



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:14 pm BST

PDB ID : 1N8Q  
Title : LIPOXYGENASE IN COMPLEX WITH PROTOCATECHUIC ACID  
Authors : Borbulevych, O.Y.; Jankun, J.; Selman, S.H.; Skrzypczak-Jankun, E.  
Deposited on : 2002-11-21  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

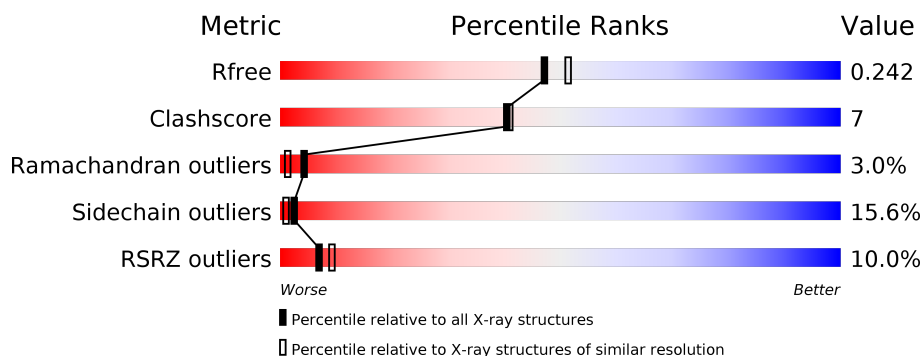
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	857	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHB	A	859	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7253 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.

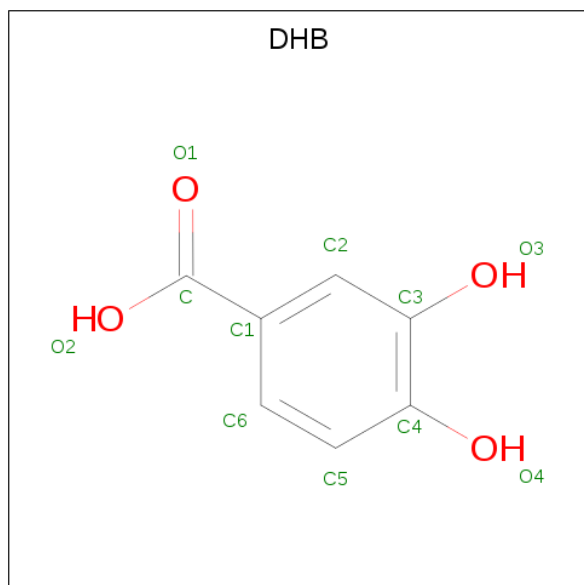
- Molecule 1 is a protein called lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6778	4329	1163	1268	18			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		

