



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 09:43 am GMT

PDB ID : 1VYV  
Title : beta4 subunit of Ca<sup>2+</sup> channel  
Authors : Chen, Y.-H.; Li, M.-H.; Zhang, Y.; He, L.-L.; Yamada, Y.; Fitzmaurice, A.;  
Yang, S.; Zhang, H.; Liang, T.; Yang, J.  
Deposited on : 2004-05-07  
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

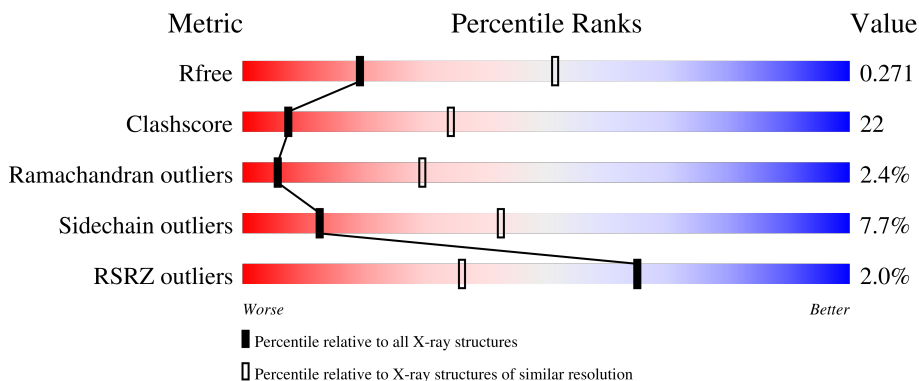
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of 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	359	
1	B	359	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4361 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 CALCIUM CHANNEL BETA-4SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	275	Total 2176	C 1384	N 382	O 402	S 4	Se 4	0	0	1
1	B	276	Total 2185	C 1389	N 383	O 405	S 4	Se 4	0	0	1



M373	F374	D375	L378	D379	E380	N381	E384	D385	A386	H389	E392	Y393	A396	R399	H402	T403	SER	SER	SER	THR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.30Å 83.20Å 72.30Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-3.00) 91.7 (29.97-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.80Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.287 0.233 , 0.271	Depositor DCC
$R_{free}$ test set	1702 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.114	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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	0.52	0/2213	0.71	1/2987 (0.0%)
1	B	0.49	1/2222 (0.0%)	0.68	0/2999
All	All	0.50	1/4435 (0.0%)	0.70	1/5986 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	MSE	CG-SE	-5.13	1.78	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ILE	N-CA-C	-5.16	97.08	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	2176	0	2213	110	0
1	B	2185	0	2219	87	0
All	All	4361	0	4432	194	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 22.

All (194) 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:246:LYS:HG3	1:B:255:ILE:HD12	1.44	0.99
1:A:159:ILE:O	1:A:163:GLN:HB2	1.61	0.98
1:B:380:GLU:O	1:B:381:ASN:HB2	1.64	0.93
1:A:246:LYS:HG2	1:A:255:ILE:HD12	1.52	0.91
1:A:256:THR:HG21	1:A:301:LEU:HD11	1.53	0.90
1:A:296:GLU:O	1:A:300:GLU:HG2	1.72	0.89
1:A:73:ARG:HG3	1:A:74:GLN:N	1.88	0.88
1:B:380:GLU:OE1	1:B:385:ASP:HB3	1.74	0.87
1:B:233:VAL:HG21	1:B:345:ILE:HG12	1.56	0.86
1:A:242:PHE:O	1:A:246:LYS:HG3	1.76	0.85
1:A:265:ALA:HB3	1:A:324:THR:HB	1.61	0.81
1:A:392:GLU:CD	1:B:343:ARG:HH21	1.84	0.81
1:A:259:THR:HG22	1:A:313:ASP:OD2	1.82	0.78
