



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 04:38 am GMT

PDB ID : 1C2B
Title : ELECTROPHORUS ELECTRICUS ACETYLCHOLINESTERASE
Authors : Bourne, Y.; Marchot, P.
Deposited on : 1999-07-26
Resolution : 4.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

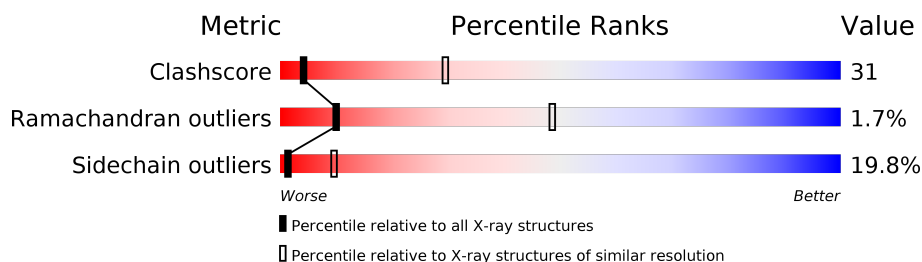
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	122078	1013 (5.28-3.72)
Ramachandran outliers	120005	1085 (5.30-3.70)
Sidechain outliers	119972	1067 (5.30-3.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	540	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4172 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 ACETYLCHOLINESTERASE.

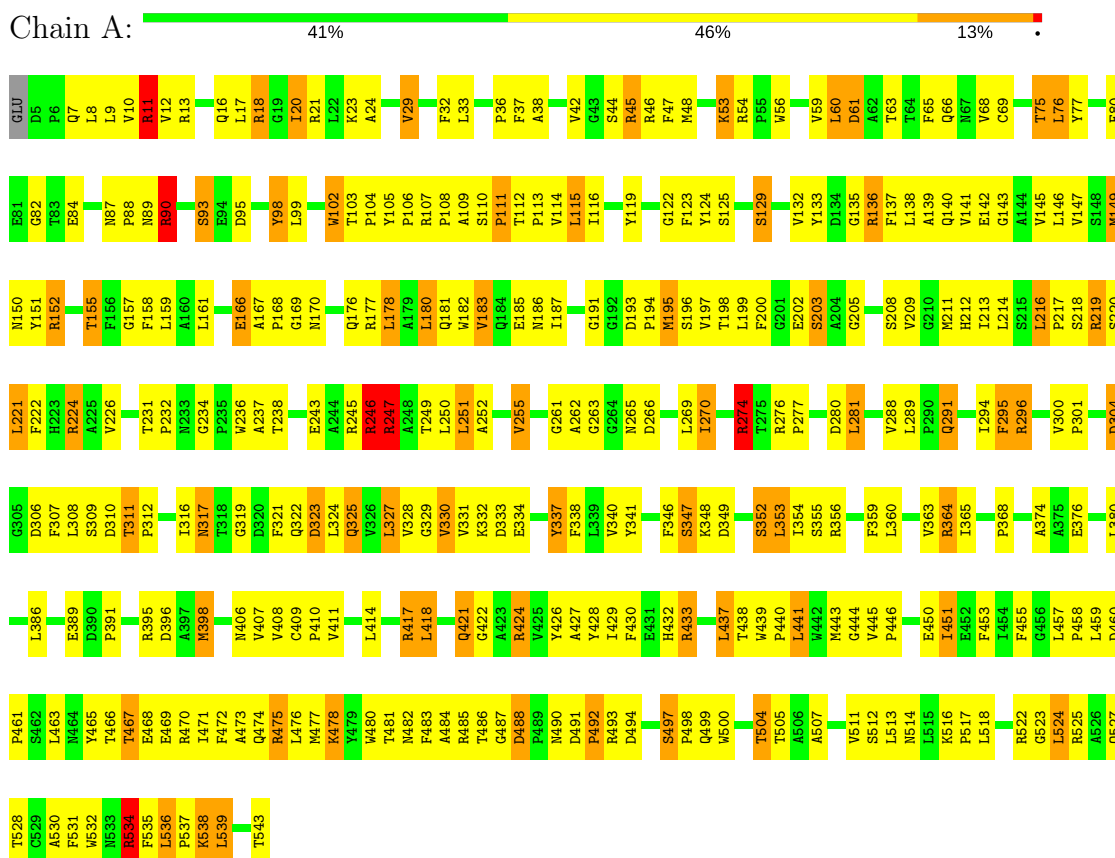
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	4172	2681	723	754	14	0	0	0

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 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.

