



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:07 AM UTC

PDB ID : 1VYV / pdb_00001vyv
Title : beta4 subunit of Ca²⁺ channel
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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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

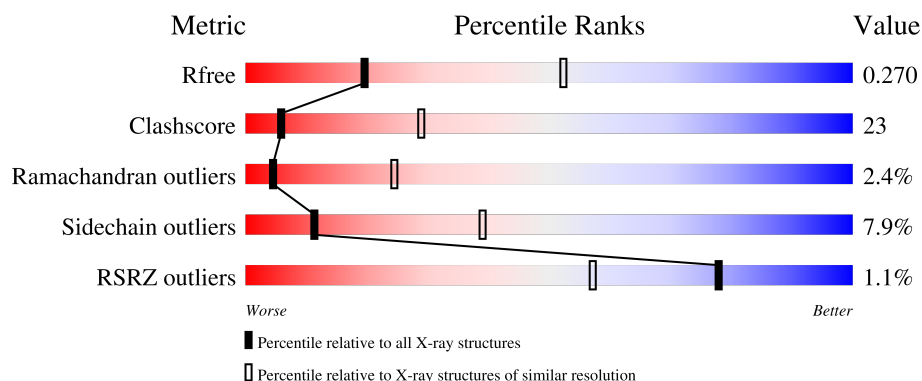
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 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
1	A	275	Total	C	N	O	S	Se	0	0	1
			2176	1384	382	402	4	4			
1	B	276	Total	C	N	O	S	Se	0	0	1
			2185	1389	383	405	4	4			

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 38% 32% 7% 23%

Chain B:

2% 40% 31% 5% 23%

GLY SER ALA ASP SER TTR THR SER ARG PRO SER ASP SER VAL SER LEU GLU ASP ASP ARG E70 A71 I72 R73 Q74 W75 Q78 Q79 A90 F94 T98 N99 V100 A105 E108 D109 P111 V117 D120 A121 K128 E129 K130 Y131 N132 W135 W136 I137

L140 L143 E143 I147 I150 I154 M158 I159 R160 I161 Q162 Q163 Q164 Q165 K166 R167 K168 ARG PHE HIS GLY LYS SER SER GLY ASN SER F94 T258 V259 A260 D261 L262 S263 L264 A265 K266 ARG SER VAL PHE LEU ASN PRO ARG ALA THR PRO THR THR ARG ALA ILE ILE GLU ARG ASN VAL THR LYS

H208 I209 M218 R219 P220 V221 V222 V223 V224 K229 G230 Y231 E232 V233 T234 D235 M236 M237 A240 K246 H247 R248 F249 I253 S254 L255 V258 T259 A260 D261 L262 S263 L264 A265 K266 ARG SER VAL PHE LEU ASN PRO ARG ALA THR PRO THR THR ARG ALA ILE ILE GLU ARG ASN VAL THR LYS

S286 S287 E290 V291 E294 I295 E296 E300 L301 S304 L305 V309 A312 D313 T314 I315 I316 H317 P318 L321 T324 A327 P328 V331 H332 V333 K334 V335 S336 S337 P338 K339 V340 L341 Q342 R343 L344 I345 K346 S347 R348 G349 K350 Q351 Q352 S353 K354 H355 L356 P357

V358	Q359	L360	V361	D364	A367	Q368	C369	P370	P371	E372	M373	F374	L378	D379	E380	N381	E384	D385	A386	E392	Y393	A396	R399	H402	T403	SER	SER	SER	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.30Å 83.20Å 72.30Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-3.00) 95.8 (30.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.287 0.234 , 0.270	Depositor DCC
R_{free} test set	1702 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4361	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.70	6/2213 (0.3%)	1.09	13/2987 (0.4%)
1	B	0.64	7/2222 (0.3%)	1.08	18/2999 (0.6%)
All	All	0.67	13/4435 (0.3%)	1.08	31/5986 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	MSE	SE-CE	-8.77	1.69	1.95
1	B	237	MSE	SE-CE	-7.44	1.73	1.95
1	A	373	MSE	SE-CE	-6.16	1.76	1.95
1	A	402	HIS	C-N	-6.08	1.24	1.33
1	A	237	MSE	SE-CE	-6.07	1.77	1.95
1	B	373	MSE	SE-CE	-5.95	1.77	1.95
1	B	237	MSE	CG-SE	-5.81	1.78	1.95
1	B	218	MSE	SE-CE	-5.56	1.78	1.95
1	B	402	HIS	C-N	-5.50	1.25	1.33
1	B	218	MSE	CG-SE	-5.44	1.79	1.95
1	A	373	MSE	CG-SE	-5.33	1.79	1.95
1	A	236	MSE	CG-SE	-5.05	1.80	1.95
1	B	373	MSE	CG-SE	-5.00	1.80	1.95