1:A:252:ARG:HA	1:A:306:GLN:OE1	1.83	0.78
1:A:164:GLU:C	1:A:166:LYS:H	1.85	0.78
1:A:228:LEU:HD11	1:A:358:VAL:HG12	1.66	0.78
1:B:332:HIS:HB2	1:B:374:PHE:CD2	2.22	0.74
1:A:140:LEU:HD13	1:A:142:LYS:HB2	1.71	0.72
1:A:233:VAL:HG21	1:A:345:ILE:HG12	1.72	0.72
1:A:249:PHE:O	1:A:253:ILE:HG22	1.90	0.71
1:A:256:THR:HG21	1:A:301:LEU:CD1	2.19	0.71
1:A:73:ARG:HG3	1:A:74:GLN:H	1.55	0.70
1:A:380:GLU:HG3	1:B:347:SER:HA	1.72	0.70
1:B:159:ILE:O	1:B:163:GLN:HG3	1.94	0.68
1:A:246:LYS:CG	1:A:255:ILE:HD12	2.25	0.67
1:A:208:HIS:HB3	1:A:209:ILE:HD12	1.77	0.67
1:A:78:GLN:O	1:A:82:ILE:HG12	1.95	0.66
1:B:380:GLU:OE2	1:B:386:ALA:HA	1.95	0.66
1:A:87:ALA:HA	1:A:90:LYS:HD2	1.78	0.65
1:A:265:ALA:HB3	1:A:324:THR:CB	2.27	0.64
1:A:243:ASP:HA	1:A:246:LYS:HD2	1.78	0.64
1:B:336:SER:OG	1:B:337:SER:N	2.31	0.63
1:B:396:ALA:O	1:B:399:ARG:HG2	1.98	0.63
1:B:287:SER:OG	1:B:290:GLU:HG3	1.98	0.63
1:A:108:GLU:C	1:A:110:VAL:H	2.02	0.62
1:B:370:PRO:HD2	1:B:373:MSE:SE	2.49	0.62
1:A:380:GLU:OE2	1:A:389:HIS:HD2	1.83	0.62
1:A:161:ILE:C	1:A:163:GLN:H	2.02	0.62
1:A:380:GLU:OE2	1:A:389:HIS:CD2	2.53	0.62
1:B:223:LEU:HD23	1:B:331:VAL:HB	1.82	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HH11	1:A:155:ARG:HG3	1.66	0.61
1:B:260:ALA:HB3	1:B:294:GLU:HG3	1.82	0.61
1:B:80:ALA:HB2	1:B:131:TYR:OH	2.01	0.61
1:B:255:ILE:HG22	1:B:255:ILE:O	2.01	0.60
1:A:332:HIS:HB2	1:A:374:PHE:CD2	2.37	0.59
1:B:262:ILE:C	1:B:264:LEU:H	2.05	0.59
1:B:380:GLU:O	1:B:381:ASN:CB	2.42	0.58
1:B:158:ASN:HB3	1:B:162:GLN:NE2	2.18	0.58
1:A:80:ALA:HB2	1:A:131:TYR:OH	2.03	0.58
1:A:110:VAL:HG22	1:A:135:TRP:CH2	2.39	0.58
1:B:94:PHE:CE2	1:B:130:LYS:HE2	2.38	0.58
1:B:258:VAL:HG11	1:B:262:ILE:HG23	1.85	0.58
1:A:94:PHE:CZ	1:A:127:ILE:HG21	2.39	0.58
1:A:262:ILE:C	1:A:264:LEU:H	2.07	0.58
1:A:155:ARG:HG3	1:A:155:ARG:NH1	2.19	0.57
1:B:258:VAL:HG11	1:B:262:ILE:CG2	2.34	0.57
1:B:379:ASP:O	1:B:380:GLU:CG	2.53	0.57
1:B:392:GLU:HG2	1:B:393:TYR:N	2.18	0.57
1:B:74:GLN:O	1:B:78:GLN:HG3	2.04	0.57
1:A:218:MSE:SE	1:A:401:THR:HG21	2.55	0.56
1:A:125:LEU:HD23	1:A:140:LEU:HA	1.86	0.56
1:A:121:ALA:O	1:A:122:LYS:HB2	2.05	0.55
1:A:220:PRO:HD2	1:A:328:PRO:HA	1.87	0.55
1:A:380:GLU:N	1:A:380:GLU:OE1	2.40	0.55
1:A:342:GLN:HG3	1:A:356:LEU:HD21	1.88	0.55
1:B:120:ASP:OD1	1:B:121:ALA:N	2.39	0.55
1:A:317:HIS:ND1	1:A:318:PRO:HD2	2.22	0.55
1:A:337:SER:OG	1:A:340:VAL:HG23	2.06	0.55
1:B:161:ILE:C	1:B:163:GLN:H	2.10	0.55
1:A:164:GLU:C	1:A:166:LYS:N	2.54	0.55