Note EDS was not executed.

• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.98Å 215.87Å 229.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 4.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-4.50)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.369 , 0.351	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4172	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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	0.66	0/4298	1.42	33/5879 (0.6%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	A	274	ARG	NE-CZ-NH2	-11.85	114.37	120.30
1	A	247	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	A	246	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	247	ARG	CD-NE-CZ	9.23	136.53	123.60
1	A	11	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	534	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	534	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	543	THR	CA-C-O	7.89	136.67	120.10
1	A	488	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	274	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	245	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	224	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	265	ASN	N-CA-CB	6.61	122.50	110.60
1	A	11	ARG	CD-NE-CZ	6.41	132.58	123.60
1	A	475	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	152	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	424	ARG	CD-NE-CZ	6.02	132.03	123.60
1	A	504	THR	CA-CB-CG2	-6.01	103.99	112.40
1	A	488	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	296	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	424	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	98	TYR	CB-CG-CD2	5.80	124.48	121.00
1	A	238	THR	N-CA-CB	5.74	121.21	110.30
1	A	102	TRP	CA-CB-CG	5.61	124.35	113.70
1	A	13	ARG	CD-NE-CZ	5.60	131.44	123.60
1	A	102	TRP	N-CA-CB	5.41	120.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	219	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	13	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	246	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	A	337	TYR	CA-CB-CG	5.09	123.08	113.40
1	A	245	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	4172	0	4052	258	37
All	All	4172	0	4052	258	37

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 31.