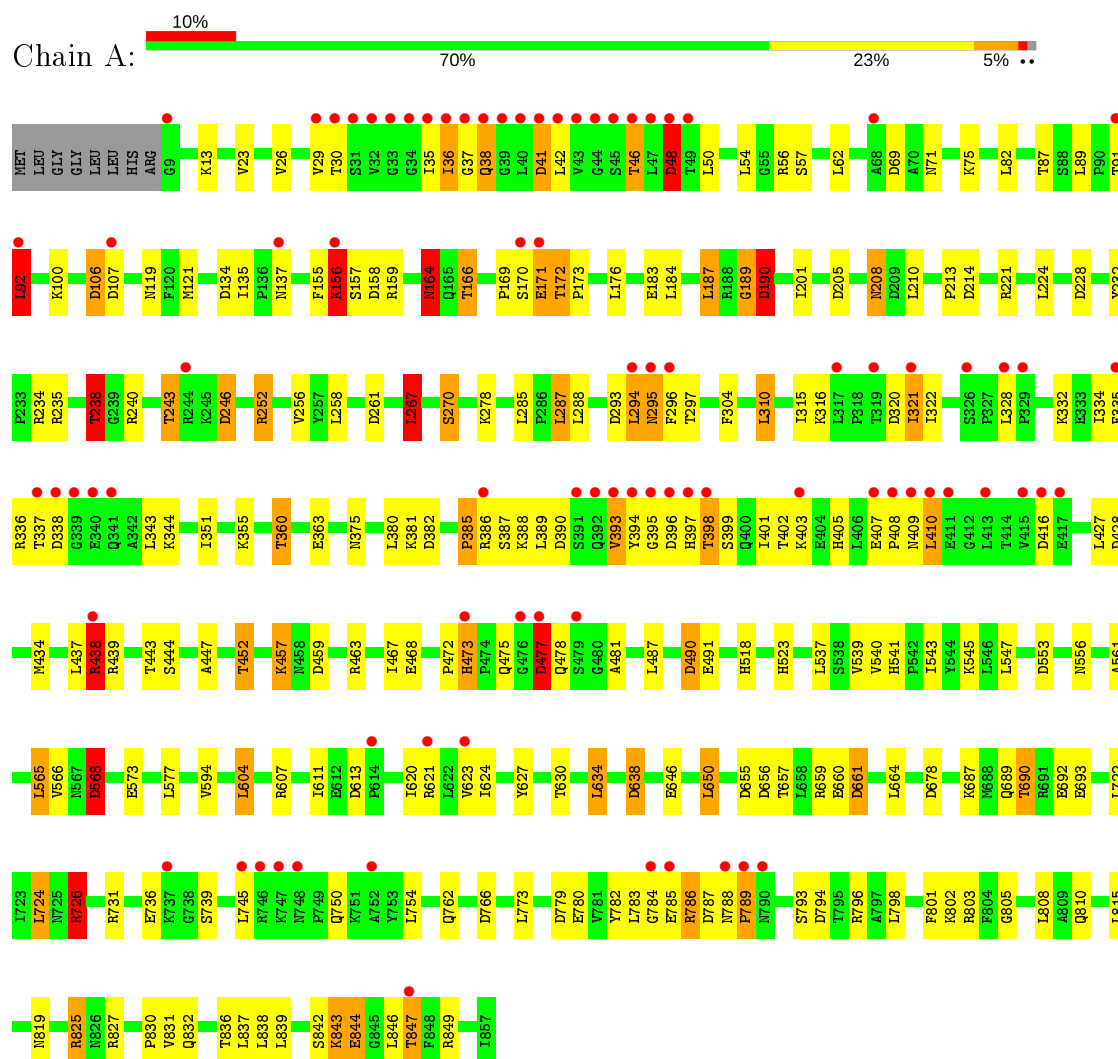
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	463	Total 463	O 463	0	0

### 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 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: lipoxxygenase-3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.64Å 136.96Å 61.80Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.10) 96.3 (48.52-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.189 , 0.245 0.187 , 0.242	Depositor DCC
$R_{free}$ test set	2659 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, DHB

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	0.67	1/6950 (0.0%)	1.13	54/9439 (0.6%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	780	GLU	CD-OE2	5.06	1.31	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ARG	NE-CZ-NH2	-13.57	113.51	120.30
1	A	234	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	A	234	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	607	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	A	41	ASP	CB-CG-OD2	10.78	128.00	118.30
1	A	240	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	294	LEU	CA-CB-CG	8.83	135.61	115.30
1	A	613	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	240	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	459	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	246	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	396	ASP	CB-CG-OD2	7.39	124.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	134	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	787	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	69	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	678	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	490	ASP	CB-CG-OD2	6.50	124.14	118.30
1	A	477	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	205	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	159	ARG	CG-CD-NE	-6.23	98.72	111.80
1	A	214	ASP	CB-CG-OD2	6.23	123.90	118.30
1	A	439	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	794	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	656	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	786	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	A	238	THR	N-CA-C	-5.76	95.44	111.00
1	A	724	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	766	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	568	ASP	C-N-CA	-5.56	110.62	122.30
1	A	107	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	270	SER	N-CA-CB	5.54	118.81	110.50
1	A	650	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	779	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	221	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	285	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	428	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	655	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	252	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	92	LEU	C-N-CA	-5.25	111.27	122.30
1	A	293	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	416	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	661	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	190	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	48	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	234	ARG	CD-NE-CZ	5.16	130.82	123.60
1	A	310	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	638	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	623	VAL	N-CA-C	-5.13	97.15	111.00
1	A	438	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	158	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	189	GLY	N-CA-C	5.07	125.78	113.10
1	A	267	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	187	LEU	CA-CB-CG	5.05	126.91	115.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	GLU	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	6778	0	6701	97	0
2	A	1	0	0	0	0
3	A	11	0	3	6	0
4	A	463	0	0	12	0
All	All	7253	0	6704	97	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 7.

