:A:685:THR:HG22	1:A:688:GLU:H	1.55	0.71
1:A:510:ILE:HD11	1:A:567:ILE:HG21	1.72	0.71
1:A:718:ILE:H	1:A:718:ILE:CD1	2.05	0.70
1:A:518:HIS:HD1	1:A:553:ASN:ND2	1.91	0.69
1:A:442:THR:HG21	1:A:572:LEU:HD11	1.76	0.68
1:A:324:PRO:O	1:A:327:LYS:HB3	1.93	0.68
1:A:715:GLY:HA2	1:A:721:ARG:HB2	1.76	0.66
1:A:832:THR:HG23	1:A:845:ARG:HB3	1.76	0.65
1:A:202:VAL:O	1:A:230:ARG:HD2	1.97	0.65
1:A:51:PHE:H	1:A:82:LYS:HD2	1.62	0.65
1:A:82:LYS:HG3	1:A:95:TYR:CE2	2.28	0.64
1:A:21:ASN:HB2	1:A:28:ILE:HB	1.78	0.63
1:A:777:TYR:HA	1:A:848:PRO:HA	1.80	0.62
1:A:518:HIS:HD1	1:A:553:ASN:HD21	1.50	0.60
1:A:727:ARG:HB2	1:A:751:THR:HG23	1.83	0.60
1:A:378:PHE:HZ	1:A:397:THR:HA	1.66	0.60
1:A:509:GLN:HA	1:A:509:GLN:NE2	2.18	0.59
1:A:400:HIS:H	1:A:400:HIS:CD2	2.18	0.59
1:A:201:ASP:HB2	1:A:232:ARG:HG3	1.85	0.58
1:A:501:VAL:HG11	1:A:721:ARG:HA	1.84	0.58
1:A:180:LEU:HB3	1:A:184:ARG:NH2	2.17	0.58
1:A:28:ILE:HD13	1:A:29:THR:H	1.66	0.58
1:A:17:VAL:HG12	1:A:123:LEU:HA	1.86	0.58
1:A:433:ARG:HD3	1:A:472:GLU:HG3	1.85	0.58
1:A:267:PHE:HB3	1:A:270:TYR:HB3	1.86	0.58
1:A:325:ILE:O	1:A:329:LEU:HB2	2.02	0.58
1:A:501:VAL:HG11	1:A:722:PRO:HD2	1.86	0.58
1:A:436:ASN:HA	1:A:440:THR:O	2.04	0.57
1:A:21:ASN:HD22	1:A:21:ASN:H	1.51	0.57
1:A:652:GLU:HA	1:A:655:LYS:HB2	1.86	0.57
1:A:302:VAL:O	1:A:305:LEU:HB2	2.04	0.57
1:A:583:VAL:HG12	1:A:586:LYS:HE2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG22	1:A:155:ARG:HG3	1.86	0.57
1:A:9:GLN:NE2	1:A:10:LYS:H	2.04	0.56
1:A:479:GLU:HG3	1:A:481:TYR:HE1	1.70	0.56
1:A:651:GLU:O	1:A:655:LYS:HE3	2.05	0.56
1:A:532:LEU:HD13	1:A:662:TRP:HB2	1.88	0.56
1:A:298:ASN:HD22	1:A:301:GLU:H	1.53	0.56
1:A:365:ALA:HB2	1:A:623:PRO:HG2	1.89	0.55
1:A:509:GLN:HE21	1:A:509:GLN:HA	1.72	0.55
1:A:436:ASN:HD21	1:A:442:THR:N	2.04	0.55
1:A:734:SER:HB2	1:A:737:TYR:H	1.71	0.55
1:A:337:PHE:HD1	1:A:338:LEU:H	1.55	0.54
1:A:823:ARG:O	1:A:830:PRO:HA	2.08	0.54
1:A:271:GLY:O	1:A:275:VAL:HG23	2.08	0.54
1:A:149:LYS:HE2	1:A:149:LYS:HA	1.91	0.53
1:A:304:LYS:HA	1:A:307:GLU:HB2	1.89	0.53
1:A:570:THR:HG21	1:A:761:ASP:HB2	1.90	0.52
1:A:566:ILE:HG21	1:A:764:ILE:HG13	1.90	0.52
1:A:9:GLN:O	1:A:100:ASP:HA	2.08	0.52
1:A:384:LEU:HD13	1:A:389:TYR:HB2	1.92	0.52
