



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:07 PM UTC

PDB ID : 1C2B / pdb_00001c2b
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 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

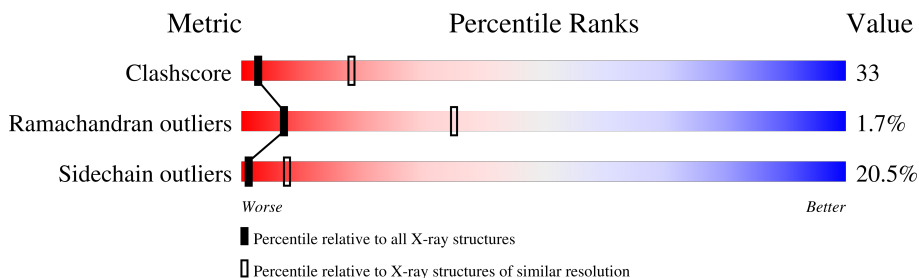
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	540	36% 43% 19% .

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.

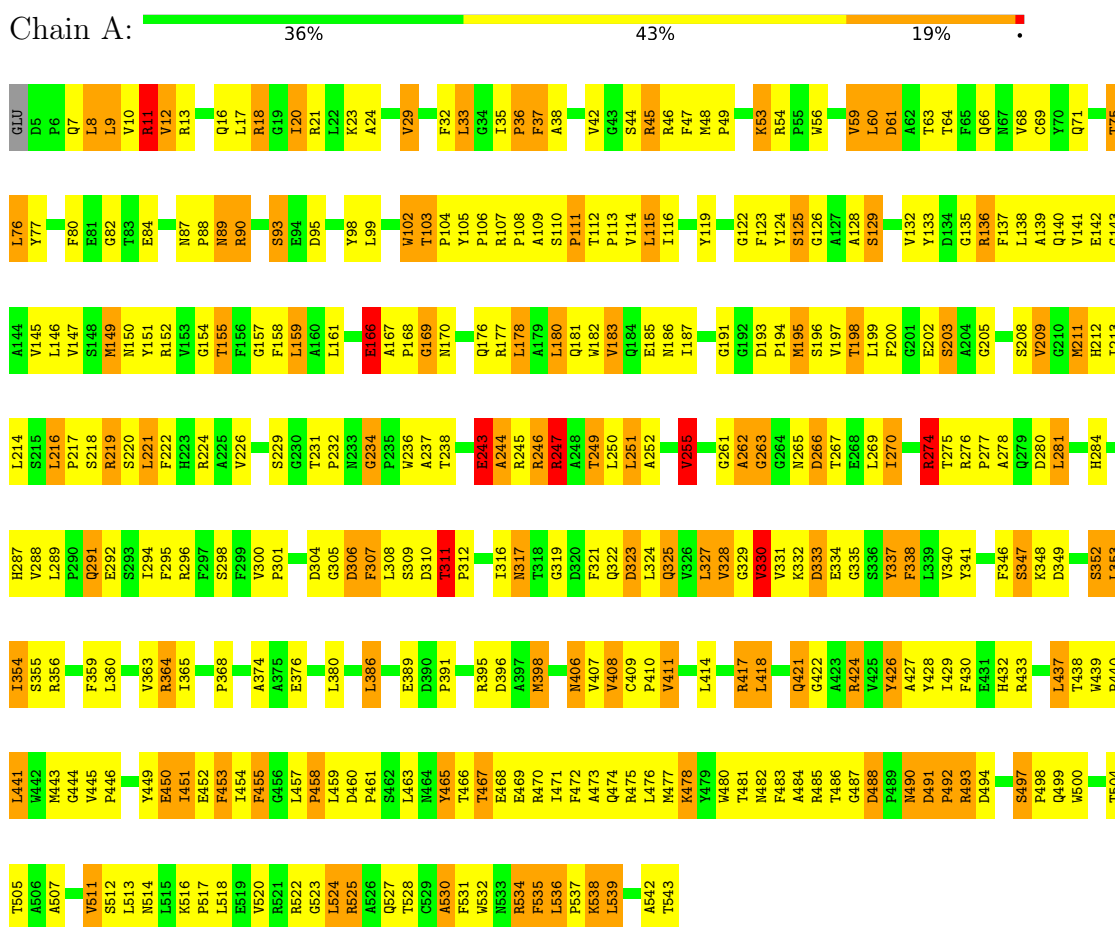
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	4172	2681	723	754	14	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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	0.85	1/4298 (0.0%)	1.80	94/5879 (1.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PHE	CA-CB	-5.32	1.46	1.54

