Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 08:32 am GMT

PDB ID	:	2WIK
Title	:	NONAGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA6
Authors	:	Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on	:	2009-05-12
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

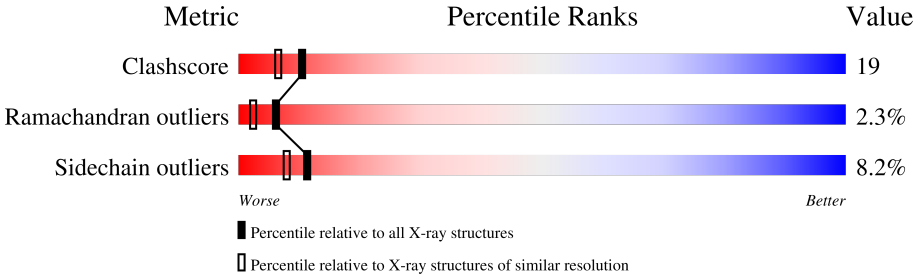
MolProbity	:	4.02b-467
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	FAILED
EDS	:	FAILED
buster-report	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	A	615	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4754 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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4205	2713	709	768	15	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276

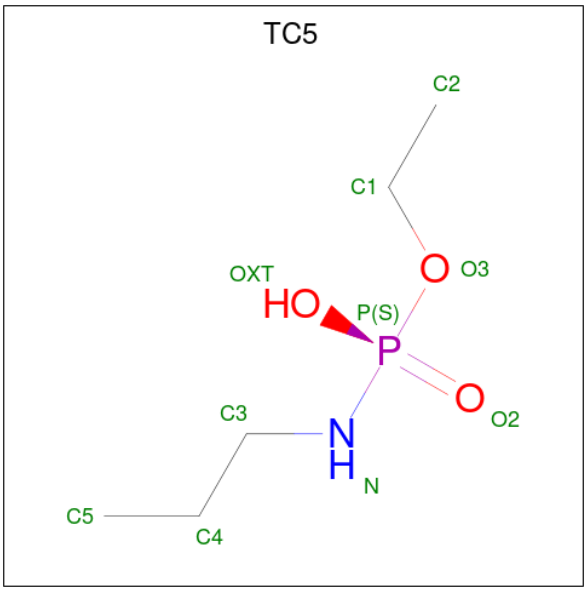
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	24	14	1	9	0	0	0

- Molecule 4 is ETHYL HYDROGEN PROPYLAMIDOPHOSPHATE (three-letter code: TC5) (formula: $C_5H_{14}NO_3P$).

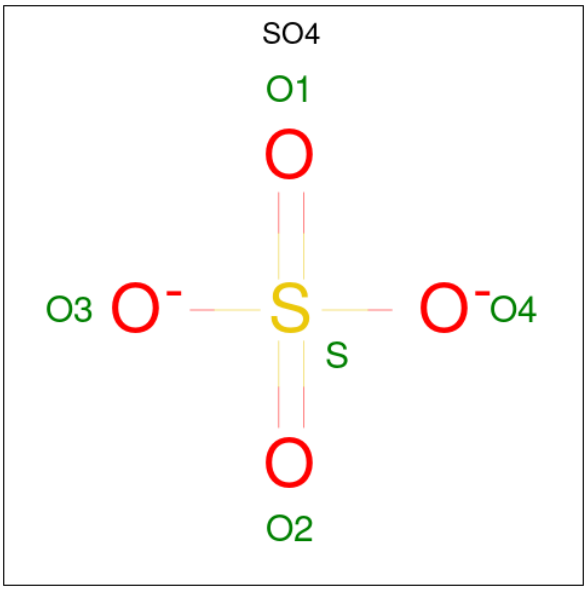


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	9	5	1	2	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	3	3	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