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ILE	N-CA-C	-10.83	97.08	112.35
1	B	164	GLU	N-CA-C	-9.61	100.12	112.23
1	B	314	THR	N-CA-C	7.88	122.16	112.54
1	B	337	SER	CA-C-N	6.93	126.62	119.82
1	B	337	SER	C-N-CA	6.93	126.62	119.82
1	A	161	ILE	N-CA-C	-6.62	105.29	111.45
1	A	336	SER	N-CA-C	6.62	122.30	111.37
1	B	108	GLU	N-CA-C	6.61	119.47	111.40
1	A	162	GLN	N-CA-C	-6.57	104.26	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	LYS	N-CA-C	-6.41	101.00	110.48
1	A	314	THR	N-CA-C	6.28	120.67	112.89
1	B	105	ALA	N-CA-C	-6.19	105.22	112.89
1	B	379	ASP	CB-CA-C	-5.84	101.27	110.79
1	A	97	LYS	N-CA-C	-5.83	99.40	108.90
1	A	209	ILE	CA-C-N	5.82	123.91	119.66
1	A	209	ILE	C-N-CA	5.82	123.91	119.66
1	B	327	ALA	CA-C-N	5.68	125.65	120.03
1	B	327	ALA	C-N-CA	5.68	125.65	120.03
1	A	105	ALA	N-CA-C	-5.66	105.88	112.89
1	B	232	GLU	N-CA-C	5.61	117.86	111.02
1	A	370	PRO	CA-C-N	5.58	126.81	119.84
1	A	370	PRO	C-N-CA	5.58	126.81	119.84
1	B	339	LYS	N-CA-C	-5.46	104.73	111.40
1	B	287	SER	N-CA-C	5.46	122.42	110.80
1	A	135	TRP	N-CA-C	5.29	117.43	109.23
1	B	135	TRP	N-CA-C	5.24	117.36	109.23
1	A	259	THR	N-CA-C	-5.21	107.09	113.50
1	B	209	ILE	N-CA-C	5.11	113.96	108.95
1	B	315	ILE	N-CA-C	5.06	116.02	108.54
1	B	98	THR	N-CA-C	5.03	118.15	110.20
1	B	71	ALA	N-CA-C	-5.00	107.25	113.55

There are no chirality outliers.

There are no planarity outliers.

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	2176	0	2213	114	0
1	B	2185	0	2219	91	0
All	All	4361	0	4432	202	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 23.