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ARG	N-CA-C	-10.87	99.53	113.12
1	A	488	ASP	CA-CB-CG	9.34	121.94	112.60
1	A	543	THR	CA-C-O	9.34	136.67	120.80
1	A	263	GLY	N-CA-C	9.05	121.45	111.85
1	A	247	ARG	CD-NE-CZ	8.66	136.53	124.40
1	A	408	VAL	N-CA-C	8.57	118.61	110.30
1	A	298	SER	N-CA-C	7.79	119.55	111.14
1	A	126	GLY	N-CA-C	7.65	119.21	111.95
1	A	154	GLY	O-C-N	-7.54	114.76	122.60
1	A	37	PHE	CA-CB-CG	7.44	121.24	113.80
1	A	490	ASN	N-CA-C	6.98	121.23	110.20
1	A	265	ASN	N-CA-CB	6.68	122.50	110.95
1	A	411	VAL	CA-C-O	6.55	128.12	121.17
1	A	335	GLY	N-CA-C	6.54	121.97	113.27
1	A	491	ASP	CA-C-N	6.53	128.00	119.84
1	A	491	ASP	C-N-CA	6.53	128.00	119.84
1	A	328	VAL	CA-C-O	-6.50	114.39	121.28
1	A	426	TYR	CA-C-O	-6.50	113.51	121.11
1	A	333	ASP	N-CA-C	6.37	117.52	108.54
1	A	406	ASN	CA-C-N	-6.28	116.81	122.97
1	A	406	ASN	C-N-CA	-6.28	116.81	122.97
1	A	36	PRO	CA-C-O	-6.22	114.54	121.32
1	A	211	MET	CA-C-N	-6.22	112.36	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	MET	C-N-CA	-6.22	112.36	120.44
1	A	386	LEU	N-CA-C	-6.19	105.56	113.23
1	A	247	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	A	166	GLU	N-CA-C	6.01	120.74	113.17
1	A	542	ALA	N-CA-C	-6.01	105.61	113.12
1	A	64	THR	N-CA-C	5.97	118.14	109.07
1	A	424	ARG	N-CA-C	-5.92	98.08	108.20
1	A	33	LEU	N-CA-CB	-5.88	100.84	109.95
1	A	11	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	411	VAL	CB-CA-C	-5.83	104.50	111.97
1	A	354	ILE	N-CA-C	5.83	116.40	110.05
1	A	37	PHE	N-CA-C	-5.79	106.07	114.12
1	A	338	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	102	TRP	N-CA-CB	5.75	120.33	110.68
1	A	238	THR	N-CA-CB	5.72	121.21	111.66
1	A	49	PRO	N-CA-C	-5.71	104.99	110.47
1	A	262	ALA	CA-C-N	-5.68	114.67	122.57
1	A	262	ALA	C-N-CA	-5.68	114.67	122.57
1	A	530	ALA	N-CA-C	-5.67	105.17	111.36
1	A	102	TRP	CA-CB-CG	5.66	124.35	113.60
1	A	450	GLU	N-CA-C	-5.64	106.53	113.41
1	A	284	HIS	CA-CB-CG	-5.62	108.18	113.80
1	A	449	TYR	CB-CA-C	5.54	119.64	111.17