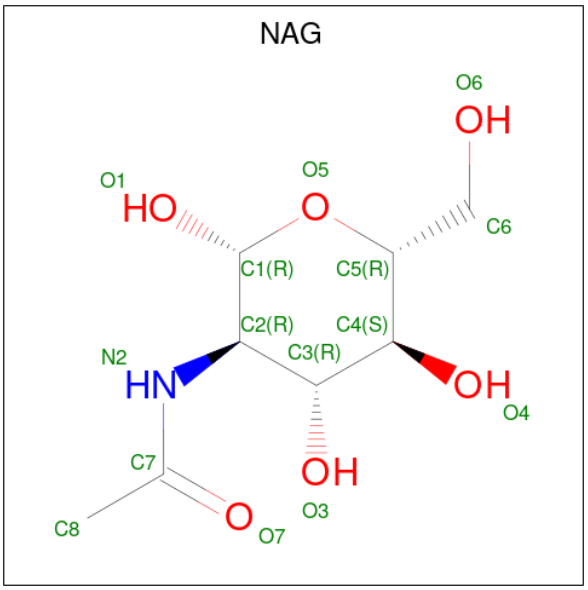


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	A	1	1	1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
			Total	C	N	O		
8	A	1	14	8	1	5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	384	384	384	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	155.24Å 155.24Å 127.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (55.05-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.213 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4754	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, TC5, NAG, SO4, FUL, NA

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	1.59	45/4330 (1.0%)	1.36	36/5879 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLU	CG-CD	10.03	1.67	1.51
1	A	398	PHE	CE2-CZ	9.74	1.55	1.37
1	A	419	TYR	CD1-CE1	8.64	1.52	1.39
1	A	371	PHE	CE1-CZ	8.53	1.53	1.37
1	A	118	PHE	CE2-CZ	7.85	1.52	1.37
1	A	197	GLU	CB-CG	7.45	1.66	1.52
1	A	255	GLU	CG-CD	7.17	1.62	1.51
1	A	404	GLU	CG-CD	7.00	1.62	1.51
1	A	255	GLU	CB-CG	6.97	1.65	1.52
1	A	231	TRP	CE3-CZ3	6.77	1.50	1.38
1	A	371	PHE	CD2-CE2	6.64	1.52	1.39
1	A	114	TYR	CE2-CZ	-6.47	1.30	1.38
1	A	90	GLU	CG-CD	-6.46	1.42	1.51
1	A	61	TYR	CD1-CE1	6.42	1.49	1.39
1	A	443	GLU	CD-OE1	6.40	1.32	1.25
1	A	268	ASP	CB-CG	6.39	1.65	1.51
1	A	419	TYR	CZ-OH	6.25	1.48	1.37
1	A	419	TYR	CD2-CE2	6.23	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	VAL	CB-CG2	-6.13	1.40	1.52
1	A	128	TYR	CD1-CE1	6.11	1.48	1.39
1	A	56	TRP	CB-CG	-5.92	1.39	1.50
1	A	474	PHE	CE2-CZ	5.88	1.48	1.37
1	A	501	LEU	C-O	5.85	1.34	1.23
1	A	490	TRP	CE3-CZ3	5.84	1.48	1.38
1	A	440	TYR	CE1-CZ	5.75	1.46	1.38
1	A	521	PHE	CE1-CZ	5.74	1.48	1.37
1	A	60	LYS	CD-CE	5.61	1.65	1.51
1	A	510	ILE	C-O	5.49	1.33	1.23
1	A	349	GLU	CB-CG	5.46	1.62	1.52
1	A	497	GLU	CD-OE2	5.38	1.31	1.25
1	A	392	VAL	CB-CG1	-5.33	1.41	1.52
1	A	115	GLY	CA-C	5.21	1.60	1.51
1	A	290	PHE	CE1-CZ	5.18	1.47	1.37
1	A	137	GLU	CD-OE2	5.17	1.31	1.25
1	A	337	PHE	CD1-CE1	5.15	1.49	1.39
1	A	232	ALA	CA-CB	-5.14	1.41	1.52
1	A	419	TYR	CB-CG	5.09	1.59	1.51
1	A	363	GLU	CG-CD	5.08	1.59	1.51
1	A	404	GLU	CD-OE1	5.08	1.31	1.25
1	A	436	VAL	CB-CG2	5.06	1.63	1.52
1	A	418	PHE	CG-CD2	5.06	1.46	1.38
1	A	332	TYR	CE1-CZ	5.04	1.45	1.38
1	A	516	ALA	CA-CB	5.01	1.62	1.52
1	A	521	PHE	CG-CD1	5.01	1.46	1.38
1	A	456	TYR	CD1-CE1	5.01	1.46	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	242	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	509	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	170	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	520	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	A	242	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	501	LEU	CB-CG-CD1	-7.71	97.89	111.00
1	A	424	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	395	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	A	359	PRO	C-N-CA	-7.08	107.43	122.30
1	A	434	MET	CG-SD-CE	6.72	110.96	100.20
1	A	91	ASP	CB-CG-OD1	6.57	124.22	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	156	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	A	515	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	509	ARG	CG-CD-NE	6.11	124.63	111.80
1	A	49	LEU	CA-CB-CG	-5.75	102.09	115.30
1	A	319	VAL	CG1-CB-CG2	-5.68	101.82	110.90
1	A	14	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	44	LYS	CD-CE-NZ	-5.60	98.83	111.70
1	A	147	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	424	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	509	ARG	CD-NE-CZ	5.51	131.32	123.60
1	A	103	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	A	470	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	91	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	301	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	466	SER	CA-CB-OG	-5.28	96.94	111.20
1	A	520	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	87	ASP	CB-CA-C	-5.24	99.92	110.40
1	A	325	GLU	C-N-CA	-5.23	111.31	122.30
1	A	135	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	156	LEU	N-CA-C	-5.19	96.99	111.00
1	A	412	TRP	C-N-CA	-5.15	111.48	122.30
1	A	360	GLY	C-N-CA	5.12	134.51	121.70
1	A	324	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	389	LEU	CB-CG-CD1	5.03	119.55	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide

