



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:18 AM GMT

PDB ID : 2BP2  
Title : THE STRUCTURE OF BOVINE PANCREATIC PROPHOSPHOLIPASE  
A2 AT 3.0 ANGSTROMS RESOLUTION  
Authors : Dijkstra, B.W.; Vannes, G.J.H.; Kalk, K.H.; Brandenburg, N.P.; Hol, W.G.J.;  
Drenth, J.  
Deposited on : 1981-06-05  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

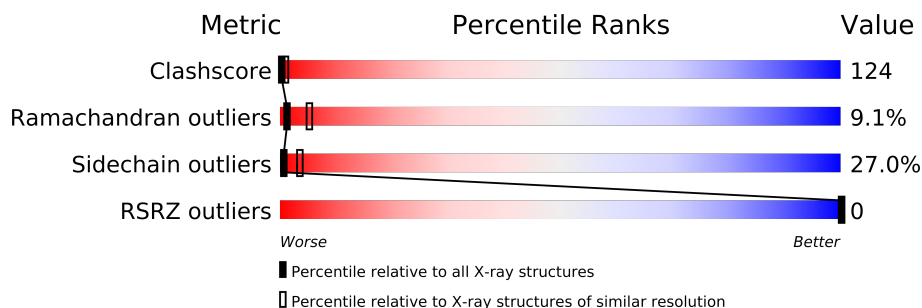
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	130	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 956 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHOLIPASE A2.

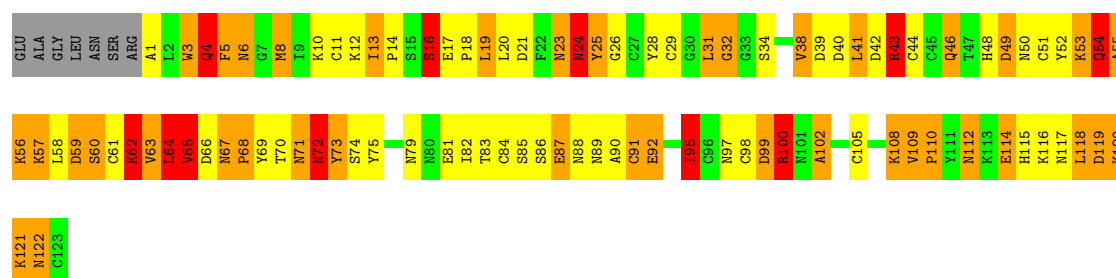
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	956	586	164	191	15	0	0	0

