



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:42 pm BST

PDB ID : 6LGX  
Title : Structure of Rabies virus glycoprotein at basic pH  
Authors : Yang, F.L.; Lin, S.; Ye, F.; Yang, J.; Qi, J.X.; Chen, Z.J.; Lin, X.; Wang, J.C.; Yue, D.; Cheng, Y.W.; Chen, Z.M.; Chen, H.; You, Y.; Zhang, Z.L.; Yang, Y.; Yang, M.; Sun, H.L.; Li, Y.H.; Cao, Y.; Yang, S.Y.; Wei, Y.Q.; Gao, G.F.; Lu, G.W.  
Deposited on : 2019-12-06  
Resolution : 3.10 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.

---

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

MolProbity : 4.02b-467  
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

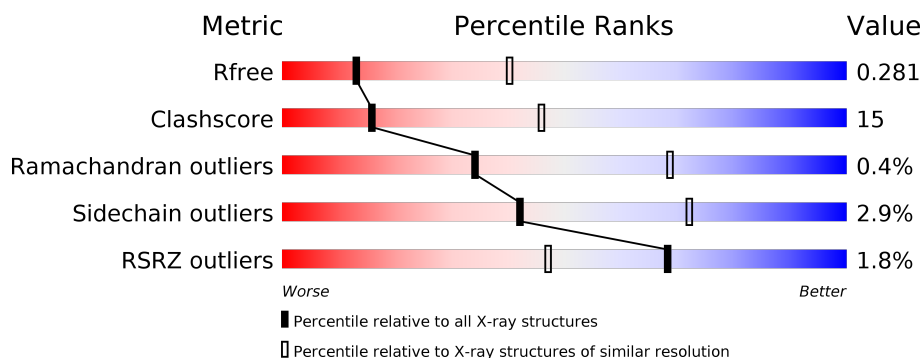
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	443	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 64%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>64%</span> <span>20%</span> <span>15%</span> </div> </div>
1	B	443	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 24%, green 53%, grey 21%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>53%</span> <span>24%</span> <span>21%</span> </div> </div>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5695 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 Glycoprotein,Glycoprotein,Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2968	1881	512	551	24			
1	B	348	Total	C	N	O	S	0	0	0
			2727	1731	473	499	24			

There are 40 discrepancies between the modelled and reference sequences:


Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q5JZZ2
A	-2	ASP	-	expression tag	UNP Q5JZZ2
A	-1	GLU	-	expression tag	UNP Q5JZZ2
A	0	PHE	-	expression tag	UNP Q5JZZ2
A	75	GLY	-	linker	UNP Q5JZZ2
A	76	GLY	-	linker	UNP Q5JZZ2
A	77	SER	-	linker	UNP Q5JZZ2
A	78	GLY	-	linker	UNP Q5JZZ2
A	79	GLY	-	linker	UNP Q5JZZ2
A	121	GLY	-	linker	UNP Q2Z2I1
A	122	GLY	-	linker	UNP Q2Z2I1
A	123	SER	-	linker	UNP Q2Z2I1
A	124	GLY	-	linker	UNP Q2Z2I1
A	125	GLY	-	linker	UNP Q2Z2I1
A	440	HIS	-	expression tag	UNP D8VEC1
A	441	HIS	-	expression tag	UNP D8VEC1
A	442	HIS	-	expression tag	UNP D8VEC1
A	443	HIS	-	expression tag	UNP D8VEC1
A	444	HIS	-	expression tag	UNP D8VEC1
A	445	HIS	-	expression tag	UNP D8VEC1
B	-3	ALA	-	expression tag	UNP Q5JZZ2
B	-2	ASP	-	expression tag	UNP Q5JZZ2
B	-1	GLU	-	expression tag	UNP Q5JZZ2
B	0	PHE	-	expression tag	UNP Q5JZZ2
B	75	GLY	-	linker	UNP Q5JZZ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLY	-	linker	UNP Q5JZZ2
B	77	SER	-	linker	UNP Q5JZZ2
B	78	GLY	-	linker	UNP Q5JZZ2
B	79	GLY	-	linker	UNP Q5JZZ2
B	121	GLY	-	linker	UNP Q2Z2I1
B	122	GLY	-	linker	UNP Q2Z2I1
B	123	SER	-	linker	UNP Q2Z2I1
B	124	GLY	-	linker	UNP Q2Z2I1
B	125	GLY	-	linker	UNP Q2Z2I1
B	440	HIS	-	expression tag	UNP D8VEC1
B	441	HIS	-	expression tag	UNP D8VEC1
B	442	HIS	-	expression tag	UNP D8VEC1
B	443	HIS	-	expression tag	UNP D8VEC1
B	444	HIS	-	expression tag	UNP D8VEC1
B	445	HIS	-	expression tag	UNP D8VEC1

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.