4.2 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	4205	0	4104	158	1
2	B	38	0	34	0	0
2	D	38	0	34	0	0
3	C	24	0	22	0	0
4	A	9	0	13	2	0
5	A	3	0	0	1	0
6	A	10	0	0	1	0
7	A	1	0	0	0	0
8	A	42	0	39	1	0
9	A	384	0	0	37	0
All	All	4754	0	4246	160	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (160) 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:495:SER:HA	9:A:2002:HOH:O	1.36	1.21
1:A:176:GLN:HB3	9:A:2007:HOH:O	1.01	1.16
1:A:50:THR:HG21	9:A:2276:HOH:O	1.41	1.16
1:A:4:ILE:HD12	1:A:4:ILE:N	1.51	1.14
1:A:4:ILE:HD12	1:A:4:ILE:H	0.92	1.07
1:A:4:ILE:H	1:A:4:ILE:CD1	1.69	1.06
1:A:518:GLN:H	1:A:518:GLN:NE2	1.66	0.93
4:A:601:TC5:H32C	4:A:601:TC5:H11C	1.52	0.92
1:A:48:SER:HA	9:A:2238:HOH:O	1.69	0.91
1:A:50:THR:O	1:A:51:LYS:HB3	1.71	0.91
1:A:495:SER:CA	9:A:2002:HOH:O	2.02	0.90
1:A:4:ILE:N	1:A:4:ILE:CD1	2.22	0.89
1:A:3:ASP:N	9:A:2001:HOH:O	2.04	0.88
1:A:496:THR:N	9:A:2002:HOH:O	2.05	0.86
1:A:518:GLN:H	1:A:518:GLN:HE21	0.87	0.86
1:A:518:GLN:HE21	1:A:518:GLN:N	1.72	0.85
1:A:494:LYS:HB2	9:A:2095:HOH:O	1.76	0.85
1:A:156:LEU:CD2	1:A:261:ILE:HD11	2.08	0.82
1:A:453:ARG:HG3	9:A:2349:HOH:O	1.80	0.82
1:A:372[A]:HIS:CE1	9:A:2113:HOH:O	2.32	0.81
1:A:377:VAL:O	1:A:377:VAL:HG23	1.78	0.81
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:HB2	9:A:2105:HOH:O	1.81	0.81
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.64	0.80
1:A:495:SER:O	1:A:496:THR:HG23	1.83	0.79
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.17	0.79
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.66	0.77
1:A:4:ILE:HG22	9:A:2171:HOH:O	1.84	0.76
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.20	0.76
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.68	0.74
1:A:453:ARG:HA	1:A:453:ARG:HE	1.53	0.74
1:A:489:SER:HB2	9:A:2133:HOH:O	1.90	0.72
1:A:377:VAL:O	1:A:377:VAL:CG2	2.39	0.70
1:A:522:TRP:O	1:A:527:PRO:HD3	1.93	0.69
1:A:270:GLN:O	1:A:274:LEU:HB2	1.93	0.68
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.29	0.68
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.08	0.67
1:A:284:THR:HG22	1:A:359:PRO:HG2	1.75	0.67
1:A:380:GLN:HB2	5:A:605:CL:CL	2.32	0.66
1:A:214:HIS:HB2	9:A:2136:HOH:O	1.95	0.66
1:A:509:ARG:HD3	9:A:2298:HOH:O	1.95	0.65
1:A:358:PHE:N	1:A:359:PRO:HD3	2.11	0.64
1:A:48:SER:CA	9:A:2238:HOH:O	2.36	0.64
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.80	0.63
1:A:157:PRO:HD2	1:A:240:ARG:CD	2.29	0.63
1:A:425:SER:O	9:A:2003:HOH:O	2.16	0.63
1:A:284:THR:CG2	1:A:359:PRO:HG2	2.28	0.63
1:A:454:ASP:O	1:A:455:GLN:HB2	1.98	0.63