### 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.

#### • Molecule 1: PHOSPHOLIPASE A2

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.95Å 46.95Å 102.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00 7.02 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 99.1 (7.02-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.219 , (Not available) 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 104.9	EDS
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 2697 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.83% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.44	5/975 (0.5%)	2.55	49/1317 (3.7%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	TRP	NE1-CE2	-7.56	1.27	1.37
1	A	114	GLU	CD-OE2	-6.40	1.18	1.25
1	A	91	CYS	CB-SG	5.57	1.91	1.82
1	A	3	TRP	CD1-NE1	5.47	1.47	1.38
1	A	28	TYR	CD1-CE1	5.07	1.47	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	CD-NE-CZ	28.70	163.79	123.60
1	A	100	ARG	NE-CZ-NH2	18.49	129.54	120.30
1	A	87	GLU	OE1-CD-OE2	15.09	141.41	123.30
1	A	100	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	A	42	ASP	CB-CG-OD1	12.39	129.45	118.30
1	A	59	ASP	CB-CG-OD1	10.05	127.35	118.30
1	A	4	GLN	CA-CB-CG	9.63	134.59	113.40
1	A	71	ASN	CA-CB-CG	-8.94	93.73	113.40
1	A	24	ASN	CA-CB-CG	-8.74	94.18	113.40
1	A	87	GLU	CG-CD-OE1	-8.62	101.07	118.30
1	A	92	GLU	OE1-CD-OE2	8.45	133.43	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	39	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	A	25	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	A	64	LEU	N-CA-C	-7.32	91.23	111.00
1	A	114	GLU	OE1-CD-OE2	7.27	132.03	123.30
1	A	4	GLN	CA-C-O	-7.26	104.85	120.10
1	A	92	GLU	CG-CD-OE1	-7.25	103.81	118.30
1	A	97	ASN	CA-CB-CG	-7.23	97.50	113.40
1	A	4	GLN	N-CA-CB	7.15	123.47	110.60
1	A	122	ASN	CA-CB-CG	-7.11	97.77	113.40
1	A	46	GLN	CA-CB-CG	-6.89	98.23	113.40
1	A	39	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	54	GLN	CA-CB-CG	-6.43	99.25	113.40
1	A	71	ASN	N-CA-CB	6.38	122.08	110.60
1	A	67	ASN	CA-CB-CG	-6.26	99.62	113.40
1	A	13	ILE	CA-CB-CG2	-6.18	98.54	110.90
1	A	40	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	43	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	64	LEU	CA-C-N	-6.09	103.80	117.20
1	A	89	ASN	CA-CB-CG	-5.93	100.36	113.40
1	A	87	GLU	CA-CB-CG	-5.90	100.41	113.40
1	A	89	ASN	OD1-CG-ND2	5.67	134.94	121.90
1	A	3	TRP	NE1-CE2-CZ2	-5.55	124.29	130.40
1	A	99	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	100	ARG	CD-NE-CZ	-5.52	115.87	123.60
1	A	5	PHE	N-CA-CB	5.51	120.52	110.60
1	A	99	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	38	VAL	CA-CB-CG2	5.43	119.05	110.90
1	A	79	ASN	CB-CG-OD1	5.33	132.26	121.60
1	A	72	ASN	CA-CB-CG	-5.32	101.69	113.40
1	A	16	SER	C-N-CA	5.29	134.92	121.70
1	A	110	PRO	CA-N-CD	-5.21	104.20	111.50
1	A	95	ILE	CA-CB-CG2	-5.14	100.61	110.90
1	A	42	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	112	ASN	N-CA-CB	-5.13	101.37	110.60
1	A	65	VAL	N-CA-CB	-5.10	100.28	111.50
1	A	73	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	102	ALA	CB-CA-C	-5.07	102.50	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ASP	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	956	0	885	228	11
All	All	956	0	885	228	11

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 124.

All (228) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:ARG:HH12	1:A:46:GLN:CG	1.04	1.55
1:A:43:ARG:NH1	1:A:46:GLN:CB	1.74	1.50
1:A:43:ARG:NH1	1:A:46:GLN:CG	1.73	1.45
1:A:67:ASN:CB	1:A:70:THR:OG1	1.78	1.28
1:A:41:LEU:O	1:A:41:LEU:HD12	1.35	1.26
1:A:43:ARG:NH1	1:A:46:GLN:HB3	1.36	1.23
1:A:62:LYS:O	1:A:65:VAL:CA	1.87	1.22
1:A:58:LEU:HD12	1:A:61:CYS:SG	1.82	1.20
1:A:60:SER:O	1:A:64:LEU:CD1	1.93	1.16
1:A:64:LEU:O	1:A:65:VAL:HG13	1.40	1.16
1:A:3:TRP:CH2	1:A:4:GLN:HG3	1.81	1.16
1:A:3:TRP:CZ2	1:A:4:GLN:HG3	1.82	1.14
1:A:64:LEU:C	1:A:65:VAL:HG13	1.62	1.13
1:A:5:PHE:CD1	1:A:99:ASP:HB3	1.86	1.10
1:A:64:LEU:C	1:A:65:VAL:CG1	2.21	1.09
1:A:67:ASN:HB3	1:A:70:THR:OG1	0.89	1.06
1:A:43:ARG:NH1	1:A:46:GLN:HG2	1.45	1.05
1:A:62:LYS:O	1:A:65:VAL:HA	1.50	1.04
1:A:43:ARG:HH11	1:A:46:GLN:CB	1.47	1.04
1:A:13:ILE:HG22	1:A:16:SER:HB2	1.39	1.03
1:A:56:LYS:HD3	1:A:68:PRO:HG3	1.38	1.03
1:A:55:ALA:O	1:A:58:LEU:HG	1.57	1.02