1:B:379:ASP:O	1:B:380:GLU:HG3	2.06	0.54
1:A:84:LEU:O	1:A:87:ALA:HB3	2.07	0.54
1:A:209:ILE:HD12	1:A:209:ILE:N	2.22	0.54
1:A:84:LEU:HD12	1:A:137:ILE:HD13	1.90	0.54
1:B:357:ASN:O	1:B:361:VAL:HG23	2.09	0.53
1:B:94:PHE:HE2	1:B:130:LYS:HE2	1.74	0.53
1:A:94:PHE:CE2	1:A:127:ILE:HG21	2.44	0.53
1:A:228:LEU:CD1	1:A:358:VAL:HG12	2.38	0.53
1:B:399:ARG:HB3	1:B:399:ARG:NH1	2.25	0.52
1:B:249:PHE:O	1:B:253:ILE:HG22	2.10	0.52
1:A:258:VAL:HG22	1:A:312:ALA:HA	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:CG2	1:B:147:ILE:HD11	2.40	0.52
1:A:378:LEU:HB3	1:A:386:ALA:HB1	1.92	0.52
1:B:164:GLU:C	1:B:166:LYS:H	2.12	0.52
1:A:350:LYS:O	1:A:354:LYS:HB2	2.09	0.52
1:B:117:VAL:CG2	1:B:150:ILE:HG12	2.40	0.52
1:A:265:ALA:CB	1:A:324:THR:HB	2.37	0.51
1:A:83:GLN:O	1:A:83:GLN:HG3	2.10	0.51
1:B:371:PRO:HG2	1:B:372:GLU:OE2	2.11	0.50
1:A:110:VAL:HG12	1:A:112:VAL:O	2.12	0.50
1:B:253:ILE:HG12	1:B:254:SER:N	2.26	0.50
1:B:75:GLU:O	1:B:79:GLN:HG2	2.11	0.50
1:B:346:LYS:C	1:B:348:ARG:H	2.14	0.50
1:A:164:GLU:O	1:A:164:GLU:HG2	2.10	0.50
1:A:379:ASP:O	1:A:380:GLU:C	2.49	0.50
1:B:73:ARG:NH2	1:B:74:GLN:HE21	2.10	0.50
1:B:128:LYS:O	1:B:129:GLU:CB	2.59	0.50
1:A:229:LYS:HE3	1:A:315:ILE:O	2.12	0.50
1:B:99:ASN:O	1:B:100:VAL:HG13	2.12	0.49
1:A:140:LEU:HD11	1:A:142:LYS:HD2	1.93	0.49
1:A:240:ALA:HB1	1:A:383:LEU:HD21	1.93	0.49
1:B:232:GLU:O	1:B:236:MSE:HG3	2.13	0.49
1:B:317:HIS:ND1	1:B:318:PRO:HD2	2.27	0.49
1:A:306:GLN:O	1:A:308:VAL:HG23	2.12	0.49
1:A:396:ALA:HA	1:A:399:ARG:NH1	2.28	0.49
1:B:304:SER:O	1:B:305:LEU:HB2	2.12	0.49
1:B:158:ASN:HB3	1:B:162:GLN:HE21	1.77	0.49
1:A:234:THR:HG23	1:A:238:GLN:HE21	1.78	0.48
1:A:287:SER:HB3	1:A:290:GLU:HG3	1.95	0.48
1:A:96:VAL:CG2	1:A:125:LEU:HB2	2.43	0.48
1:A:248:ARG:NH1	1:A:395:GLU:OE1	2.43	0.48
1:B:364:ASP:O	1:B:368:GLN:HG3	2.14	0.48
1:A:84:LEU:HD13	1:A:149:PHE:CE1	2.49	0.48
1:A:134:ASP:C	1:A:135:TRP:CD1	2.87	0.48
1:B:291:VAL:O	1:B:295:ILE:HG12	2.14	0.48
1:B:117:VAL:HG21	1:B:150:ILE:HG12	1.96	0.47
1:A:384:GLU:H	1:A:384:GLU:HG2	1.23	0.47
1:B:358:VAL:HG23	1:B:359:GLN:N	2.28	0.47
1:A:143:GLU:OE2	1:A:399:ARG:HD2	2.14	0.47
1:A:266:LYS:HG2	1:A:266:LYS:O	2.14	0.47
1:A:346:LYS:C	1:A:348:ARG:H	2.17	0.47
1:A:218:MSE:HE2	1:A:305:LEU:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLN:O	1:A:296:GLU:HG3	2.14	0.47
1:B:399:ARG:NH1	1:B:399:ARG:CB	2.78	0.47
1:A:232:GLU:OE1	1:A:352:GLN:HG3	2.15	0.47
1:B:131:TYR:CD2	1:B:132:ASN:ND2	2.83	0.47
1:A:71:ALA:N	1:A:73:ARG:HG2	2.30	0.46