All (258) 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:116:ILE:HD11	1:A:183:VAL:HG11	1.43	0.97
1:A:429:ILE:HD11	1:A:524:LEU:HD21	1.46	0.96
1:A:497:SER:CB	1:A:498:PRO:HD3	2.06	0.85
1:A:44:SER:HA	1:A:274:ARG:HD2	1.60	0.82
1:A:11:ARG:HB2	1:A:11:ARG:HH11	1.44	0.81
1:A:36:PRO:HB2	1:A:53:LYS:HG2	1.62	0.79
1:A:112:THR:HG23	1:A:113:PRO:HD2	1.65	0.78
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.63	0.78
1:A:319:GLY:O	1:A:421:GLN:HG2	1.83	0.78
1:A:507:ALA:HA	1:A:522:ARG:HH21	1.46	0.78
1:A:294:ILE:HG12	1:A:365:ILE:HG22	1.68	0.75
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.68	0.74
1:A:36:PRO:HB2	1:A:53:LYS:CG	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE2	1:A:246:ARG:HD3	1.90	0.72
1:A:226:VAL:HG11	1:A:480:TRP:HE1	1.54	0.72
1:A:36:PRO:HA	1:A:98:TYR:HD1	1.54	0.72
1:A:329:GLY:HA3	1:A:428:TYR:CE1	2.26	0.71
1:A:68:VAL:HG11	1:A:88:PRO:HB3	1.73	0.71
1:A:21:ARG:HH21	1:A:23:LYS:NZ	1.89	0.71
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.73	0.70
1:A:167:ALA:HB3	1:A:270:ILE:HD12	1.73	0.70
1:A:37:PHE:HD1	1:A:178:LEU:HD13	1.55	0.70
1:A:56:TRP:NE1	1:A:60:LEU:HB2	2.08	0.69
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.28	0.69
1:A:103:THR:HG23	1:A:104:PRO:HD2	1.75	0.68
1:A:488:ASP:OD1	1:A:490:ASN:HB2	1.92	0.68
1:A:18:ARG:HB2	1:A:18:ARG:HH21	1.58	0.68
1:A:365:ILE:O	1:A:368:PRO:HD3	1.94	0.67
1:A:428:TYR:HB2	1:A:513:LEU:HD23	1.78	0.66
1:A:142:GLU:CB	1:A:481:THR:HG21	2.25	0.66
1:A:440:PRO:HD2	1:A:443:MET:SD	2.36	0.66
1:A:478:LYS:HZ3	1:A:478:LYS:HB3	1.61	0.66
1:A:66:GLN:HB3	1:A:98:TYR:HD2	1.60	0.66
1:A:407:VAL:O	1:A:411:VAL:HG23	1.96	0.65
1:A:528:THR:O	1:A:531:PHE:HB3	1.96	0.65
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.31	0.65
1:A:470:ARG:O	1:A:474:GLN:HG3	1.96	0.65
1:A:89:ASN:O	1:A:90:ARG:HD3	1.96	0.65
1:A:534:ARG:HH11	1:A:534:ARG:HG3	1.62	0.65
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.77	0.65
1:A:497:SER:CB	1:A:498:PRO:CD	2.75	0.64
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.79	0.64
1:A:36:PRO:HA	1:A:98:TYR:CD1	2.32	0.64
1:A:53:LYS:HD2	1:A:54:ARG:O	1.98	0.63
1:A:331:VAL:HB	1:A:445:VAL:HG12	1.81	0.63
1:A:116:ILE:HD12	1:A:197:VAL:HG13	1.80	0.63
1:A:473:ALA:O	1:A:477:MET:HG3	1.99	0.62
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.00	0.62
1:A:426:TYR:HB3	1:A:500:TRP:NE1	2.14	0.61
1:A:322:GLN:O	1:A:323:ASP:HB3	1.99	0.61
1:A:251:LEU:HD21	1:A:281:LEU:HD12	1.83	0.61
1:A:132:VAL:HG23	1:A:133:TYR:CD1	2.35	0.61
1:A:112:THR:CG2	1:A:113:PRO:HD2	2.31	0.61
1:A:149:MET:HE2	1:A:176:GLN:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:HG23	1:A:341:TYR:CD1	2.36	0.60
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.37	0.60
1:A:114:VAL:HG12	1:A:145:VAL:HB	1.84	0.60
1:A:311:THR:HG22	1:A:312:PRO:HD2	1.83	0.60
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.01	0.60
1:A:114:VAL:HG23	1:A:197:VAL:HA	1.84	0.59
1:A:122:GLY:O	1:A:123:PHE:HB2	2.01	0.59