1	A	103	THR	O-C-N	5.53	125.81	121.88
1	A	128	ALA	O-C-N	-5.52	115.76	122.22
1	A	33	LEU	O-C-N	-5.50	116.60	123.04
1	A	305	GLY	N-CA-C	-5.48	106.09	115.08
1	A	244	ALA	CA-C-O	5.48	126.76	121.00
1	A	9	LEU	CA-C-N	-5.48	115.32	122.94
1	A	9	LEU	C-N-CA	-5.48	115.32	122.94
1	A	219	ARG	N-CA-C	5.48	117.69	111.11
1	A	71	GLN	N-CA-CB	-5.46	103.10	111.56
1	A	255	VAL	N-CA-CB	-5.46	105.22	112.26
1	A	287	HIS	CA-C-N	-5.45	114.56	122.69
1	A	287	HIS	C-N-CA	-5.45	114.56	122.69
1	A	424	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	209	VAL	CB-CA-C	-5.43	104.92	112.04
1	A	49	PRO	CA-C-O	-5.43	116.99	120.90
1	A	71	GLN	N-CA-C	5.42	117.09	108.79
1	A	543	THR	CB-CA-C	5.41	121.00	109.10
1	A	169	GLY	N-CA-C	5.40	119.48	112.68
1	A	465	TYR	N-CA-C	-5.40	101.58	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	274	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	A	159	LEU	CA-C-N	-5.34	113.48	122.29
1	A	159	LEU	C-N-CA	-5.34	113.48	122.29
1	A	234	GLY	O-C-N	-5.34	116.43	121.77
1	A	307	PHE	CA-C-O	-5.33	114.90	120.55
1	A	311	THR	CB-CA-C	-5.32	99.69	110.17
1	A	125	SER	CA-C-O	-5.30	115.74	121.36
1	A	266	ASP	CB-CA-C	5.29	119.56	110.79
1	A	449	TYR	CA-CB-CG	-5.23	104.48	113.90
1	A	249	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	234	GLY	N-CA-C	5.22	122.98	112.34
1	A	535	PHE	N-CA-C	5.20	117.74	111.40
1	A	511	VAL	N-CA-C	5.14	116.77	108.85
1	A	455	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	33	LEU	N-CA-C	5.13	117.91	109.76
1	A	229	SER	CA-C-O	-5.11	115.61	121.54
1	A	337	TYR	CA-CB-CG	5.10	123.08	113.90
1	A	89	ASN	CA-C-O	5.09	125.48	119.48
1	A	292	GLU	CA-C-O	-5.07	115.48	121.16
1	A	306	ASP	CA-C-N	-5.06	113.50	120.28
1	A	306	ASP	C-N-CA	-5.06	113.50	120.28
1	A	520	VAL	N-CA-C	5.06	116.74	109.51
1	A	243	GLU	O-C-N	5.05	128.48	122.27
1	A	330	VAL	N-CA-CB	-5.05	102.63	110.96
1	A	13	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	458	PRO	CB-CA-C	5.01	119.00	111.68
1	A	154	GLY	CA-C-N	5.00	126.98	120.28
1	A	154	GLY	C-N-CA	5.00	126.98	120.28