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:ILE:O	1:A:16:SER:HB2	1.59	1.02
1:A:121:LYS:HE3	1:A:121:LYS:HA	1.43	1.01
1:A:59:ASP:O	1:A:62:LYS:HB2	1.61	1.00
1:A:60:SER:O	1:A:64:LEU:HD11	1.61	0.97
1:A:55:ALA:O	1:A:58:LEU:CG	2.14	0.95
1:A:43:ARG:HH12	1:A:46:GLN:CB	1.54	0.94
1:A:62:LYS:O	1:A:65:VAL:N	2.01	0.93
1:A:1:ALA:N	1:A:71:ASN:O	2.02	0.93
1:A:8:MET:HE1	1:A:99:ASP:HB2	1.48	0.92
1:A:3:TRP:HE1	1:A:72:ASN:ND2	1.67	0.92
1:A:13:ILE:HG22	1:A:13:ILE:O	1.71	0.91
1:A:60:SER:C	1:A:64:LEU:HD11	1.89	0.91
1:A:41:LEU:O	1:A:44:CYS:HB2	1.70	0.91
1:A:1:ALA:H1	1:A:71:ASN:N	1.70	0.90
1:A:67:ASN:OD1	1:A:70:THR:N	2.05	0.90
1:A:121:LYS:HE3	1:A:121:LYS:CA	2.02	0.88
1:A:38:VAL:HG11	1:A:118:LEU:CD1	2.05	0.87
1:A:3:TRP:HE1	1:A:72:ASN:HD21	0.90	0.87
1:A:52:TYR:OH	1:A:99:ASP:OD2	1.92	0.86
1:A:119:ASP:OD1	1:A:121:LYS:HB2	1.74	0.86
1:A:5:PHE:HE1	1:A:99:ASP:O	1.58	0.86
1:A:56:LYS:HD3	1:A:68:PRO:CG	2.05	0.86
1:A:8:MET:CE	1:A:99:ASP:HB2	2.06	0.85
1:A:1:ALA:H1	1:A:71:ASN:H	1.24	0.85
1:A:41:LEU:C	1:A:41:LEU:HD12	1.96	0.85
1:A:43:ARG:HH12	1:A:46:GLN:HG2	0.69	0.85
1:A:66:ASP:CG	1:A:67:ASN:N	2.30	0.83
1:A:5:PHE:CE1	1:A:99:ASP:HB3	2.12	0.83
1:A:43:ARG:HH11	1:A:46:GLN:HB3	0.68	0.83
1:A:119:ASP:O	1:A:121:LYS:N	2.12	0.83
1:A:1:ALA:CB	1:A:71:ASN:O	2.27	0.83
1:A:120:LYS:N	1:A:120:LYS:HD3	1.93	0.83
1:A:59:ASP:HA	1:A:62:LYS:HD3	1.60	0.82
1:A:58:LEU:O	1:A:62:LYS:HD2	1.80	0.81
1:A:49:ASP:O	1:A:53:LYS:HG2	1.80	0.80
1:A:67:ASN:HB3	1:A:70:THR:HG1	1.47	0.78
1:A:3:TRP:CE2	1:A:4:GLN:HG3	2.19	0.77
1:A:4:GLN:OE1	1:A:4:GLN:N	2.16	0.77
1:A:60:SER:O	1:A:64:LEU:HG	1.86	0.76
1:A:5:PHE:CD1	1:A:99:ASP:CB	2.68	0.76
1:A:60:SER:O	1:A:64:LEU:CG	2.33	0.76
1:A:26:GLY:HA2	1:A:118:LEU:HD12	1.65	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:ASN:ND2	1:A:19:LEU:HG	2.02	0.74
1:A:60:SER:O	1:A:64:LEU:HD12	1.87	0.74
1:A:3:TRP:CZ2	1:A:4:GLN:CG	2.68	0.74
1:A:119:ASP:OD1	1:A:121:LYS:N	2.19	0.74
1:A:67:ASN:OD1	1:A:70:THR:HG23	1.89	0.73
1:A:67:ASN:HB3	1:A:70:THR:CB	2.16	0.73
1:A:13:ILE:O	1:A:16:SER:CB	2.35	0.73
1:A:58:LEU:CD1	1:A:61:CYS:SG	2.71	0.73
1:A:1:ALA:N	1:A:71:ASN:N	2.36	0.72