1:A:327:LEU:HD23	1:A:328:VAL:N	2.18	0.59
1:A:138:LEU:HG	1:A:477:MET:HE3	1.85	0.59
1:A:329:GLY:HA3	1:A:428:TYR:CD1	2.38	0.59
1:A:337:TYR:O	1:A:340:VAL:HG22	2.03	0.58
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.38	0.58
1:A:42:VAL:O	1:A:45:ARG:HB2	2.04	0.58
1:A:17:LEU:HD23	1:A:60:LEU:HB3	1.84	0.58
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.85	0.58
1:A:123:PHE:HB2	1:A:300:VAL:HG12	1.85	0.58
1:A:167:ALA:CB	1:A:270:ILE:HD12	2.34	0.58
1:A:444:GLY:O	1:A:446:PRO:HD3	2.03	0.58
1:A:66:GLN:CB	1:A:98:TYR:HD2	2.16	0.58
1:A:231:THR:HB	1:A:232:PRO:HD2	1.86	0.58
1:A:18:ARG:NH2	1:A:59:VAL:HG11	2.18	0.57
1:A:472:PHE:CE1	1:A:476:LEU:HD11	2.40	0.57
1:A:426:TYR:HD2	1:A:500:TRP:CD1	2.23	0.57
1:A:437:LEU:CD1	1:A:439:TRP:H	2.18	0.57
1:A:453:PHE:HB3	1:A:476:LEU:HD13	1.86	0.57
1:A:330:VAL:HG23	1:A:411:VAL:HG21	1.87	0.57
1:A:181:GLN:O	1:A:185:GLU:HG2	2.05	0.56
1:A:317:ASN:HB2	1:A:417:ARG:NH1	2.20	0.56
1:A:138:LEU:HD11	1:A:455:PHE:HA	1.87	0.56
1:A:180:LEU:O	1:A:183:VAL:HG12	2.06	0.56
1:A:328:VAL:CG1	1:A:411:VAL:HG13	2.36	0.56
1:A:317:ASN:HA	1:A:417:ARG:HH11	1.70	0.56
1:A:103:THR:CG2	1:A:104:PRO:HD2	2.36	0.55
1:A:363:VAL:N	1:A:398:MET:HE1	2.22	0.55
1:A:450:GLU:HG2	1:A:451:ILE:N	2.20	0.55
1:A:124:TYR:CD1	1:A:125:SER:HB3	2.42	0.55
1:A:266:ASP:O	1:A:270:ILE:HG12	2.06	0.54
1:A:66:GLN:CG	1:A:98:TYR:CD2	2.90	0.54
1:A:322:GLN:HA	1:A:422:GLY:HA3	1.90	0.54
1:A:66:GLN:CB	1:A:98:TYR:CD2	2.90	0.54
1:A:250:LEU:HG	1:A:288:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HH22	1:A:59:VAL:HG11	1.71	0.54
1:A:99:LEU:HD12	1:A:99:LEU:C	2.28	0.54
1:A:330:VAL:CG2	1:A:411:VAL:HG21	2.38	0.54
1:A:535:PHE:O	1:A:538:LYS:HG2	2.07	0.54
1:A:478:LYS:NZ	1:A:478:LYS:HB3	2.23	0.53
1:A:114:VAL:HG11	1:A:187:ILE:HG12	1.89	0.53
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.90	0.53
1:A:124:TYR:CE1	1:A:125:SER:HB3	2.44	0.53
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.23	0.53
1:A:66:GLN:HB3	1:A:98:TYR:CD2	2.43	0.53
1:A:142:GLU:HB3	1:A:481:THR:HG21	1.90	0.53
1:A:20:ILE:HG22	1:A:63:THR:HA	1.89	0.53
1:A:328:VAL:O	1:A:427:ALA:HA	2.09	0.53
1:A:116:ILE:HD13	1:A:180:LEU:HD12	1.90	0.52
1:A:18:ARG:NH2	1:A:18:ARG:HB2	2.24	0.52
1:A:328:VAL:HG12	1:A:329:GLY:N	2.24	0.52
1:A:205:GLY:O	1:A:208:SER:HB2	2.09	0.52
1:A:325:GLN:HB3	1:A:483:PHE:CE1	2.45	0.51
1:A:354:ILE:CD1	1:A:359:PHE:HB2	2.41	0.51
1:A:197:VAL:HG11	1:A:221:LEU:O	2.10	0.51
1:A:29:VAL:HG12	1:A:103:THR:O	2.11	0.51
1:A:110:SER:OG	1:A:111:PRO:HD2	2.11	0.51
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.76	0.51
1:A:346:PHE:HA	1:A:352:SER:HB3	1.93	0.51
1:A:317:ASN:HA	1:A:417:ARG:HD2	1.92	0.51
1:A:89:ASN:OD1	1:A:129:SER:HB2	2.11	0.50
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.93	0.50
1:A:532:TRP:O	1:A:537:PRO:HD3	2.11	0.50
1:A:432:HIS:HB3	1:A:472:PHE:HE2	1.76	0.50
1:A:409:CYS:N	1:A:410:PRO:CD	2.75	0.50
1:A:68:VAL:HG12	1:A:69:CYS:O	2.12	0.50
1:A:213:ILE:HG23	1:A:219:ARG:NH1	2.26	0.50