All (202) 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:392:GLU:CD	1:B:343:ARG:HH21	1.84	0.85
1:A:242:PHE:O	1:A:246:LYS:HG3	1.76	0.85
1:A:164:GLU:C	1:A:166:LYS:H	1.85	0.83
1:A:265:ALA:HB3	1:A:324:THR:HB	1.61	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: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:108:GLU:C	1:A:110:VAL:H	2.02	0.67
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:161:ILE:C	1:A:163:GLN:H	2.02	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:262:ILE:C	1:A:264:LEU:H	2.07	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:380:GLU:OE2	1:A:389:HIS:CD2	2.53	0.62
1:B:262:ILE:C	1:B:264:LEU:H	2.05	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:HD23	1:B:331:VAL:HB	1.82	0.61
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:164:GLU:C	1:A:166:LYS:N	2.54	0.59
1:B:161:ILE:C	1:B:163:GLN:H	2.10	0.59
1:A:332:HIS:HB2	1:A:374:PHE:CD2	2.37	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: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:B:164:GLU:C	1:B:166:LYS:H	2.12	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:B:346:LYS:C	1:B:348:ARG:H	2.14	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: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:379:ASP:O	1:A:380:GLU:C	2.49	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:A:134:ASP:C	1:A:135:TRP:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:350:LYS:O	1:A:354:LYS:HB2	2.09	0.52
1:A:346:LYS:C	1:A:348:ARG:H	2.17	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:108:GLU:C	1:A:110:VAL:N	2.69	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:A:265:ALA:O	1:A:266:LYS:C	2.54	0.50
1:B:75:GLU:O	1:B:79:GLN:HG2	2.11	0.50
1:A:164:GLU:O	1:A:164:GLU:HG2	2.10	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:A:262:ILE:C	1:A:264:LEU:N	2.70	0.50
1:B:262:ILE:C	1:B:264:LEU:N	2.69	0.50
1:A:380:GLU:H	1:A:380:GLU:CD	2.18	0.49
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:389:HIS:C	1:A:389:HIS:ND1	2.71	0.48
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:B:108:GLU:C	1:B:110:VAL:H	2.22	0.48
1:B:291:VAL:O	1:B:295:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:HG21	1:B:150:ILE:HG12	1.96	0.47
1:B:164:GLU:C	1:B:166:LYS:N	2.70	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:218:MSE:HE2	1:A:305:LEU:O	2.14	0.47
1:A:292:GLN:O	1:A:296:GLU:HG3	2.14	0.47
1:A:392:GLU:CD	1:B:343:ARG:NH2	2.63	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:247:HIS:ND1	1:A:247:HIS:C	2.72	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:77:GLU:O	1:A:78:GLN:C	2.58	0.46
1:A:161:ILE:C	1:A:163:GLN:N	2.71	0.46
1:A:80:ALA:CB	1:A:131:TYR:OH	2.64	0.46
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: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:237:MSE:O	1:B:240:ALA:HB3	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:TYR:HD2	1:B:132:ASN:ND2	2.16	0.43
1:B:346:LYS:C	1:B:348:ARG:N	2.76	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:158:ASN:O	1:B:159:ILE:C	2.61	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:B:232:GLU:HG3	1:B:352:GLN:CD	2.43	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:312:ALA:O	1:B:313:ASP:C	2.63	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:138:GLY:O	1:A:147:ILE:HG13	2.21	0.41
1:B:109:ASP:OD1	1:B:109:ASP:N	2.50	0.41
1:B:335:VAL:HG11	1:B:341:LEU:HB2	2.03	0.41
1:A:110:VAL:CG1	1:A:112:VAL:O	2.68	0.41
1:A:82:ILE:C	1:A:84:LEU:N	2.77	0.41
1:A:85:GLU:C	1:A:87:ALA:N	2.78	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:A:230:GLY:C	1:A:235:ASP:OD2	2.65	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 [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	269/359 (75%)	239 (89%)	24 (9%)	6 (2%)	5	26
1	B	270/359 (75%)	234 (87%)	29 (11%)	7 (3%)	4	23
All	All	539/718 (75%)	473 (88%)	53 (10%)	13 (2%)	4	24

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%)	222 (92%)	19 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	242/312 (78%)	223 (92%)	19 (8%)	11	39
All	All	483/624 (77%)	445 (92%)	38 (8%)	11	39

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	A	79	GLN
1	A	85	GLU
1	A	86	ARG
1	A	89	SER
1	A	117	VAL
1	A	140	LEU
1	A	233	VAL
1	A	234	THR
1	A	247	HIS
1	A	248	ARG
1	A	256	THR
1	A	258	VAL
1	A	301	LEU
1	A	335	VAL
1	A	383	LEU
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	147	ILE
1	B	154	LEU
1	B	160	ARG
1	B	161	ILE
1	B	208	HIS
1	B	224	VAL
1	B	233	VAL
1	B	247	HIS
1	B	287	SER
1	B	301	LEU
1	B	313	ASP
1	B	336	SER
1	B	343	ARG

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Mol	Chain	Res	Type
1	B	357	ASN
1	B	392	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	238	GLN
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	163	GLN
1	B	165	GLN
1	B	292	GLN
1	B	332	HIS
1	B	342	GLN
1	B	359	GLN
1	B	368	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 ⓘ

There are no oligosaccharides 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 [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, 95th 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 ²)	Q<0.9
1	A	271/359 (75%)	-0.19	0	100 100	17, 41, 80, 107	0
1	B	272/359 (75%)	-0.05	6 (2%)	62 39	23, 46, 83, 105	0
All	All	543/718 (75%)	-0.12	6 (1%)	78 57	17, 45, 82, 107	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	SER	3.0
1	B	260	ALA	2.9
1	B	259	THR	2.8
1	B	70	GLU	2.3
1	B	264	LEU	2.2
1	B	357	ASN	2.1

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 oligosaccharides 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.