All (97) 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:36:ILE:HG22	1:A:37:GLY:H	1.34	0.91
1:A:541:HIS:HD2	1:A:543:ILE:H	1.20	0.90
1:A:785:GLU:HB2	1:A:805:GLY:HA3	1.51	0.90
1:A:842:SER:OG	1:A:847:THR:HG21	1.79	0.82
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.61	0.79
1:A:36:ILE:HG22	1:A:37:GLY:N	2.03	0.72
1:A:294:LEU:HD23	1:A:295:ASN:N	2.05	0.71
1:A:294:LEU:HD23	1:A:295:ASN:H	1.56	0.70
1:A:785:GLU:OE2	1:A:802:LYS:HA	1.91	0.69
1:A:56:ARG:NH1	4:A:1493:HOH:O	2.24	0.69
1:A:646:GLU:OE2	1:A:803:ARG:NH2	2.26	0.68
1:A:294:LEU:HD23	1:A:296:PHE:H	1.59	0.66
1:A:335:PHE:CD1	1:A:343:LEU:HD11	2.31	0.65
1:A:385:PRO:HD2	1:A:399:SER:HB3	1.78	0.65
1:A:847:THR:HG23	1:A:849:ARG:HG2	1.79	0.63
1:A:238:THR:HG21	4:A:1091:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ILE:HD11	1:A:468:GLU:HB2	1.82	0.61
1:A:773:LEU:CD1	3:A:859:DHB:H5	2.29	0.61
1:A:36:ILE:HG21	1:A:267:LEU:HB3	1.81	0.61
1:A:438:ARG:HD2	1:A:473:HIS:CE1	2.35	0.60
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.83	0.59
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.84	0.59
1:A:208:ASN:H	1:A:208:ASN:HD22	1.49	0.59
1:A:541:HIS:CD2	1:A:543:ILE:H	2.11	0.59
1:A:785:GLU:HB2	1:A:805:GLY:CA	2.27	0.59
1:A:773:LEU:HD11	3:A:859:DHB:H5	1.84	0.59
1:A:360:THR:HG22	1:A:363:GLU:H	1.68	0.58
1:A:657:THR:HG21	4:A:941:HOH:O	2.03	0.58
1:A:213:PRO:HG2	1:A:243:THR:HG21	1.84	0.58
1:A:164:ASN:HD22	1:A:793:SER:HB3	1.70	0.57
1:A:294:LEU:CD2	1:A:296:PHE:H	2.18	0.56
1:A:437:LEU:HD23	1:A:472:PRO:HD3	1.86	0.56
1:A:385:PRO:HD2	1:A:399:SER:CB	2.36	0.56
1:A:169:PRO:HG2	1:A:661:ASP:OD1	2.06	0.56
1:A:437:LEU:HB3	1:A:472:PRO:HG3	1.86	0.56
1:A:788:ASN:CB	1:A:789:PRO:HD3	2.36	0.55
1:A:819:ASN:ND2	1:A:827:ARG:HE	2.05	0.55
1:A:783:LEU:O	1:A:785:GLU:N	2.39	0.54
1:A:402:THR:H	1:A:405:HIS:HD2	1.54	0.54
1:A:170:SER:HB3	4:A:1001:HOH:O	2.08	0.53
1:A:208:ASN:ND2	1:A:235:ARG:HH21	2.06	0.53
1:A:726:ARG:HD3	4:A:1228:HOH:O	2.08	0.52
1:A:788:ASN:HB3	1:A:789:PRO:HD3	1.91	0.52
1:A:36:ILE:CG2	1:A:37:GLY:N	2.71	0.52
1:A:155:PHE:O	1:A:156:LYS:HG2	2.09	0.51
1:A:690:THR:HG22	1:A:693:GLU:H	1.76	0.51
1:A:37:GLY:C	1:A:38:GLN:HE21	2.14	0.51
1:A:561:ALA:HA	1:A:565:LEU:HB2	1.92	0.51
1:A:304:PHE:H	1:A:750:GLN:NE2	2.08	0.51
1:A:26:VAL:O	1:A:30:THR:HG23	2.11	0.50
1:A:119:ASN:OD1	1:A:121:MET:HB2	2.12	0.49
1:A:568:ASP:O	1:A:573:GLU:OE1	2.30	0.49