- Chain A: 

- Chain B:

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.44Å 138.45Å 61.44Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	47.40 – 3.10 47.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.40-3.10) 99.2 (47.39-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, $R_{free}$	0.242 , 0.285 0.244 , 0.281	Depositor DCC
$R_{free}$ test set	1344 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.1	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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](#)

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	0.30	0/3041	0.52	0/4118
1	B	0.32	0/2796	0.58	3/3788 (0.1%)
All	All	0.31	0/5837	0.55	3/7906 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	PRO	CA-N-CD	-5.32	104.06	111.50
1	B	397	HIS	C-N-CD	5.19	139.29	128.40
1	B	158	LYS	N-CA-C	5.03	124.59	111.00

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	2968	0	2927	76	1
1	B	2727	0	2695	89	1
All	All	5695	0	5622	165	1

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 15.

All (165) 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:35:CYS:SG	1:B:200:ALA:O	1.95	1.24
1:B:155:PRO:O	1:B:158:LYS:HB2	1.58	1.01
1:B:148:SER:HA	1:B:160:SER:O	1.59	1.00
1:B:397:HIS:CG	1:B:398:PRO:HD3	1.98	0.99
1:A:333:ARG:NH2	1:A:334:THR:CG2	2.30	0.94
1:B:32:ASP:OD1	1:B:33:GLU:N	2.04	0.91
1:A:333:ARG:CZ	1:A:334:THR:HG23	2.03	0.88
1:A:333:ARG:NH2	1:A:334:THR:HG21	1.89	0.87
1:A:27:ASN:OD1	1:A:276:LEU:CD2	2.23	0.86
1:A:26:ASN:OD1	1:A:28:LEU:HB2	1.74	0.85
1:A:27:ASN:HD22	1:A:308:VAL:HG21	1.46	0.80
1:B:145:TYR:OH	1:B:252:CYS:O	1.99	0.80
1:A:333:ARG:CZ	1:A:334:THR:CG2	2.61	0.79
1:B:406:PHE:O	1:B:407:LYS:HG2	1.84	0.77
1:B:402:PRO:O	1:B:403:SER:HB2	1.86	0.76
1:A:233:LEU:HD11	1:A:246:SER:HB3	1.67	0.76
1:A:231:LEU:O	1:A:244:GLN:NE2	2.20	0.74
1:A:27:ASN:HD22	1:A:308:VAL:CG2	2.00	0.74
1:B:403:SER:OG	1:B:404:THR:N	2.20	0.73
1:B:8:PRO:HB3	1:B:327:ALA:HB1	1.71	0.72
1:B:397:HIS:CD2	1:B:397:HIS:H	2.08	0.71
1:B:146:ASP:OD2	1:B:148:SER:HB2	1.91	0.70
1:A:27:ASN:ND2	1:A:308:VAL:HG21	2.06	0.69
1:B:35:CYS:SG	1:B:201:SER:C	2.70	0.69
1:B:397:HIS:CD2	1:B:398:PRO:HD3	2.28	0.69
1:A:231:LEU:HD12	1:A:244:GLN:HG3	1.74	0.68
1:B:397:HIS:ND1	1:B:398:PRO:HD3	2.08	0.67
1:A:27:ASN:ND2	1:A:308:VAL:CG2	2.58	0.67
1:A:17:ILE:HD13	1:A:324:GLU:HB3	1.78	0.66
1:A:105:ASP:O	1:A:107:ARG:NH1	2.29	0.65
1:A:319:ASN:O	1:A:320:LYS:HB2	1.95	0.65
1:A:173:HIS:HD1	1:A:176:THR:HG1	1.42	0.64
1:A:85:LYS:HG3	1:A:86:HIS:H	1.62	0.64
1:B:162:ILE:HG13	1:B:162:ILE:O	1.96	0.64
1:A:410:ASP:OD1	1:A:410:ASP:N	2.32	0.63
1:B:148:SER:O	1:B:149:LEU:HD23	1.97	0.63
1:A:27:ASN:OD1	1:A:276:LEU:HD23	1.98	0.62
1:B:402:PRO:O	1:B:403:SER:CB	2.45	0.62
1:A:333:ARG:HH22	1:A:334:THR:HG21	1.63	0.62
1:B:400:ALA:HB3	1:B:402:PRO:HD3	1.82	0.62
1:B:341:SER:OG	1:B:342:LYS:N	2.33	0.61
1:B:11:LEU:HD23	1:B:347:VAL:HG11	1.82	0.61