1:A:227:PHE:CD2	1:A:227:PHE:C	2.72	0.62
1:A:105:LYS:HG3	9:A:2014:HOH:O	1.99	0.61
1:A:403:LEU:O	1:A:407:LYS:HG3	2.01	0.61
1:A:55:ILE:HD11	9:A:2360:HOH:O	2.01	0.60
1:A:49:LEU:HD12	1:A:50:THR:H	1.67	0.60
1:A:355:LYS:HG2	1:A:366:LYS:HE3	1.83	0.60
1:A:262:LYS:HG2	1:A:265:ARG:HH22	1.65	0.60
1:A:105:LYS:NZ	9:A:2014:HOH:O	2.34	0.59
1:A:425:SER:HB3	1:A:428:LEU:HD23	1.84	0.59
1:A:69:ILE:HG22	1:A:70:ASP:N	2.17	0.59
1:A:361:VAL:O	1:A:366:LYS:NZ	2.36	0.59
1:A:510:ILE:HD13	1:A:510:ILE:N	2.15	0.58
1:A:277:ALA:CB	9:A:2105:HOH:O	2.47	0.58
1:A:156:LEU:HD23	1:A:261:ILE:HD11	1.83	0.58
1:A:39:GLY:O	1:A:265:ARG:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLU:HG2	9:A:2167:HOH:O	2.05	0.57
1:A:176:GLN:NE2	9:A:2016:HOH:O	2.38	0.57
1:A:372[A]:HIS:HE1	1:A:518:GLN:HA	1.70	0.57
1:A:276:GLU:O	1:A:279:VAL:HG22	2.04	0.57
4:A:601:TC5:H32C	4:A:601:TC5:C1	2.32	0.57
1:A:378:ASP:O	1:A:380:GLN:N	2.37	0.56
1:A:116:GLY:HA3	1:A:120:THR:O	2.06	0.56
1:A:4:ILE:HG12	1:A:17:GLN:OE1	2.06	0.56
1:A:378:ASP:C	1:A:380:GLN:H	2.10	0.55
1:A:256:ASN:OD1	8:A:615:NAG:H3	2.07	0.55
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.06	0.55
1:A:357:PHE:C	1:A:359:PRO:HD3	2.27	0.55
1:A:509:ARG:HG2	9:A:2298:HOH:O	2.06	0.55
1:A:253:SER:O	1:A:254:ARG:HD3	2.06	0.55
1:A:17:GLN:HE21	1:A:24:THR:HG21	1.72	0.55
1:A:69:ILE:CG2	1:A:70:ASP:N	2.70	0.54
1:A:278:PHE:C	1:A:280:VAL:H	2.11	0.54
1:A:251:GLY:HA2	9:A:2230:HOH:O	2.07	0.53
1:A:383:GLU:CD	1:A:383:GLU:H	2.11	0.53
1:A:453:ARG:HE	1:A:453:ARG:CA	2.19	0.53
1:A:234:THR:O	1:A:293:THR:HG22	2.08	0.53
1:A:502:THR:OG1	1:A:509:ARG:NH1	2.42	0.53
1:A:214:HIS:HE1	9:A:2264:HOH:O	1.92	0.53
1:A:137:GLU:OE2	1:A:465:ARG:NH1	2.40	0.52
1:A:280:VAL:HG13	1:A:282:TYR:O	2.10	0.52
1:A:495:SER:O	1:A:496:THR:CG2	2.57	0.52
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.45	0.51
1:A:176:GLN:CG	9:A:2007:HOH:O	2.44	0.51
1:A:198:SER:HA	1:A:224:SER:O	2.10	0.50
1:A:385:TYR:HD2	9:A:2201:HOH:O	1.94	0.50
1:A:262:LYS:HD2	1:A:262:LYS:O	2.12	0.50
1:A:74:PRO:HA	9:A:2179:HOH:O	2.11	0.50
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.94	0.50
1:A:280:VAL:CG1	1:A:282:TYR:O	2.60	0.50
1:A:372[A]:HIS:CE1	1:A:518:GLN:HA	2.47	0.50
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.93	0.49
1:A:452:ARG:C	1:A:454:ASP:H	2.16	0.49
1:A:240:ARG:O	1:A:241:ASN:C	2.51	0.49
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.48	0.48
1:A:393:VAL:O	1:A:397:ASN:HB2	2.13	0.48
1:A:502:THR:O	1:A:508:THR:HB	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.49	0.48