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	273	37
All	All	4172	0	4052	273	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 33.

All (273) 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:HH11	1:A:11:ARG:HB2	1.44	0.81
1:A:36:PRO:HB2	1:A:53:LYS:HG2	1.62	0.79
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.63	0.78
1:A:112:THR:HG23	1:A:113:PRO:HD2	1.65	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:138:LEU:HG	1:A:477:MET:HE3	1.69	0.73
1:A:36:PRO:HB2	1:A:53:LYS:CG	2.18	0.73
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:HH21	1:A:18:ARG:HB2	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:66:GLN:HB3	1:A:98:TYR:HD2	1.60	0.66
1:A:440:PRO:HD2	1:A:443:MET:SD	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LYS:HZ3	1:A:478:LYS:HB3	1.61	0.66
1:A:407:VAL:O	1:A:411:VAL:HG23	1.96	0.65
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.31	0.65
1:A:528:THR:O	1:A:531:PHE:HB3	1.96	0.65
1:A:89:ASN:O	1:A:90:ARG:HD3	1.96	0.65
1:A:470:ARG:O	1:A:474:GLN:HG3	1.96	0.65
1:A:534:ARG:HG3	1:A:534:ARG:HH11	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: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: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:17:LEU:HD23	1:A:60:LEU:HB3	1.84	0.58
1:A:42:VAL:O	1:A:45:ARG:HB2	2.04	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:99:LEU:C	1:A:99:LEU:HD12	2.28	0.58
1:A:231:THR:HB	1:A:232:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:MET:HE2	1:A:176:GLN:HB3	1.87	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: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:363:VAL:N	1:A:398:MET:HE1	2.23	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:18:ARG:HH22	1:A:59:VAL:HG11	1.71	0.54
1:A:250:LEU:HG	1:A:288:VAL:HG12	1.89	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:HB3	1:A:478:LYS:NZ	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:149:MET:HE2	1:A:176:GLN:HA	1.91	0.53
1:A:66:GLN:HB3	1:A:98:TYR:CD2	2.43	0.53
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.23	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:450:GLU:HG2	1:A:451:ILE:N	2.20	0.52
1:A:18:ARG:HB2	1:A:18:ARG:NH2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:O	1:A:159:LEU:C	2.52	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:HG3	1:A:107:ARG:HH11	1.76	0.51
1:A:317:ASN:HA	1:A:417:ARG:HD2	1.92	0.51
1:A:346:PHE:HA	1:A:352:SER:HB3	1.93	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:106:PRO:O	1:A:107:ARG:C	2.54	0.50
1:A:432:HIS:HB3	1:A:472:PHE:HE2	1.76	0.50
1:A:68:VAL:HG12	1:A:69:CYS:O	2.12	0.50
1:A:409:CYS:N	1:A:410:PRO:CD	2.75	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:407:VAL:C	1:A:410:PRO:HD2	2.37	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
1:A:363:VAL:HG23	1:A:398:MET:HE1	1.94	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: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:236:TRP:CZ3	1:A:237:ALA:HB2	2.48	0.48
1:A:36:PRO:HB2	1:A:53:LYS:HG3	1.95	0.48
1:A:249:THR:OG1	1:A:250:LEU:N	2.46	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:75:THR:O	1:A:77:TYR:N	2.47	0.48
1:A:146:LEU:C	1:A:146:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:THR:OG1	1:A:487:GLY:N	2.47	0.48
1:A:247:ARG:HB3	1:A:288:VAL:CG2	2.44	0.47
1:A:208:SER:O	1:A:209:VAL:C	2.57	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:211:MET:HG2	1:A:308:LEU:HD21	1.97	0.47
1:A:328:VAL:HG11	1:A:411:VAL:HG13	1.95	0.47
1:A:445:VAL:HG12	1:A:445:VAL:O	2.14	0.47
1:A:77:TYR:CD2	1:A:348:LYS:HD3	2.50	0.47
1:A:202:GLU:O	1:A:203:SER:C	2.57	0.46
1:A:255:VAL:HG13	1:A:276:ARG:HD2	1.98	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:68:VAL:HG21	1:A:88:PRO:HB3	1.97	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:45:ARG:NH1	1:A:45:ARG:HG3	2.29	0.46
1:A:10:VAL:HG23	1:A:32:PHE:CE2	2.51	0.46