1:A:3:TRP:CZ3	1:A:4:GLN:HG3	2.24	0.72
1:A:1:ALA:HB3	1:A:71:ASN:O	1.87	0.72
1:A:10:LYS:HG2	1:A:18:PRO:HD3	1.71	0.72
1:A:43:ARG:CZ	1:A:46:GLN:HG2	2.20	0.72
1:A:60:SER:C	1:A:64:LEU:CD1	2.53	0.71
1:A:121:LYS:HA	1:A:121:LYS:CE	2.20	0.71
1:A:43:ARG:NH1	1:A:46:GLN:CD	2.42	0.71
1:A:64:LEU:C	1:A:66:ASP:N	2.40	0.70
1:A:13:ILE:CG2	1:A:16:SER:HB2	2.20	0.70
1:A:24:ASN:HB3	1:A:117:ASN:ND2	2.07	0.69
1:A:5:PHE:CE1	1:A:99:ASP:O	2.45	0.69
1:A:121:LYS:HE3	1:A:121:LYS:N	2.06	0.69
1:A:43:ARG:NH1	1:A:46:GLN:OE1	2.26	0.69
1:A:1:ALA:H3	1:A:71:ASN:C	1.96	0.68
1:A:43:ARG:CZ	1:A:46:GLN:OE1	2.41	0.68
1:A:119:ASP:O	1:A:119:ASP:OD1	2.12	0.67
1:A:6:ASN:HD22	1:A:19:LEU:CD2	2.08	0.67
1:A:118:LEU:HD22	1:A:122:ASN:HB2	1.78	0.65
1:A:23:ASN:ND2	1:A:24:ASN:H	1.94	0.65
1:A:5:PHE:HD1	1:A:99:ASP:HB3	1.56	0.65
1:A:55:ALA:O	1:A:58:LEU:CB	2.45	0.64
1:A:63:VAL:HG23	1:A:63:VAL:O	1.98	0.63
1:A:56:LYS:CD	1:A:68:PRO:HG3	2.22	0.63
1:A:59:ASP:HA	1:A:62:LYS:CD	2.27	0.63
1:A:10:LYS:HD2	1:A:18:PRO:CD	2.29	0.63
1:A:120:LYS:C	1:A:121:LYS:HE3	2.19	0.63
1:A:55:ALA:C	1:A:58:LEU:HG	2.19	0.63
1:A:61:CYS:O	1:A:66:ASP:N	2.33	0.62
1:A:43:ARG:NH1	1:A:46:GLN:CA	2.61	0.61
1:A:55:ALA:HA	1:A:58:LEU:HD11	1.83	0.60
1:A:51:CYS:O	1:A:54:GLN:HB3	2.01	0.60
1:A:105:CYS:O	1:A:108:LYS:HB2	2.01	0.60
1:A:114:GLU:OE2	1:A:114:GLU:N	2.33	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:62:LYS:C	1:A:65:VAL:H	2.04	0.59
1:A:24:ASN:HB3	1:A:116:LYS:HZ2	1.67	0.59
1:A:12:LYS:C	1:A:14:PRO:HD3	2.22	0.59
1:A:38:VAL:HG11	1:A:118:LEU:HD11	1.83	0.59
1:A:10:LYS:CG	1:A:18:PRO:HD3	2.31	0.59
1:A:122:ASN:ND2	1:A:122:ASN:N	2.45	0.59
1:A:59:ASP:C	1:A:62:LYS:HB2	2.23	0.58
1:A:64:LEU:O	1:A:65:VAL:CG1	2.30	0.58
1:A:12:LYS:O	1:A:14:PRO:HD3	2.03	0.58
1:A:8:MET:O	1:A:11:CYS:HB3	2.04	0.58
1:A:55:ALA:HA	1:A:58:LEU:CD1	2.34	0.57
1:A:24:ASN:HB2	1:A:116:LYS:NZ	2.19	0.57
1:A:6:ASN:HD22	1:A:19:LEU:HD23	1.69	0.57
1:A:13:ILE:N	1:A:14:PRO:HD3	2.15	0.57
1:A:10:LYS:HD2	1:A:18:PRO:HD2	1.87	0.56
1:A:38:VAL:HG21	1:A:115:HIS:HB3	1.86	0.56
1:A:4:GLN:OE1	1:A:4:GLN:CA	2.53	0.56
1:A:24:ASN:CB	1:A:116:LYS:HZ2	2.19	0.56