1:A:102:ASP:CG	1:A:103:SER:H	2.13	0.52
1:A:445:THR:H	1:A:503:ASN:ND2	2.07	0.52
1:A:424:HIS:HB3	1:A:503:ASN:HD22	1.74	0.52
1:A:121:PHE:HE1	1:A:123:LEU:HB2	1.74	0.51
1:A:482:VAL:HG13	1:A:483:PRO:HD2	1.92	0.51
1:A:273:LYS:HB2	1:A:555:LEU:HD11	1.93	0.51
1:A:13:GLY:HA3	1:A:99:PHE:HE2	1.75	0.51
1:A:277:GLN:HE22	1:A:558:LYS:HE2	1.75	0.51
1:A:107:ILE:HD12	1:A:131:ILE:HD11	1.90	0.51
1:A:378:PHE:CZ	1:A:397:THR:HA	2.44	0.51
1:A:230:ARG:HA	1:A:522:GLU:HG2	1.94	0.50
1:A:9:GLN:CD	1:A:10:LYS:H	2.14	0.50
1:A:164:LEU:HD23	3:A:2090:HOH:O	2.11	0.50
1:A:468:HIS:CD2	1:A:474:TYR:HB2	2.47	0.50
1:A:570:THR:CG2	1:A:761:ASP:HB2	2.42	0.49
1:A:335:GLU:HG2	1:A:336:GLN:H	1.77	0.49
1:A:275:VAL:HA	1:A:279:VAL:HB	1.94	0.49
1:A:832:THR:HG22	1:A:844:PHE:O	2.13	0.49
1:A:597:ASN:O	1:A:601:LYS:HG2	2.13	0.49
1:A:319:ASN:HB2	1:A:320:ILE:HD12	1.95	0.48
1:A:375:ILE:HG23	1:A:380:LEU:HD11	1.95	0.48
1:A:718:ILE:N	1:A:718:ILE:HD13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:HB	1:A:322:PRO:HG3	1.95	0.48
1:A:298:ASN:ND2	1:A:301:GLU:N	2.62	0.48
1:A:714:TYR:CE1	1:A:829:MET:SD	3.06	0.48
1:A:410:VAL:O	1:A:414:ILE:HG23	2.14	0.48
1:A:350:LYS:HD2	3:A:2062:HOH:O	2.14	0.47
1:A:198:TYR:HB2	1:A:530:ARG:HG3	1.97	0.47
1:A:445:THR:H	1:A:503:ASN:HD21	1.60	0.47
1:A:298:ASN:ND2	1:A:301:GLU:H	2.13	0.46
1:A:693:SER:O	1:A:697:ILE:HG13	2.15	0.46
1:A:327:LYS:C	1:A:329:LEU:H	2.17	0.46
1:A:513:HIS:CD2	1:A:513:HIS:C	2.87	0.46
1:A:310:VAL:HB	1:A:338:LEU:HB3	1.98	0.46
1:A:499:TYR:OH	1:A:751:THR:HG21	2.16	0.45
1:A:664:LYS:O	1:A:668:GLU:HB2	2.16	0.45
1:A:436:ASN:HD21	1:A:442:THR:H	1.63	0.45
1:A:183:VAL:O	1:A:197:ILE:HA	2.16	0.45
1:A:757:GLU:HA	1:A:760:ILE:HG12	1.97	0.45
1:A:253:LEU:HD21	1:A:258:ALA:CB	2.35	0.45
1:A:479:GLU:HG3	1:A:481:TYR:CE1	2.51	0.45
1:A:19:GLN:O	1:A:22:VAL:HB	2.17	0.45
1:A:115:ASN:HB2	1:A:145:VAL:HG12	1.98	0.45
1:A:779:GLY:C	1:A:781:ARG:H	2.18	0.45
1:A:672:GLY:HA2	1:A:675:LYS:HB3	1.99	0.45
1:A:389:TYR:HB3	1:A:392:HIS:CE1	2.52	0.44
1:A:14:THR:HG23	1:A:127:ILE:HG13	1.99	0.44
1:A:424:HIS:HA	1:A:427:TYR:CE2	2.52	0.44
1:A:417:LYS:HG2	1:A:618:LEU:HD13	1.99	0.44
1:A:400:HIS:N	1:A:400:HIS:CD2	2.85	0.44
1:A:278:ASP:HB3	1:A:323:ILE:HG12	1.99	0.44