1:A:294:LEU:HD21	1:A:296:PHE:CD2	2.47	0.49
1:A:75:LYS:NZ	4:A:1279:HOH:O	2.45	0.49
1:A:287:LEU:HD23	1:A:321:ILE:HG23	1.95	0.48
1:A:659:ARG:NH1	1:A:689:GLN:O	2.46	0.48
1:A:825:ARG:NH1	4:A:1233:HOH:O	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ARG:HB2	1:A:344:LYS:HB3	1.95	0.47
1:A:843:LYS:O	1:A:844:GLU:HB2	2.14	0.47
1:A:360:THR:HG21	1:A:830:PRO:HG3	1.96	0.47
1:A:394:TYR:HB3	1:A:481:ALA:CB	2.44	0.47
1:A:410:LEU:HG	1:A:457:LYS:HG2	1.98	0.46
1:A:393:VAL:HB	1:A:397:HIS:HB2	1.98	0.46
1:A:166:THR:HG21	4:A:868:HOH:O	2.15	0.46
1:A:156:LYS:HB3	1:A:156:LYS:HE2	1.42	0.45
1:A:166:THR:HG22	1:A:545:LYS:HZ2	1.81	0.45
1:A:37:GLY:O	1:A:38:GLN:NE2	2.49	0.44
1:A:172:THR:HB	1:A:173:PRO:HD3	1.99	0.44
1:A:782:TYR:O	1:A:786:ARG:HB2	2.17	0.44
1:A:518:HIS:HE1	3:A:859:DHB:C5	2.30	0.44
1:A:106:ASP:OD1	1:A:106:ASP:N	2.50	0.43
1:A:169:PRO:C	1:A:171:GLU:N	2.66	0.43
1:A:46:THR:H	1:A:48:ASP:HB2	1.82	0.43
1:A:773:LEU:HD13	3:A:859:DHB:H5	1.98	0.43
1:A:137:ASN:HB2	4:A:1039:HOH:O	2.17	0.43
1:A:541:HIS:HE1	1:A:661:ASP:OD2	2.02	0.43
1:A:381:LYS:HD3	1:A:381:LYS:HA	1.83	0.43
1:A:785:GLU:CB	1:A:805:GLY:HA3	2.36	0.42
1:A:189:GLY:O	1:A:190:ASP:HB3	2.19	0.42
1:A:473:HIS:CD2	1:A:477:ASP:HA	2.55	0.42
1:A:36:ILE:HA	1:A:36:ILE:HD13	1.90	0.42
1:A:611:ILE:HD11	1:A:621:ARG:HD3	2.01	0.42
1:A:478:GLN:NE2	4:A:1115:HOH:O	2.51	0.42
1:A:385:PRO:O	1:A:398:THR:HB	2.20	0.42
1:A:452:THR:HB	1:A:467:ILE:HG12	2.02	0.42
1:A:620:ILE:HD11	1:A:634:LEU:HD21	2.01	0.41
1:A:288:LEU:HD12	1:A:288:LEU:HA	1.87	0.41
1:A:523:HIS:CE1	3:A:859:DHB:O3	2.73	0.41
1:A:518:HIS:HE1	3:A:859:DHB:C4	2.33	0.41
1:A:189:GLY:HA3	1:A:201:ILE:HG23	2.03	0.41
1:A:57:SER:HB3	1:A:121:MET:HG3	2.02	0.41
1:A:785:GLU:HG2	1:A:801:PHE:CE2	2.55	0.41
1:A:164:ASN:ND2	4:A:1080:HOH:O	2.54	0.41
1:A:836:THR:HA	1:A:839:LEU:HD13	2.03	0.41
1:A:604:LEU:HD11	1:A:630:THR:OG1	2.20	0.40
1:A:443:THR:HG22	4:A:1277:HOH:O	2.20	0.40
1:A:243:THR:HG22	1:A:246:ASP:O	2.21	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	847/857 (99%)	773 (91%)	49 (6%)	25 (3%)	<b>4</b> <b>1</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	A	408	PRO
1	A	477	ASP
1	A	784	GLY
1	A	789	PRO
1	A	844	GLU
1	A	35	ILE
1	A	42	LEU
1	A	46	THR
1	A	48	ASP
1	A	164	ASN
1	A	190	ASP
1	A	270	SER
1	A	295	ASN
1	A	36	ILE
1	A	41	ASP
1	A	156	LYS
1	A	261	ASP
1	A	398	THR
1	A	390	ASP
1	A	92	LEU
1	A	157	SER
1	A	473	HIS
1	A	624	ILE
1	A	393	VAL