1:B:73:ARG:HH21	1:B:74:GLN:HE21	1.63	0.46
1:A:256:THR:OG1	1:A:257:ARG:N	2.48	0.46
1:A:322:ILE:HG22	1:A:323:LYS:HG3	1.98	0.46
1:A:90:LYS:O	1:A:128:LYS:HE2	2.15	0.46
1:A:87:ALA:O	1:A:128:LYS:HD3	2.16	0.46
1:A:108:GLU:C	1:A:110:VAL:N	2.69	0.46
1:A:80:ALA:CB	1:A:131:TYR:OH	2.64	0.46
1:A:265:ALA:O	1:A:266:LYS:C	2.54	0.45
1:A:71:ALA:N	1:A:74:GLN:HG3	2.32	0.45
1:A:128:LYS:O	1:A:129:GLU:CB	2.63	0.45
1:B:364:ASP:O	1:B:367:ALA:HB3	2.16	0.45
1:B:163:GLN:O	1:B:166:LYS:HB2	2.15	0.45
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.82	0.45
1:A:370:PRO:HA	1:A:371:PRO:HD3	1.85	0.45
1:B:143:GLU:OE2	1:B:399:ARG:HD3	2.17	0.45
1:B:253:ILE:HD11	1:B:255:ILE:HD11	1.99	0.45
1:B:399:ARG:HB3	1:B:399:ARG:CZ	2.46	0.45
1:A:380:GLU:H	1:A:380:GLU:CD	2.18	0.45
1:B:220:PRO:HD2	1:B:328:PRO:HA	1.98	0.45
1:A:258:VAL:O	1:A:258:VAL:CG2	2.65	0.45
1:A:83:GLN:OE1	1:A:86:ARG:NH2	2.51	0.44
1:B:109:ASP:OD1	1:B:109:ASP:N	2.50	0.44
1:B:237:MSE:O	1:B:240:ALA:HB3	2.18	0.44
1:B:262:ILE:C	1:B:264:LEU:N	2.69	0.44
1:B:164:GLU:C	1:B:166:LYS:N	2.70	0.44
1:A:389:HIS:ND1	1:A:389:HIS:C	2.71	0.44
1:A:98:THR:HG21	1:A:119:PHE:CD1	2.53	0.44
1:A:96:VAL:HG23	1:A:125:LEU:HB2	2.00	0.43
1:A:262:ILE:C	1:A:264:LEU:N	2.70	0.43
1:B:219:ARG:HA	1:B:220:PRO:HD3	1.75	0.43
1:B:378:LEU:HB3	1:B:386:ALA:HB1	1.99	0.43
1:B:230:GLY:N	1:B:235:ASP:OD1	2.36	0.43
1:A:288:LEU:O	1:A:292:GLN:HG3	2.18	0.43
1:A:110:VAL:HA	1:A:135:TRP:CH2	2.54	0.43
1:A:135:TRP:CD1	1:A:135:TRP:N	2.87	0.43
1:B:108:GLU:C	1:B:110:VAL:H	2.22	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:TYR:HD2	1:B:132:ASN:ND2	2.16	0.43
1:B:305:LEU:O	1:B:402:HIS:NE2	2.51	0.43
1:B:384:GLU:OE1	1:B:384:GLU:N	2.45	0.43
1:B:110:VAL:HG22	1:B:135:TRP:CH2	2.53	0.43
1:B:350:LYS:O	1:B:354:LYS:HB2	2.18	0.43
1:A:74:GLN:O	1:A:77:GLU:HB3	2.19	0.43
1:B:364:ASP:OD1	1:B:368:GLN:NE2	2.52	0.42
1:A:164:GLU:HG3	1:A:168:LYS:HB2	2.00	0.42
1:A:392:GLU:CD	1:B:343:ARG:NH2	2.63	0.42
1:B:231:TYR:CD1	1:B:231:TYR:N	2.87	0.42
1:A:117:VAL:CG2	1:A:118:SER:N	2.82	0.42
1:B:233:VAL:HG21	1:B:345:ILE:CG1	2.40	0.42
1:B:356:LEU:HD11	1:B:360:LEU:HD11	2.01	0.42
1:A:123:ASP:OD1	1:A:140:LEU:HD21	2.20	0.42
1:B:221:VAL:HB	1:B:309:VAL:HG22	2.02	0.42
1:B:332:HIS:CE1	1:B:334:LYS:HE3	2.55	0.42
1:A:138:GLY:O	1:A:147:ILE:HA	2.21	0.41
1:A:87:ALA:O	1:A:90:LYS:HB2	2.20	0.41
1:A:247:HIS:ND1	1:A:247:HIS:C	2.72	0.41
1:A:138:GLY:O	1:A:147:ILE:HG13	2.21	0.41
1:B:335:VAL:HG11	1:B:341:LEU:HB2	2.03	0.41
1:A:77:GLU:O	1:A:78:GLN:C	2.58	0.41