1:A:224:SER:OG	1:A:325:GLU:OE2	2.22	0.48
1:A:347:ARG:HD2	1:A:385:TYR:OH	2.14	0.48
1:A:3:ASP:HA	1:A:4:ILE:HD12	1.96	0.47
1:A:495:SER:C	9:A:2002:HOH:O	2.33	0.47
1:A:238:GLU:O	1:A:242:ARG:HG3	2.15	0.47
1:A:295:ASP:OD1	1:A:295:ASP:N	2.44	0.47
1:A:448:LEU:N	1:A:449:PRO:CD	2.78	0.47
1:A:245:ASN:O	1:A:249:LEU:HD12	2.16	0.46
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.51	0.46
1:A:48:SER:CB	9:A:2238:HOH:O	2.61	0.46
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.51	0.46
1:A:117:GLY:O	1:A:118:PHE:HB2	2.16	0.45
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.97	0.45
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.46	0.45
1:A:524:SER:O	1:A:528:LYS:HE3	2.16	0.45
1:A:458:LYS:HA	1:A:458:LYS:HD2	1.58	0.45
1:A:322:ASN:O	1:A:325:GLU:HG2	2.16	0.45
1:A:176:GLN:CB	9:A:2007:HOH:O	1.87	0.45
1:A:17:GLN:NE2	1:A:24:THR:HG21	2.32	0.45
1:A:452:ARG:O	1:A:454:ASP:N	2.50	0.45
1:A:18:LEU:HD11	1:A:27:ALA:HB2	1.98	0.44
1:A:157:PRO:HG2	1:A:236:LEU:HG	2.00	0.44
1:A:25:VAL:HG13	1:A:99:ILE:O	2.18	0.43
1:A:248:LYS:O	1:A:251:GLY:N	2.52	0.43
1:A:262:LYS:HD2	1:A:262:LYS:C	2.39	0.43
1:A:279:VAL:HG21	1:A:290:PHE:CE2	2.54	0.43
1:A:348:LYS:HB3	9:A:2144:HOH:O	2.18	0.43
1:A:13:VAL:HG23	1:A:28:PHE:HD2	1.84	0.43
1:A:49:LEU:HD12	1:A:50:THR:N	2.33	0.42
1:A:247:ALA:O	1:A:248:LYS:C	2.57	0.42
1:A:21:PHE:N	9:A:2005:HOH:O	2.23	0.42
1:A:217:PHE:O	1:A:313:LYS:HE2	2.20	0.42
1:A:415:ASN:HB2	6:A:606:SO4:O3	2.20	0.42
1:A:497:GLU:H	1:A:497:GLU:HG3	1.34	0.42
1:A:509:ARG:CG	9:A:2298:HOH:O	2.66	0.42
1:A:197:GLU:HA	1:A:223:GLN:O	2.20	0.42
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.20	0.41
1:A:28:PHE:N	1:A:28:PHE:CD1	2.88	0.41
1:A:341:ASN:C	1:A:341:ASN:OD1	2.59	0.41
1:A:391:ASP:O	1:A:392:VAL:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ALA:HB1	1:A:505:THR:HB	2.00	0.41
1:A:110:LEU:HB3	1:A:195:PHE:CE1	2.56	0.41
1:A:328:ALA:HA	1:A:434:MET:CE	2.51	0.41
1:A:509:ARG:CD	9:A:2298:HOH:O	2.63	0.41
1:A:378:ASP:CG	1:A:379:ASP:H	2.24	0.41
1:A:347:ARG:HB2	1:A:385:TYR:OH	2.21	0.41
1:A:518:GLN:NE2	1:A:518:GLN:N	2.47	0.41
1:A:140:ILE:HG22	1:A:141:VAL:N	2.36	0.41
1:A:407:LYS:HG2	1:A:493:PHE:HE1	1.85	0.41
1:A:157:PRO:HD2	1:A:240:ARG:HD3	2.04	0.40
1:A:24:THR:O	1:A:101:ALA:HB3	2.21	0.40
1:A:184:ALA:N	9:A:2023:HOH:O	2.45	0.40
1:A:268:ASP:HA	1:A:269:PRO:HD2	1.84	0.40
1:A:39:GLY:O	1:A:265:ARG:CD	2.69	0.40
1:A:495:SER:O	1:A:496:THR:CB	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:OE1	1:A:367:GLU:OE1[5_555]	2.17	0.03