1:A:431:TYR:O	1:A:435:ILE:HG13	2.18	0.44
1:A:843:THR:HB	1:A:845:ARG:HG2	1.99	0.44
1:A:364:ILE:CD1	1:A:372:ILE:HG21	2.48	0.44
1:A:84:THR:HA	1:A:88:ILE:HD11	1.99	0.44
1:A:743:ASN:HA	1:A:744:PRO:HD3	1.75	0.44
1:A:85:LEU:N	1:A:86:PRO:HA	2.33	0.43
1:A:563:ALA:O	1:A:564:ASP:HB2	2.18	0.43
1:A:545:HIS:CE1	1:A:849:ASN:HD22	2.36	0.43
1:A:545:HIS:HE1	1:A:849:ASN:HD22	1.65	0.43
1:A:328:GLU:HA	1:A:331:ARG:CA	2.41	0.43
1:A:653:LEU:CD1	1:A:689:LEU:HD12	2.43	0.43
1:A:121:PHE:CE1	1:A:123:LEU:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HG21	1:A:372:ILE:HD12	2.01	0.43
1:A:436:ASN:ND2	1:A:442:THR:H	2.17	0.43
1:A:382:SER:OG	1:A:384:LEU:HG	2.18	0.43
1:A:10:LYS:HA	1:A:99:PHE:O	2.18	0.43
1:A:807:ILE:O	1:A:811:LEU:HD13	2.19	0.43
1:A:101:TRP:CZ3	1:A:106:GLY:O	2.72	0.43
1:A:147:ASN:HD22	1:A:149:LYS:H	1.66	0.43
1:A:81:GLY:HA3	1:A:96:ASP:HB3	2.01	0.43
1:A:382:SER:HB2	1:A:392:HIS:O	2.19	0.42
1:A:349:ASP:HB3	1:A:352:ALA:HB2	2.01	0.42
1:A:776:PHE:HD1	1:A:781:ARG:HB3	1.85	0.42
1:A:536:HIS:O	1:A:540:LYS:HG3	2.19	0.42
1:A:65:LYS:NZ	1:A:104:ASP:HA	2.34	0.42
1:A:717:LEU:HG	1:A:719:LEU:HB2	2.01	0.42
1:A:325:ILE:C	1:A:327:LYS:H	2.23	0.42
1:A:663:TRP:O	1:A:667:VAL:HG22	2.20	0.42
1:A:491:TYR:CD2	1:A:744:PRO:HB2	2.55	0.42
1:A:625:ALA:O	1:A:629:LEU:HD22	2.20	0.42
1:A:25:ILE:H	1:A:25:ILE:HD12	1.84	0.42
1:A:21:ASN:H	1:A:21:ASN:ND2	2.17	0.41
1:A:14:THR:HG23	1:A:127:ILE:CG1	2.50	0.41
1:A:817:ASP:OD1	1:A:820:LEU:HG	2.20	0.41
1:A:396:ILE:HD11	1:A:463:GLU:N	2.35	0.41
1:A:604:VAL:HG21	1:A:622:TYR:HE2	1.84	0.41
1:A:51:PHE:CZ	1:A:117:MET:SD	3.14	0.41
1:A:695:THR:O	1:A:698:TRP:HB3	2.21	0.41
1:A:396:ILE:HD12	1:A:461:ALA:HB1	2.03	0.41
1:A:174:LYS:O	1:A:178:GLU:HB2	2.20	0.41
1:A:779:GLY:O	1:A:781:ARG:N	2.38	0.41
1:A:734:SER:H	1:A:737:TYR:HB3	1.86	0.41
1:A:803:ASN:O	1:A:807:ILE:HG13	2.20	0.41
1:A:60:LEU:O	1:A:73:VAL:HA	2.21	0.41
1:A:770:ARG:HG2	1:A:842:LEU:HB2	2.03	0.40
1:A:589:VAL:HG13	1:A:679:TRP:CD2	2.56	0.40
1:A:496:ALA:O	1:A:500:VAL:HG23	2.20	0.40
1:A:366:GLY:HA2	1:A:714:TYR:CE2	2.56	0.40
1:A:462:ILE:HD12	1:A:493:TRP:CZ3	2.57	0.40
1:A:569:LYS:HD3	1:A:569:LYS:HA	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	829/853 (97%)	714 (86%)	81 (10%)	34 (4%)	3 3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	48	THR