### 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	743/749 (99%)	627 (84%)	116 (16%)	<b>2</b> <b>1</b>

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	23	VAL
1	A	29	VAL
1	A	38	GLN
1	A	50	LEU
1	A	54	LEU
1	A	62	LEU
1	A	71	ASN
1	A	82	LEU
1	A	87	THR
1	A	89	LEU
1	A	91	THR
1	A	92	LEU
1	A	100	LYS
1	A	106	ASP
1	A	135	ILE
1	A	156	LYS
1	A	164	ASN
1	A	166	THR
1	A	176	LEU
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	190	ASP
1	A	208	ASN
1	A	210	LEU
1	A	224	LEU
1	A	228	ASP
1	A	232	TYR
1	A	238	THR

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Mol	Chain	Res	Type
1	A	243	THR
1	A	252	ARG
1	A	256	VAL
1	A	258	LEU
1	A	267	LEU
1	A	278	LYS
1	A	287	LEU
1	A	297	THR
1	A	310	LEU
1	A	315	ILE
1	A	316	LYS
1	A	320	ASP
1	A	321	ILE
1	A	322	ILE
1	A	328	LEU
1	A	332	LYS
1	A	334	ILE
1	A	337	THR
1	A	338	ASP
1	A	351	ILE
1	A	355	LYS
1	A	360	THR
1	A	375	ASN
1	A	380	LEU
1	A	382	ASP
1	A	385	PRO
1	A	386	ARG
1	A	388	LYS
1	A	389	LEU
1	A	403	LYS
1	A	407	GLU
1	A	409	ASN
1	A	410	LEU
1	A	427	LEU
1	A	434	MET
1	A	438	ARG
1	A	444	SER
1	A	452	THR
1	A	457	LYS
1	A	463	ARG
1	A	475	GLN
1	A	487	LEU

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Mol	Chain	Res	Type
1	A	490	ASP
1	A	491	GLU
1	A	537	LEU
1	A	539	VAL
1	A	540	VAL
1	A	547	LEU
1	A	553	ASP
1	A	556	ASN
1	A	565	LEU
1	A	566	VAL
1	A	568	ASP
1	A	594	VAL
1	A	604	LEU
1	A	627	TYR
1	A	634	LEU
1	A	638	ASP
1	A	650	LEU
1	A	660	GLU
1	A	664	LEU
1	A	687	LYS
1	A	690	THR
1	A	692	GLU
1	A	722	LEU
1	A	724	LEU
1	A	726	ARG
1	A	731	ARG
1	A	736	GLU
1	A	739	SER
1	A	745	LEU
1	A	754	LEU
1	A	762	GLN
1	A	796	ARG
1	A	798	LEU
1	A	808	LEU
1	A	810	GLN
1	A	815	LEU
1	A	825	ARG
1	A	831	VAL
1	A	832	GLN
1	A	837	LEU
1	A	838	LEU
1	A	843	LYS