1:A:45:ARG:O	1:A:48:MET:HB2	2.11	0.50
1:A:478:LYS:O	1:A:482:ASN:HB2	2.12	0.50
1:A:99:LEU:HA	1:A:149:MET:HA	1.94	0.49
1:A:119:TYR:CE1	1:A:151:TYR:CE1	3.00	0.49
1:A:213:ILE:HG23	1:A:219:ARG:HH12	1.77	0.49
1:A:476:LEU:CD2	1:A:513:LEU:HD12	2.43	0.49
1:A:155:THR:HG22	1:A:159:LEU:HD12	1.93	0.49
1:A:252:ALA:CB	1:A:269:LEU:HD21	2.43	0.49
1:A:348:LYS:O	1:A:440:PRO:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:CD2	1:A:418:LEU:HD12	2.48	0.49
1:A:478:LYS:HE2	1:A:482:ASN:ND2	2.28	0.49
1:A:56:TRP:CE2	1:A:60:LEU:HD23	2.47	0.49
1:A:60:LEU:HD12	1:A:61:ASP:N	2.27	0.49
1:A:236:TRP:CZ3	1:A:237:ALA:HB2	2.48	0.48
1:A:249:THR:OG1	1:A:250:LEU:N	2.46	0.48
1:A:363:VAL:HG23	1:A:398:MET:HE1	1.95	0.48
1:A:36:PRO:HB2	1:A:53:LYS:HG3	1.95	0.48
1:A:84:GLU:O	1:A:87:ASN:HB2	2.13	0.48
1:A:8:LEU:HD23	1:A:8:LEU:N	2.28	0.48
1:A:139:ALA:O	1:A:143:GLY:HA2	2.14	0.48
1:A:354:ILE:HD11	1:A:359:PHE:HB2	1.95	0.48
1:A:7:GLN:HG3	1:A:105:TYR:CE1	2.49	0.48
1:A:197:VAL:HB	1:A:222:PHE:HA	1.96	0.48
1:A:445:VAL:O	1:A:445:VAL:HG12	2.14	0.48
1:A:486:THR:OG1	1:A:487:GLY:N	2.47	0.48
1:A:75:THR:O	1:A:77:TYR:N	2.47	0.48
1:A:247:ARG:HB3	1:A:288:VAL:CG2	2.44	0.47
1:A:277:PRO:HG2	1:A:280:ASP:OD1	2.13	0.47
1:A:226:VAL:HG11	1:A:480:TRP:NE1	2.25	0.47
1:A:294:ILE:HG12	1:A:365:ILE:CG2	2.42	0.47
1:A:115:LEU:HD11	1:A:484:ALA:HB2	1.96	0.47
1:A:328:VAL:HG11	1:A:411:VAL:HG13	1.95	0.47
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.97	0.47
1:A:77:TYR:CD2	1:A:348:LYS:HD3	2.50	0.47
1:A:255:VAL:HG13	1:A:276:ARG:HD2	1.98	0.46
1:A:158:PHE:O	1:A:159:LEU:C	2.52	0.46
1:A:198:THR:OG1	1:A:224:ARG:HB2	2.14	0.46
1:A:433:ARG:NH2	1:A:441:LEU:HA	2.31	0.46
1:A:457:LEU:N	1:A:458:PRO:CD	2.78	0.46
1:A:152:ARG:O	1:A:157:GLY:HA3	2.15	0.46
1:A:180:LEU:HD11	1:A:199:LEU:CD2	2.46	0.46
1:A:68:VAL:HG21	1:A:88:PRO:HB3	1.97	0.46
1:A:45:ARG:NH1	1:A:45:ARG:HG3	2.29	0.46
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.81	0.46
1:A:138:LEU:HG	1:A:477:MET:CE	2.44	0.46
1:A:10:VAL:HG23	1:A:32:PHE:CE2	2.51	0.46
1:A:476:LEU:HD21	1:A:513:LEU:HD12	1.96	0.46
1:A:316:ILE:HG21	1:A:414:LEU:CD1	2.46	0.46
1:A:136:ARG:HG2	1:A:137:PHE:N	2.31	0.46
1:A:291:GLN:HB2	1:A:291:GLN:HE21	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:O	1:A:107:ARG:C	2.54	0.45
1:A:66:GLN:OE1	1:A:98:TYR:CE2	2.69	0.45
1:A:38:ALA:HA	1:A:53:LYS:N	2.32	0.45
1:A:334:GLU:HG3	1:A:407:VAL:HB	1.99	0.45
1:A:317:ASN:HA	1:A:417:ARG:NH1	2.31	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.99	0.45
1:A:161:LEU:HD13	1:A:270:ILE:CD1	2.47	0.45
1:A:16:GLN:HB3	1:A:59:VAL:HG22	1.99	0.45
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.70	0.45
1:A:37:PHE:CD1	1:A:178:LEU:HD13	2.44	0.44
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.89	0.44
1:A:407:VAL:C	1:A:410:PRO:HD2	2.37	0.44
1:A:141:VAL:HG21	1:A:459:LEU:HD22	1.99	0.44
1:A:347:SER:OG	1:A:349:ASP:N	2.46	0.44
1:A:534:ARG:HH11	1:A:534:ARG:CG	2.30	0.44