1	A	75	LYS
1	A	84	THR
1	A	186	ASP
1	A	380	LEU
1	A	398	LYS
1	A	780	GLN
1	A	55	SER
1	A	82	LYS
1	A	103	SER
1	A	130	ASP
1	A	185	GLY
1	A	53	ALA
1	A	80	ARG
1	A	110	ALA
1	A	327	LYS
1	A	403	PRO
1	A	564	ASP
1	A	831	TYR
1	A	167	GLU
1	A	308	GLY
1	A	437	ALA
1	A	468	HIS
1	A	486	GLU
1	A	508	HIS
1	A	30	SER
1	A	326	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	LEU
1	A	160	ASN
1	A	406	GLY
1	A	742	LYS
1	A	85	LEU
1	A	379	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	724/739 (98%)	638 (88%)	86 (12%)	6 8

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	ILE
1	A	14	THR
1	A	21	ASN
1	A	22	VAL
1	A	23	LEU
1	A	25	ILE
1	A	28	ILE
1	A	48	THR
1	A	52	LEU
1	A	55	SER
1	A	57	SER
1	A	67	ASP
1	A	80	ARG
1	A	100	ASP
1	A	101	TRP
1	A	174	LYS
1	A	177	GLU
1	A	194	TRP
1	A	214	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	PRO
1	A	230	ARG
1	A	253	LEU
1	A	254	PRO
1	A	263	LYS
1	A	272	ILE
1	A	281	PRO
1	A	292	LEU
1	A	294	LEU
1	A	295	ASP
1	A	298	ASN
1	A	312	LEU
1	A	317	LEU
1	A	321	THR
1	A	324	PRO
1	A	337	PHE
1	A	346	MET
1	A	350	LYS
1	A	356	ASP
1	A	361	ARG
1	A	364	ILE
1	A	370	ASN
1	A	377	GLU
1	A	380	LEU
1	A	395	ILE
1	A	400	HIS
1	A	421	ILE
1	A	422	LEU
1	A	442	THR
1	A	479	GLU
1	A	486	GLU
1	A	495	LEU
1	A	509	GLN
1	A	535	VAL
1	A	555	LEU
1	A	558	LYS
1	A	564	ASP
1	A	572	LEU
1	A	575	ARG
1	A	578	LEU
1	A	579	GLU
1	A	583	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	606	VAL
1	A	622	TYR
1	A	629	LEU
1	A	630	GLU
1	A	655	LYS
1	A	659	LEU
1	A	676	ASP
1	A	689	LEU
1	A	691	GLU
1	A	703	LEU
1	A	718	ILE
1	A	719	LEU
1	A	721	ARG
1	A	727	ARG
1	A	749	LEU
1	A	751	THR
1	A	780	GLN
1	A	785	ASP
1	A	794	LEU
1	A	802	LYS
1	A	810	LYS
1	A	832	THR
1	A	840	GLU
1	A	853	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	21	ASN
1	A	147	ASN
1	A	277	GLN
1	A	298	ASN
1	A	336	GLN
1	A	347	GLN
1	A	370	ASN
1	A	392	HIS
1	A	404	ASN
1	A	436	ASN
1	A	503	ASN
1	A	509	GLN
1	A	529	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	553	ASN
1	A	593	GLN
1	A	660	GLN
1	A	711	GLN
1	A	822	ASN
1	A	849	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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