1:A:43:ARG:HH12	1:A:46:GLN:CA	2.18	0.55
1:A:73:TYR:HB3	1:A:92:GLU:HB2	1.88	0.55
1:A:71:ASN:OD1	1:A:92:GLU:HB2	2.07	0.55
1:A:3:TRP:CH2	1:A:4:GLN:CG	2.74	0.55
1:A:102:ALA:O	1:A:105:CYS:HB3	2.07	0.55
1:A:71:ASN:OD1	1:A:92:GLU:CB	2.56	0.54
1:A:64:LEU:N	1:A:65:VAL:HG12	2.22	0.54
1:A:10:LYS:CG	1:A:18:PRO:CD	2.86	0.54
1:A:73:TYR:OH	1:A:99:ASP:OD1	2.18	0.54
1:A:43:ARG:HH12	1:A:46:GLN:C	2.11	0.53
1:A:64:LEU:C	1:A:66:ASP:H	2.09	0.53
1:A:5:PHE:CE1	1:A:99:ASP:CB	2.87	0.53
1:A:38:VAL:HG11	1:A:118:LEU:HD13	1.85	0.53
1:A:119:ASP:C	1:A:119:ASP:OD1	2.45	0.53
1:A:24:ASN:O	1:A:116:LYS:HD2	2.07	0.53
1:A:10:LYS:HD2	1:A:18:PRO:HD3	1.89	0.53
1:A:24:ASN:CB	1:A:116:LYS:NZ	2.71	0.53
1:A:3:TRP:CE2	1:A:4:GLN:CG	2.90	0.53
1:A:67:ASN:OD1	1:A:69:TYR:C	2.47	0.52
1:A:8:MET:CE	1:A:99:ASP:CB	2.83	0.52
1:A:38:VAL:HG23	1:A:115:HIS:ND1	2.25	0.52
1:A:119:ASP:OD1	1:A:121:LYS:CB	2.53	0.51
1:A:23:ASN:ND2	1:A:24:ASN:N	2.57	0.51
1:A:3:TRP:CG	1:A:4:GLN:N	2.78	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:TYR:HB3	1:A:29:CYS:HB2	1.91	0.51
1:A:10:LYS:HD2	1:A:17:GLU:HA	1.92	0.51
1:A:19:LEU:HD23	1:A:19:LEU:N	2.26	0.51
1:A:19:LEU:O	1:A:23:ASN:HB2	2.10	0.51
1:A:118:LEU:HD22	1:A:122:ASN:CB	2.40	0.51
1:A:1:ALA:HB3	1:A:4:GLN:HE22	1.76	0.51
1:A:68:PRO:O	1:A:71:ASN:N	2.41	0.51
1:A:68:PRO:C	1:A:70:THR:H	2.15	0.50
1:A:66:ASP:OD2	1:A:67:ASN:N	2.44	0.50
1:A:4:GLN:NE2	1:A:72:ASN:HD22	2.09	0.50
1:A:38:VAL:HG21	1:A:115:HIS:CB	2.41	0.50
1:A:119:ASP:C	1:A:121:LYS:H	2.14	0.50
1:A:10:LYS:CD	1:A:18:PRO:CD	2.89	0.50
1:A:6:ASN:ND2	1:A:19:LEU:CG	2.74	0.49
1:A:66:ASP:CG	1:A:71:ASN:HD22	2.16	0.49
1:A:6:ASN:HD22	1:A:19:LEU:CG	2.26	0.49
1:A:67:ASN:O	1:A:71:ASN:N	2.45	0.49
1:A:64:LEU:C	1:A:65:VAL:HG12	2.21	0.49
1:A:95:ILE:O	1:A:95:ILE:CG2	2.60	0.49
1:A:55:ALA:O	1:A:58:LEU:HB2	2.11	0.49
1:A:60:SER:CA	1:A:64:LEU:HD11	2.42	0.48
1:A:6:ASN:O	1:A:10:LYS:HG3	2.14	0.48
1:A:17:GLU:O	1:A:20:LEU:HB2	2.13	0.48
1:A:1:ALA:CA	1:A:71:ASN:O	2.61	0.48
1:A:38:VAL:HG21	1:A:115:HIS:CG	2.48	0.48
1:A:84:CYS:SG	1:A:100:ARG:HG3	2.53	0.48
1:A:59:ASP:O	1:A:62:LYS:CB	2.49	0.47
1:A:43:ARG:CZ	1:A:46:GLN:CG	2.79	0.47