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.81	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:517:PRO:O	1:A:518:LEU:C	2.59	0.46
1:A:138:LEU:HG	1:A:477:MET:CE	2.44	0.46
1:A:136:ARG:HG2	1:A:137:PHE:N	2.31	0.46
1:A:182:TRP:O	1:A:183:VAL:C	2.60	0.45
1:A:291:GLN:HE21	1:A:291:GLN:HB2	1.61	0.45
1:A:477:MET:HE2	1:A:477:MET:HB3	1.79	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:16:GLN:HB3	1:A:59:VAL:HG22	1.99	0.45
1:A:161:LEU:HD13	1:A:270:ILE:CD1	2.47	0.45
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.70	0.45
1:A:490:ASN:O	1:A:491:ASP:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG21	1:A:459:LEU:HD22	1.99	0.44
1:A:149:MET:HE2	1:A:176:GLN:CB	2.47	0.44
1:A:211:MET:HE1	1:A:301:PRO:HG2	2.00	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:124:TYR:CD1	1:A:124:TYR:C	2.96	0.43
1:A:407:VAL:O	1:A:410:PRO:HD2	2.18	0.43
1:A:451:ILE:H	1:A:451:ILE:HG12	1.55	0.43
1:A:306:ASP:O	1:A:307:PHE:C	2.57	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: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:453:PHE:O	1:A:454:ILE:C	2.62	0.43
1:A:21:ARG:HH21	1:A:23:LYS:HZ1	1.63	0.43
1:A:208:SER:O	1:A:211:MET:N	2.52	0.43
1:A:33:LEU:CD1	1:A:33:LEU:N	2.82	0.43
1:A:56:TRP:CD1	1:A:60:LEU:HB2	2.53	0.42
1:A:116:ILE:CD1	1:A:183:VAL:HG11	2.32	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:HD12	1:A:418:LEU:HA	1.91	0.42
1:A:216:LEU:O	1:A:217:PRO:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ALA:O	1:A:245:ARG:C	2.60	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:243:GLU:OE1	1:A:247:ARG:NH2	2.48	0.42
1:A:451:ILE:O	1:A:452:GLU:C	2.63	0.42
1:A:159:LEU:C	1:A:159:LEU:HD23	2.45	0.42
1:A:93:SER:OG	1:A:95:ASP:N	2.46	0.41
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:317:ASN:CB	1:A:417:ARG:NH1	2.84	0.41
1:A:364:ARG:HH11	1:A:364:ARG:HD3	1.69	0.41
1:A:374:ALA:HA	1:A:539:LEU:HD13	2.02	0.41
1:A:475:ARG:HH11	1:A:475:ARG:HD3	1.66	0.41
1:A:170:ASN:ND2	1:A:304:ASP:OD2	2.52	0.41
1:A:193:ASP:HA	1:A:194:PRO:HD2	1.92	0.41
1:A:406:ASN:O	1:A:410:PRO:HG2	2.21	0.41
1:A:60:LEU:HD12	1:A:61:ASP:O	2.21	0.41
1:A:212:HIS:HD2	1:A:218:SER:OG	2.02	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:8:LEU:HD11	1:A:21:ARG:HB2	2.02	0.41
1:A:75:THR:HB	1:A:76:LEU:H	1.75	0.41
1:A:132:VAL:HG23	1:A:133:TYR:CE1	2.55	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:35:ILE:O	1:A:36:PRO:C	2.61	0.40
1:A:180:LEU:HD11	1:A:199:LEU:HD21	2.03	0.40
1:A:249:THR:O	1:A:250:LEU:C	2.62	0.40
1:A:277:PRO:O	1:A:278:ALA:C	2.64	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
1:A:524:LEU:O	1:A:525:ARG:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:ALA:CB	1:A:109:ALA:CB[3_555]	2.03	0.17
1:A:262:ALA:N	1:A:262:ALA:N[11_555]	2.03	0.17
1:A:21:ARG:CZ	1:A:21:ARG:NH1[4_565]	2.07	0.13
1:A:261:GLY:N	1:A:263:GLY:O[11_555]	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%)	7 35

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%)	345 (80%)	89 (20%)	1 7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	VAL
1	A	18	ARG
1	A	20	ILE
1	A	29	VAL
1	A	45	ARG
1	A	53	LYS
1	A	59	VAL
1	A	60	LEU
1	A	61	ASP
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	198	THR
1	A	214	LEU
1	A	216	LEU
1	A	220	SER
1	A	221	LEU
1	A	243	GLU
1	A	246	ARG
1	A	247	ARG
1	A	251	LEU
1	A	255	VAL
1	A	267	THR
1	A	270	ILE
1	A	274	ARG
1	A	275	THR
1	A	281	LEU
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	296	ARG
1	A	309	SER
1	A	311	THR
1	A	317	ASN
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	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

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Mol	Chain	Res	Type
1	A	536	LEU
1	A	538	LYS
1	A	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	181	GLN
1	A	212	HIS
1	A	228	GLN
1	A	291	GLN
1	A	317	ASN
1	A	421	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 oligosaccharides 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.