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.83	0.44
1:A:492:PRO:HB2	1:A:493:ARG:H	1.44	0.44
1:A:146:LEU:HD23	1:A:147:VAL:N	2.32	0.44
1:A:166:GLU:HG3	1:A:270:ILE:HG13	2.00	0.44
1:A:481:THR:O	1:A:484:ALA:HB3	2.18	0.44
1:A:20:ILE:HG13	1:A:21:ARG:N	2.33	0.43
1:A:407:VAL:O	1:A:410:PRO:HD2	2.18	0.43
1:A:451:ILE:HG12	1:A:451:ILE:H	1.55	0.43
1:A:457:LEU:N	1:A:458:PRO:HD3	2.33	0.43
1:A:408:VAL:O	1:A:411:VAL:HB	2.18	0.43
1:A:433:ARG:NH2	1:A:440:PRO:O	2.51	0.43
1:A:467:THR:HG23	1:A:470:ARG:NH1	2.33	0.43
1:A:169:GLY:O	1:A:170:ASN:HB2	2.17	0.43
1:A:327:LEU:HD23	1:A:328:VAL:H	1.84	0.43
1:A:439:TRP:HB3	1:A:440:PRO:HD2	2.00	0.43
1:A:103:THR:HG23	1:A:108:PRO:HD3	2.00	0.43
1:A:7:GLN:CB	1:A:105:TYR:HE1	2.32	0.43
1:A:146:LEU:C	1:A:146:LEU:HD23	2.39	0.43
1:A:295:PHE:CE2	1:A:338:PHE:CZ	3.07	0.43
1:A:216:LEU:CB	1:A:217:PRO:HD3	2.48	0.43
1:A:316:ILE:HG13	1:A:317:ASN:N	2.33	0.43
1:A:208:SER:O	1:A:209:VAL:C	2.57	0.43
1:A:208:SER:O	1:A:211:MET:N	2.52	0.43
1:A:21:ARG:HH21	1:A:23:LYS:HZ1	1.63	0.43
1:A:33:LEU:N	1:A:33:LEU:CD1	2.82	0.43
1:A:116:ILE:CD1	1:A:183:VAL:HG11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TRP:CD1	1:A:60:LEU:HB2	2.53	0.42
1:A:21:ARG:HH21	1:A:23:LYS:HZ2	1.62	0.42
1:A:458:PRO:HB3	1:A:465:TYR:CG	2.54	0.42
1:A:310:ASP:OD1	1:A:311:THR:N	2.53	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.91	0.42
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.82	0.42
1:A:468:GLU:HA	1:A:471:ILE:HD12	2.01	0.42
1:A:108:PRO:HG2	1:A:191:GLY:HA3	2.01	0.42
1:A:193:ASP:OD1	1:A:195:MET:HB2	2.20	0.42
1:A:437:LEU:HD12	1:A:439:TRP:H	1.82	0.42
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.54	0.42
1:A:500:TRP:HB2	1:A:518:LEU:HD11	2.02	0.42
1:A:338:PHE:CD1	1:A:338:PHE:N	2.88	0.42
1:A:202:GLU:O	1:A:203:SER:C	2.57	0.42
1:A:243:GLU:OE1	1:A:247:ARG:NH2	2.48	0.42
1:A:135:GLY:CA	1:A:146:LEU:HD13	2.50	0.41
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.50	0.41
1:A:93:SER:OG	1:A:95:ASP:N	2.46	0.41
1:A:364:ARG:HD3	1:A:364:ARG:HH11	1.69	0.41
1:A:317:ASN:CB	1:A:417:ARG:NH1	2.84	0.41
1:A:475:ARG:HH11	1:A:475:ARG:HD3	1.66	0.41
1:A:374:ALA:HA	1:A:539:LEU:HD13	2.02	0.41
1:A:193:ASP:HA	1:A:194:PRO:HD2	1.92	0.41
1:A:170:ASN:ND2	1:A:304:ASP:OD2	2.52	0.41
1:A:406:ASN:O	1:A:410:PRO:HG2	2.21	0.41
1:A:212:HIS:HD2	1:A:218:SER:OG	2.02	0.41
1:A:517:PRO:O	1:A:518:LEU:C	2.59	0.41
1:A:60:LEU:HD12	1:A:61:ASP:O	2.21	0.41
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.20	0.41
1:A:527:GLN:O	1:A:530:ALA:N	2.53	0.41
1:A:132:VAL:HG23	1:A:133:TYR:CE1	2.55	0.41
1:A:75:THR:HB	1:A:76:LEU:H	1.75	0.41
1:A:8:LEU:HD11	1:A:21:ARG:HB2	2.02	0.41
1:A:182:TRP:O	1:A:183:VAL:C	2.60	0.41
1:A:46:ARG:HD3	1:A:47:PHE:CZ	2.56	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.91	0.41
1:A:180:LEU:HD11	1:A:199:LEU:HD21	2.03	0.40
1:A:306:ASP:O	1:A:307:PHE:C	2.57	0.40
1:A:212:HIS:CD2	1:A:218:SER:OG	2.74	0.40
1:A:491:ASP:HA	1:A:492:PRO:HD2	1.77	0.40