1:A:55:ALA:O	1:A:58:LEU:CD1	2.62	0.47
1:A:119:ASP:C	1:A:121:LYS:N	2.66	0.47
1:A:54:GLN:OE1	1:A:54:GLN:HA	1.96	0.47
1:A:64:LEU:O	1:A:66:ASP:N	2.48	0.46
1:A:8:MET:HE3	1:A:99:ASP:HB2	1.92	0.46
1:A:63:VAL:O	1:A:64:LEU:HD23	2.14	0.46
1:A:62:LYS:O	1:A:65:VAL:CB	2.61	0.46
1:A:10:LYS:CD	1:A:18:PRO:HD3	2.46	0.46
1:A:4:GLN:NE2	1:A:72:ASN:ND2	2.65	0.45
1:A:108:LYS:N	1:A:108:LYS:HD3	2.27	0.45
1:A:52:TYR:O	1:A:56:LYS:HG3	2.16	0.45
1:A:46:GLN:HG3	1:A:46:GLN:O	2.17	0.45
1:A:65:VAL:O	1:A:65:VAL:CG2	2.64	0.45
1:A:68:PRO:C	1:A:70:THR:N	2.70	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:ARG:NH2	1:A:46:GLN:HG2	2.31	0.45
1:A:6:ASN:HB2	1:A:19:LEU:HD21	1.99	0.45
1:A:50:ASN:O	1:A:54:GLN:HB2	2.17	0.45
1:A:105:CYS:O	1:A:109:VAL:HG22	2.17	0.45
1:A:66:ASP:CG	1:A:67:ASN:H	2.15	0.44
1:A:108:LYS:HD2	1:A:108:LYS:HA	1.30	0.44
1:A:55:ALA:CA	1:A:58:LEU:HG	2.48	0.44
1:A:66:ASP:OD2	1:A:67:ASN:C	2.56	0.44
1:A:71:ASN:OD1	1:A:72:ASN:N	2.50	0.44
1:A:23:ASN:HA	1:A:23:ASN:HD22	1.42	0.44
1:A:118:LEU:HD23	1:A:119:ASP:H	1.83	0.43
1:A:24:ASN:HB3	1:A:117:ASN:HD22	1.82	0.43
1:A:68:PRO:HA	1:A:95:ILE:HG13	2.00	0.43
1:A:119:ASP:O	1:A:122:ASN:N	2.38	0.42
1:A:88:ASN:HD22	1:A:88:ASN:HA	1.57	0.42
1:A:3:TRP:CD2	1:A:4:GLN:N	2.87	0.42
1:A:4:GLN:HB3	1:A:75:TYR:HE2	1.84	0.42
1:A:31:LEU:C	1:A:32:GLY:O	2.58	0.42
1:A:43:ARG:HA	1:A:46:GLN:HB3	2.01	0.42
1:A:52:TYR:HE1	1:A:98:CYS:HB3	1.83	0.42
1:A:73:TYR:HB3	1:A:92:GLU:O	2.19	0.42
1:A:48:HIS:HB2	1:A:102:ALA:HB2	2.01	0.42
1:A:54:GLN:OE1	1:A:54:GLN:CA	2.57	0.42
1:A:12:LYS:HD2	1:A:12:LYS:HA	1.66	0.42
1:A:46:GLN:O	1:A:46:GLN:CG	2.64	0.42
1:A:67:ASN:CG	1:A:70:THR:HG23	2.40	0.42
1:A:116:LYS:HZ2	1:A:117:ASN:ND2	2.17	0.42
1:A:10:LYS:CD	1:A:18:PRO:HD2	2.49	0.41
1:A:67:ASN:O	1:A:70:THR:C	2.58	0.41
1:A:65:VAL:HG22	1:A:65:VAL:O	2.20	0.41
1:A:66:ASP:OD2	1:A:68:PRO:N	2.54	0.41
1:A:85:SER:OG	1:A:87:GLU:HB2	2.20	0.41
1:A:43:ARG:NH1	1:A:46:GLN:C	2.72	0.41
1:A:82:ILE:HG22	1:A:83:THR:N	2.35	0.41
1:A:52:TYR:CE1	1:A:98:CYS:HB3	2.56	0.40
1:A:58:LEU:HB2	1:A:61:CYS:SG	2.61	0.40
1:A:57:LYS:O	1:A:62:LYS:HE2	2.21	0.40
1:A:25:TYR:CD1	1:A:25:TYR:C	2.95	0.40