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:HD11	1:B:372:LEU:HD23	1.81	0.61
1:A:62:THR:OG1	1:A:133:ILE:HG23	2.00	0.61
1:B:142:LEU:HD11	1:B:147:LYS:HA	1.83	0.61
1:B:100:TRP:HE3	1:B:105:ASP:HB3	1.66	0.61
1:B:148:SER:CA	1:B:160:SER:O	2.45	0.61
1:B:338:ILE:HG22	1:B:339:ILE:HG13	1.82	0.61
1:A:201:SER:O	1:A:202:ASN:HB3	2.01	0.60
1:A:2:PHE:CZ	1:A:27:ASN:OD1	2.54	0.59
1:A:405:VAL:HG23	1:A:405:VAL:O	2.03	0.59
1:B:234:ARG:NH1	1:B:238:GLY:O	2.36	0.59
1:B:146:ASP:O	1:B:147:LYS:HB2	2.02	0.59
1:B:31:GLU:O	1:B:31:GLU:HG2	2.02	0.58
1:A:27:ASN:HD21	1:A:308:VAL:HG11	1.67	0.58
1:A:281:GLU:HA	1:A:284:LEU:HD12	1.86	0.57
1:B:37:ASN:O	1:B:200:ALA:HA	2.03	0.57
1:A:67:GLU:HB2	1:A:83:LYS:HG3	1.85	0.57
1:B:368:ASP:OD1	1:B:368:ASP:N	2.38	0.57
1:B:397:HIS:CD2	1:B:397:HIS:N	2.73	0.56
1:B:282:GLU:OE2	1:B:282:GLU:N	2.33	0.56
1:B:354:HIS:HB3	1:B:359:PHE:CE1	2.41	0.56
1:A:282:GLU:OE1	1:A:282:GLU:N	2.31	0.56
1:A:358:VAL:HG12	1:A:364:ILE:HG22	1.87	0.56
1:A:224:ARG:HH21	1:A:248:GLU:HA	1.71	0.55
1:B:407:LYS:O	1:B:407:LYS:HG3	2.05	0.55
1:A:27:ASN:OD1	1:A:276:LEU:HD22	2.03	0.55
1:B:101:LYS:HD3	1:B:134:ILE:HG12	1.88	0.54
1:B:346:LYS:HE2	1:B:349:GLY:HA2	1.89	0.54
1:A:155:PRO:HG2	1:A:158:LYS:HD2	1.89	0.54
1:A:201:SER:HA	1:A:206:THR:HA	1.90	0.54
1:B:397:HIS:CE1	1:B:398:PRO:HD3	2.43	0.54
1:B:372:LEU:CD1	1:B:377:GLN:HG3	2.38	0.53
1:B:372:LEU:HD12	1:B:377:GLN:HG3	1.90	0.53
1:B:334:THR:O	1:B:337:GLU:HG2	2.09	0.53
1:A:368:ASP:OD1	1:A:368:ASP:N	2.41	0.53
1:B:332:VAL:HG21	1:B:338:ILE:HD11	1.90	0.53
1:A:363:ILE:HG12	1:A:373:ILE:HG12	1.90	0.52
1:B:288:GLU:O	1:B:292:THR:OG1	2.20	0.51
1:B:405:VAL:O	1:B:407:LYS:NZ	2.41	0.51
1:B:199:ARG:O	1:B:208:GLY:O	2.28	0.51
1:B:32:ASP:O	1:B:33:GLU:HB2	2.09	0.51
1:B:39:SER:O	1:B:198:LYS:HA	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASN:C	1:B:38:LEU:HD22	2.31	0.51
1:B:62:THR:HG23	1:B:133:ILE:HB	1.93	0.51
1:B:392:VAL:HG12	1:B:393:ILE:H	1.76	0.50
1:A:368:ASP:OD2	1:A:370:HIS:ND1	2.44	0.50
1:B:196:ARG:HB2	1:B:196:ARG:HH11	1.77	0.50
1:A:273:VAL:HG22	1:A:276:LEU:HG	1.93	0.50
1:A:27:ASN:ND2	1:A:308:VAL:CG1	2.75	0.50
1:B:293:THR:HG23	1:B:295:SER:H	1.76	0.50
1:B:96:ALA:O	1:B:100:TRP:HD1	1.94	0.50
1:A:66:THR:HG22	1:A:84:ARG:HB3	1.94	0.49
1:A:202:ASN:CG	1:A:203:GLY:H	2.15	0.49
1:A:2:PHE:HZ	1:A:27:ASN:OD1	1.94	0.49
1:A:224:ARG:NH2	1:A:248:GLU:HG2	2.28	0.49
1:A:8:PRO:O	1:A:347:VAL:HG23	2.13	0.48
1:A:347:VAL:HG12	1:A:352:HIS:HB2	1.94	0.48
1:A:334:THR:O	1:A:337:GLU:HG2	2.14	0.48
1:B:319:ASN:O	1:B:320:LYS:HG3	2.13	0.48
1:A:375:GLU:N	1:A:375:GLU:OE1	2.43	0.48
1:A:60:THR:HB	1:A:135:ILE:HB	1.95	0.48
1:B:204:ASN:N	1:B:204:ASN:OD1	2.46	0.48