All (37) 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:261:GLY:C	1:A:262:ALA:C[11_555]	0.70	1.50
1:A:262:ALA:N	1:A:262:ALA:C[11_555]	0.78	1.42
1:A:262:ALA:N	1:A:262:ALA:CA[11_555]	0.79	1.41
1:A:262:ALA:CA	1:A:262:ALA:CA[11_555]	0.83	1.37
1:A:261:GLY:CA	1:A:263:GLY:N[11_555]	0.85	1.35
1:A:261:GLY:CA	1:A:263:GLY:CA[11_555]	0.92	1.28
1:A:261:GLY:C	1:A:263:GLY:N[11_555]	0.95	1.25
1:A:21:ARG:CD	1:A:21:ARG:NH1[4_565]	1.28	0.92
1:A:21:ARG:NE	1:A:21:ARG:CZ[4_565]	1.30	0.90
1:A:21:ARG:CZ	1:A:21:ARG:CZ[4_565]	1.35	0.85
1:A:261:GLY:C	1:A:262:ALA:O[11_555]	1.47	0.73
1:A:261:GLY:N	1:A:263:GLY:N[11_555]	1.55	0.65
1:A:21:ARG:NE	1:A:21:ARG:NH2[4_565]	1.59	0.61
1:A:261:GLY:O	1:A:262:ALA:O[11_555]	1.65	0.55
1:A:262:ALA:CA	1:A:262:ALA:CB[11_555]	1.65	0.55
1:A:21:ARG:NE	1:A:21:ARG:NH1[4_565]	1.67	0.53
1:A:261:GLY:O	1:A:262:ALA:C[11_555]	1.69	0.51
1:A:262:ALA:N	1:A:263:GLY:N[11_555]	1.72	0.48
1:A:261:GLY:CA	1:A:263:GLY:C[11_555]	1.75	0.45
1:A:262:ALA:CB	1:A:262:ALA:CB[11_555]	1.75	0.45
1:A:261:GLY:C	1:A:263:GLY:CA[11_555]	1.78	0.42
1:A:262:ALA:N	1:A:262:ALA:CB[11_555]	1.81	0.39
1:A:262:ALA:N	1:A:262:ALA:O[11_555]	1.85	0.35
1:A:262:ALA:O	1:A:262:ALA:O[11_555]	1.93	0.27
1:A:105:TYR:CE2	1:A:105:TYR:OH[4_565]	1.94	0.26
1:A:261:GLY:O	1:A:263:GLY:N[11_555]	2.01	0.19
1:A:262:ALA:CA	1:A:262:ALA:C[11_555]	2.02	0.18
1:A:262:ALA:N	1:A:262:ALA:N[11_555]	2.03	0.17
1:A:109:ALA:CB	1:A:109:ALA:CB[3_555]	2.03	0.17
1:A:261:GLY:N	1:A:263:GLY:O[11_555]	2.07	0.13
1:A:21:ARG:CZ	1:A:21:ARG:NH1[4_565]	2.07	0.13
1:A:21:ARG:CD	1:A:21:ARG:CZ[4_565]	2.12	0.08
1:A:21:ARG:NH1	1:A:21:ARG:NH1[4_565]	2.14	0.06
1:A:21:ARG:CZ	1:A:21:ARG:NH2[4_565]	2.17	0.03
1:A:261:GLY:O	1:A:263:GLY:CA[11_555]	2.19	0.01
1:A:261:GLY:CA	1:A:263:GLY:O[11_555]	2.19	0.01
1:A:261:GLY:N	1:A:263:GLY:CA[11_555]	2.19	0.01