All (11) 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	Distance(Å)	Clash(Å)
1:A:63:VAL:CB	1:A:114:GLU:CG[2_655]	1.35	0.85
1:A:64:LEU:CD2	1:A:115:HIS:CE1[2_655]	1.42	0.78
1:A:63:VAL:CG2	1:A:115:HIS:CD2[2_655]	1.46	0.74
1:A:63:VAL:CG2	1:A:115:HIS:NE2[2_655]	1.57	0.63
1:A:63:VAL:CG1	1:A:114:GLU:CB[2_655]	1.72	0.48
1:A:63:VAL:CG1	1:A:114:GLU:CG[2_655]	1.74	0.46
1:A:63:VAL:CA	1:A:114:GLU:CG[2_655]	1.98	0.22
1:A:63:VAL:CG2	1:A:115:HIS:CG[2_655]	1.99	0.21
1:A:64:LEU:CD2	1:A:115:HIS:NE2[2_655]	2.06	0.14
1:A:63:VAL:CG2	1:A:115:HIS:CE1[2_655]	2.12	0.08
1:A:75:TYR:OH	1:A:87:GLU:OE2[5_556]	2.12	0.08

## 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	121/130 (93%)	100 (83%)	10 (8%)	11 (9%)	<b>1</b> <b>5</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	A	32	GLY
1	A	54	GLN
1	A	62	LYS
1	A	63	VAL
1	A	91	CYS
1	A	112	ASN
1	A	90	ALA
1	A	55	ALA
1	A	65	VAL
1	A	68	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	111/116 (96%)	81 (73%)	30 (27%)	<b>1</b> <b>3</b>

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	ASN
1	A	8	MET
1	A	16	SER
1	A	19	LEU
1	A	23	ASN
1	A	24	ASN
1	A	31	LEU
1	A	34	SER
1	A	41	LEU
1	A	43	ARG
1	A	53	LYS
1	A	56	LYS
1	A	57	LYS
1	A	60	SER
1	A	62	LYS
1	A	64	LEU
1	A	65	VAL
1	A	72	ASN
1	A	74	SER
1	A	81	GLU
1	A	86	SER
1	A	95	ILE
1	A	100	ARG
1	A	108	LYS
1	A	109	VAL
1	A	110	PRO
1	A	118	LEU
1	A	119	ASP
1	A	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	23	ASN
1	A	72	ASN
1	A	88	ASN
1	A	117	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

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	123/130 (94%)	-0.47	0 100 100	2, 10, 28, 41	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.