1:B:65:VAL:HG13	1:B:85:LYS:HB3	1.96	0.48
1:B:401:ASP:N	1:B:402:PRO:CD	2.77	0.47
1:A:27:ASN:ND2	1:A:308:VAL:HG11	2.27	0.47
1:A:316:THR:HB	1:A:360:PHE:HA	1.96	0.47
1:B:22:LEU:HD21	1:B:322:LEU:HD21	1.95	0.47
1:B:35:CYS:SG	1:B:201:SER:CA	3.02	0.47
1:B:153:VAL:HG22	1:B:171:THR:HG23	1.96	0.47
1:B:397:HIS:CG	1:B:398:PRO:CD	2.85	0.47
1:B:46:LEU:HB2	1:B:51:ILE:HG12	1.96	0.47
1:A:101:LYS:HD2	1:A:106:PRO:HG2	1.97	0.47
1:B:58:GLY:HA3	1:B:178:TRP:CZ2	2.49	0.47
1:B:405:VAL:HG12	1:B:406:PHE:N	2.29	0.47
1:B:155:PRO:O	1:B:158:LYS:CB	2.47	0.46
1:B:405:VAL:HG12	1:B:407:LYS:H	1.81	0.46
1:A:385:MET:O	1:A:389:LYS:N	2.36	0.46
1:B:286:ALA:O	1:B:290:ILE:HG13	2.15	0.46
1:A:151:SER:H	1:A:157:GLY:HA2	1.81	0.46
1:A:306:LYS:HG2	1:A:308:VAL:O	2.16	0.46
1:B:97:ALA:O	1:B:101:LYS:HD2	2.14	0.46
1:B:60:THR:O	1:B:134:ILE:HA	2.16	0.45
1:A:17:ILE:HB	1:A:21:HIS:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:HH21	1:A:249:THR:H	1.65	0.45
1:B:392:VAL:HG12	1:B:393:ILE:N	2.32	0.45
1:A:202:ASN:CG	1:A:203:GLY:N	2.70	0.45
1:A:62:THR:HG22	1:A:176:THR:OG1	2.17	0.45
1:A:372:LEU:HD12	1:A:372:LEU:O	2.17	0.45
1:A:66:THR:O	1:A:128:THR:HA	2.17	0.44
1:A:2:PHE:HZ	1:A:276:LEU:HD23	1.83	0.44
1:B:208:GLY:HA2	1:B:219:LEU:HG	1.98	0.44
1:A:286:ALA:O	1:A:290:ILE:HG13	2.18	0.44
1:B:196:ARG:NH1	1:B:196:ARG:HB2	2.33	0.44
1:B:41:PHE:CE2	1:B:43:TYR:HB3	2.53	0.44
1:B:30:VAL:HG11	1:B:218:SER:HB3	1.99	0.43
1:B:319:ASN:C	1:B:320:LYS:CG	2.87	0.43
1:B:398:PRO:HD2	1:B:399:LEU:HD23	2.01	0.43
1:A:184:ARG:HG2	1:A:185:PRO:HD3	2.01	0.43
1:A:333:ARG:CZ	1:A:334:THR:HG21	2.39	0.43
1:A:341:SER:OG	1:A:342:LYS:N	2.51	0.43
1:A:38:LEU:HG	1:A:200:ALA:HB2	2.01	0.43
1:A:85:LYS:HG3	1:A:86:HIS:N	2.30	0.43
1:A:27:ASN:ND2	1:A:27:ASN:C	2.71	0.42
1:B:383:GLN:O	1:B:387:LEU:HD23	2.18	0.42
1:B:35:CYS:SG	1:B:202:ASN:N	2.92	0.42
1:A:277:VAL:HG13	1:A:280:ARG:HH21	1.84	0.42
1:B:306:LYS:NZ	1:B:311:PHE:O	2.38	0.42
1:B:405:VAL:CG1	1:B:406:PHE:N	2.82	0.42
1:A:342:LYS:HG3	1:A:343:GLY:N	2.33	0.42
1:A:226:LYS:HG2	1:A:231:LEU:HD23	2.01	0.42
1:B:173:HIS:ND1	1:B:176:THR:HG23	2.35	0.42
1:B:289:SER:O	1:B:293:THR:HG22	2.19	0.41
1:B:375:GLU:OE1	1:B:375:GLU:N	2.48	0.41
1:B:280:ARG:O	1:B:284:LEU:HG	2.20	0.41
1:B:166:SER:C	1:B:168:TYR:H	2.24	0.41
1:B:404:THR:OG1	1:B:404:THR:O	2.32	0.41
1:B:32:ASP:CG	1:B:33:GLU:H	2.10	0.41
1:A:58:GLY:HA3	1:A:178:TRP:CZ2	2.56	0.41
1:A:43:TYR:HE2	1:A:45:GLU:HB3	1.84	0.41
1:A:397:HIS:HB3	1:A:400:ALA:HB3	2.02	0.41
1:A:153:VAL:HG23	1:A:154:PHE:CD1	2.56	0.40
1:A:211:ASP:N	1:A:211:ASP:OD1	2.51	0.40
1:B:97:ALA:C	1:B:101:LYS:HD2	2.41	0.40
1:B:255:ASP:OD1	1:B:255:ASP:N	2.54	0.40