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Mol	Chain	Res	Type
1	A	846	LEU
1	A	847	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	102	ASN
1	A	122	GLN
1	A	164	ASN
1	A	208	ASN
1	A	282	GLN
1	A	308	HIS
1	A	375	ASN
1	A	405	HIS
1	A	473	HIS
1	A	521	ASN
1	A	534	ASN
1	A	541	HIS
1	A	556	ASN
1	A	574	GLN
1	A	618	HIS
1	A	665	GLN
1	A	725	ASN
1	A	750	GLN
1	A	762	GLN
1	A	810	GLN
1	A	813	ASN
1	A	819	ASN
1	A	832	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DHB	A	859	-	9,11,11	1.69	3 (33%)	12,15,15	1.57	4 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DHB	A	859	-	-	0/0/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	859	DHB	O4-C4	-2.90	1.30	1.36
3	A	859	DHB	O3-C3	-2.53	1.31	1.36
3	A	859	DHB	C4-C3	-2.40	1.36	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	859	DHB	C6-C1-C2	3.09	122.54	118.16
3	A	859	DHB	C5-C6-C1	-2.62	117.36	121.13
3	A	859	DHB	C1-C2-C3	-2.31	118.84	120.68
3	A	859	DHB	C2-C1-C	-2.03	117.69	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	859	DHB	6	0

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	849/857 (99%)	0.52	85 (10%) 7 9	12, 26, 63, 80	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	26.1
1	A	43	VAL	14.1
1	A	40	LEU	11.8
1	A	45	SER	11.3
1	A	36	ILE	10.6
1	A	397	HIS	10.3
1	A	41	ASP	10.3
1	A	409	ASN	9.4
1	A	395	GLY	9.0
1	A	9	GLY	8.8
1	A	32	VAL	8.3
1	A	47	LEU	8.1
1	A	33	GLY	7.8
1	A	35	ILE	7.7
1	A	31	SER	7.6
1	A	38	GLN	7.5
1	A	784	GLY	7.3
1	A	34	GLY	7.2
1	A	410	LEU	7.2
1	A	46	THR	6.9
1	A	396	ASP	6.8
1	A	37	GLY	5.5
1	A	394	TYR	5.4
1	A	785	GLU	5.1
1	A	42	LEU	5.1
1	A	296	PHE	4.8
1	A	107	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	49	THR	4.6
1	A	411	GLU	4.6
1	A	393	VAL	4.3
1	A	341	GLN	4.3
1	A	39	GLY	4.2
1	A	790	ASN	4.1
1	A	339	GLY	4.0
1	A	413	LEU	3.8
1	A	407	GLU	3.6
1	A	317	LEU	3.6
1	A	479	SER	3.5
1	A	171	GLU	3.4
1	A	747	LYS	3.3
1	A	473	HIS	3.3
1	A	408	PRO	3.3
1	A	737	LYS	3.2
1	A	335	PHE	3.2
1	A	137	ASN	3.1
1	A	170	SER	3.1
1	A	415	VAL	3.1
1	A	338	ASP	3.0
1	A	745	LEU	3.0
1	A	92	LEU	2.9
1	A	321	ILE	2.9
1	A	326	SER	2.9
1	A	476	GLY	2.8
1	A	295	ASN	2.8
1	A	752	ALA	2.8
1	A	337	THR	2.7
1	A	156	LYS	2.7
1	A	746	ARG	2.7
1	A	48	ASP	2.7
1	A	789	PRO	2.6
1	A	91	THR	2.6
1	A	614	PRO	2.6
1	A	340	GLU	2.5
1	A	416	ASP	2.5
1	A	417	GLU	2.5
1	A	438	ARG	2.5
1	A	391	SER	2.5
1	A	788	ASN	2.4
1	A	621	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	403	LYS	2.3
1	A	398	THR	2.3
1	A	30	THR	2.3
1	A	748	ASN	2.3
1	A	847	THR	2.3
1	A	29	VAL	2.3
1	A	319	THR	2.2
1	A	329	PRO	2.2
1	A	244	ARG	2.2
1	A	68	ALA	2.2
1	A	294	LEU	2.1
1	A	386	ARG	2.1
1	A	623	VAL	2.1
1	A	477	ASP	2.1
1	A	392	GLN	2.0
1	A	328	LEU	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DHB	A	859	11/11	0.61	0.46	59,61,63,63	11
2	FE2	A	858	1/1	0.86	0.09	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.