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	537/540 (99%)	470 (88%)	58 (11%)	9 (2%)	10	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	323	ASP
1	A	492	PRO
1	A	494	ASP
1	A	497	SER
1	A	111	PRO
1	A	203	SER
1	A	234	GLY
1	A	523	GLY

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	434/441 (98%)	348 (80%)	86 (20%)	1	9

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ARG

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Mol	Chain	Res	Type
1	A	18	ARG
1	A	20	ILE
1	A	29	VAL
1	A	45	ARG
1	A	53	LYS
1	A	60	LEU
1	A	61	ASP
1	A	65	PHE
1	A	75	THR
1	A	90	ARG
1	A	93	SER
1	A	102	TRP
1	A	115	LEU
1	A	129	SER
1	A	136	ARG
1	A	149	MET
1	A	155	THR
1	A	166	GLU
1	A	168	PRO
1	A	178	LEU
1	A	180	LEU
1	A	183	VAL
1	A	195	MET
1	A	196	SER
1	A	214	LEU
1	A	216	LEU
1	A	220	SER
1	A	221	LEU
1	A	246	ARG
1	A	247	ARG
1	A	251	LEU
1	A	255	VAL
1	A	270	ILE
1	A	274	ARG
1	A	281	LEU
1	A	291	GLN
1	A	295	PHE
1	A	296	ARG
1	A	304	ASP
1	A	309	SER
1	A	311	THR
1	A	317	ASN

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	325	GLN
1	A	327	LEU
1	A	330	VAL
1	A	332	LYS
1	A	333	ASP
1	A	347	SER
1	A	352	SER
1	A	353	LEU
1	A	355	SER
1	A	356	ARG
1	A	360	LEU
1	A	364	ARG
1	A	376	GLU
1	A	380	LEU
1	A	386	LEU
1	A	389	GLU
1	A	398	MET
1	A	417	ARG
1	A	418	LEU
1	A	421	GLN
1	A	424	ARG
1	A	433	ARG
1	A	437	LEU
1	A	438	THR
1	A	441	LEU
1	A	451	ILE
1	A	467	THR
1	A	478	LYS
1	A	485	ARG
1	A	499	GLN
1	A	504	THR
1	A	505	THR
1	A	512	SER
1	A	514	ASN
1	A	516	LYS
1	A	524	LEU
1	A	525	ARG
1	A	534	ARG
1	A	536	LEU
1	A	538	LYS
1	A	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	212	HIS
1	A	291	GLN
1	A	317	ASN
1	A	421	GLN
1	A	464	ASN
1	A	482	ASN
1	A	499	GLN

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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.