1:A:110:VAL:CG1	1:A:112:VAL:O	2.68	0.41
1:A:242:PHE:HB3	1:A:246:LYS:HE3	2.03	0.41
1:B:260:ALA:O	1:B:262:ILE:N	2.54	0.41
1:A:265:ALA:HB3	1:A:324:THR:CG2	2.51	0.41
1:B:296:GLU:O	1:B:300:GLU:HB2	2.21	0.41
1:B:317:HIS:HA	1:B:318:PRO:HD3	1.96	0.41
1:B:337:SER:HA	1:B:338:PRO:HD3	1.86	0.41
1:B:160:ARG:HE	1:B:161:ILE:HG13	1.86	0.40
1:B:321:LEU:HA	1:B:324:THR:HG23	2.04	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	269/359 (75%)	239 (89%)	24 (9%)	6 (2%)	6	31
1	B	270/359 (75%)	234 (87%)	29 (11%)	7 (3%)	5	27
All	All	539/718 (75%)	473 (88%)	53 (10%)	13 (2%)	6	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	LYS
1	B	167	ARG
1	B	261	ASP
1	B	336	SER
1	A	261	ASP
1	A	347	SER
1	A	380	GLU
1	A	109	ASP
1	A	129	GLU
1	B	129	GLU
1	B	287	SER
1	B	347	SER
1	B	109	ASP

### 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	241/312 (77%)	225 (93%)	16 (7%)	16	49
1	B	242/312 (78%)	221 (91%)	21 (9%)	10	37
All	All	483/624 (77%)	446 (92%)	37 (8%)	13	42

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	A	79	GLN
1	A	83	GLN
1	A	85	GLU
1	A	89	SER
1	A	117	VAL
1	A	140	LEU
1	A	233	VAL
1	A	247	HIS
1	A	248	ARG
1	A	256	THR
1	A	258	VAL
1	A	335	VAL
1	A	384	GLU
1	A	388	GLU
1	A	389	HIS
1	B	108	GLU
1	B	109	ASP
1	B	111	PRO
1	B	140	LEU
1	B	154	LEU
1	B	157	GLU
1	B	160	ARG
1	B	161	ILE
1	B	208	HIS
1	B	224	VAL
1	B	233	VAL
1	B	235	ASP
1	B	247	HIS
1	B	287	SER
1	B	313	ASP
1	B	336	SER
1	B	343	ARG
1	B	357	ASN
1	B	375	ASP
1	B	389	HIS
1	B	392	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	238	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	292	GLN
1	A	342	GLN
1	A	359	GLN
1	A	381	ASN
1	A	382	GLN
1	A	389	HIS
1	A	402	HIS
1	B	74	GLN
1	B	78	GLN
1	B	162	GLN
1	B	165	GLN
1	B	292	GLN
1	B	306	GLN
1	B	320	GLN
1	B	332	HIS
1	B	342	GLN
1	B	359	GLN
1	B	368	GLN
1	B	382	GLN
1	B	402	HIS

### 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 monosaccharides 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	271/359 (75%)	-0.32	5 (1%) 68 40	17, 41, 80, 107	0
1	B	272/359 (75%)	-0.29	6 (2%) 62 33	23, 46, 83, 105	0
All	All	543/718 (75%)	-0.30	11 (2%) 65 36	17, 45, 82, 107	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	GLU	3.6
1	A	71	ALA	2.8
1	A	168	LYS	2.6
1	A	165	GLN	2.6
1	B	168	LYS	2.6
1	B	167	ARG	2.4
1	B	208	HIS	2.2
1	B	250	ASP	2.1
1	B	286	SER	2.1
1	A	73	ARG	2.0
1	A	164	GLU	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 monosaccharides 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.