All (1) 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:A:320:LYS:O	1:B:395:LEU:CD1[1_556]	1.91	0.29

## 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	369/443 (83%)	345 (94%)	24 (6%)	0	100	100
1	B	340/443 (77%)	313 (92%)	24 (7%)	3 (1%)	17	52
All	All	709/886 (80%)	658 (93%)	48 (7%)	3 (0%)	34	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	ASP
1	B	403	SER
1	B	398	PRO

### 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	336/390 (86%)	328 (98%)	8 (2%)	49	76
1	B	309/390 (79%)	298 (96%)	11 (4%)	35	67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	645/780 (83%)	626 (97%)	19 (3%)	42 72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	184	ARG
1	A	207	CYS
1	A	209	PHE
1	A	213	ARG
1	A	330	LYS
1	A	333	ARG
1	A	397	HIS
1	B	131	SER
1	B	159	CYS
1	B	160	SER
1	B	209	PHE
1	B	213	ARG
1	B	294	LYS
1	B	321	THR
1	B	356	ASN
1	B	397	HIS
1	B	398	PRO
1	B	407	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	B	397	HIS

### 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](#)

There are no ligands in this entry.

## 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](#)

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	377/443 (85%)	-0.22	5 (1%) 77 59	61, 117, 176, 218	0
1	B	348/443 (78%)	-0.11	8 (2%) 60 39	69, 122, 191, 211	0
All	All	725/886 (81%)	-0.17	13 (1%) 68 47	61, 119, 183, 218	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	4.7
1	B	163	THR	3.2
1	B	132	LEU	3.1
1	B	66	THR	3.0
1	A	82	PHE	3.0
1	A	108	TYR	2.8
1	A	83	LYS	2.7
1	B	64	VAL	2.5
1	A	33	GLU	2.4
1	A	27	ASN	2.3
1	B	367	PRO	2.3
1	B	162	ILE	2.2
1	B	204	ASN	2.2

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.