4.3 Torsion angles (i)

4.3.1 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	527/529 (100%)	475 (90%)	40 (8%)	12 (2%)	6 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	LYS
1	A	379	ASP
1	A	496	THR
1	A	249	LEU
1	A	453	ARG
1	A	506	GLU
1	A	281	PRO
1	A	9	LYS
1	A	361	VAL
1	A	279	VAL
1	A	251	GLY

4.3.2 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	452/454 (100%)	415 (92%)	37 (8%)	11 8

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

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	13	VAL
1	A	16	MET
1	A	51	LYS
1	A	69	ILE
1	A	91	ASP
1	A	138	ARG
1	A	156	LEU
1	A	195	PHE
1	A	214	HIS
1	A	236	LEU
1	A	240	ARG
1	A	248	LYS
1	A	254	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	LYS
1	A	265	ARG
1	A	274	LEU
1	A	280	VAL
1	A	286	LEU
1	A	299	LEU
1	A	359	PRO
1	A	361	VAL
1	A	375	ASP
1	A	376	TRP
1	A	387	GLU
1	A	428	LEU
1	A	453	ARG
1	A	454	ASP
1	A	455	GLN
1	A	489	SER
1	A	492	VAL
1	A	497	GLU
1	A	506	GLU
1	A	509	ARG
1	A	518	GLN
1	A	529	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	289	ASN
1	A	380	GLN
1	A	518	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

Mogul was not executed - this section is therefore empty.

4.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

4.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

4.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.