



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:50 AM GMT

PDB ID : 2JGI  
Title : CRYSTAL STRUCTURE OF MOUSE ACETYLCHOLINESTERASE INHIBITED BY NON-AGED DIISOPROPYL FLUOROPHOSPHATE (DFP)  
Authors : Hornberg, A.; Tunemalm, A.-K.; Ekstrom, F.  
Deposited on : 2007-02-13  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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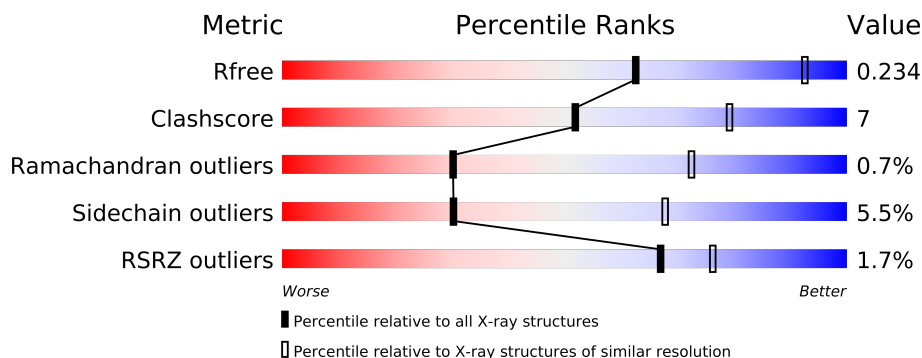
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	1544	-	X

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8441 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

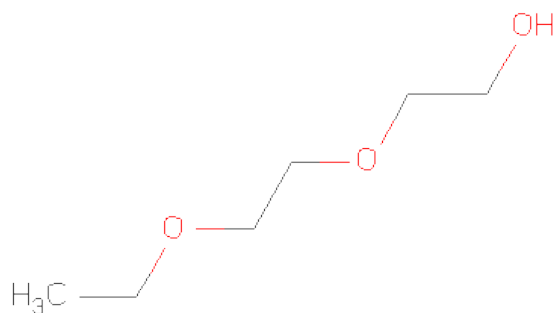
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	535	4191	2688	726	762	1	14	0	0	0
1	B	532	4167	2675	720	757	1	14	0	0	0

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 3 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula:  $C_6H_{14}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is water.

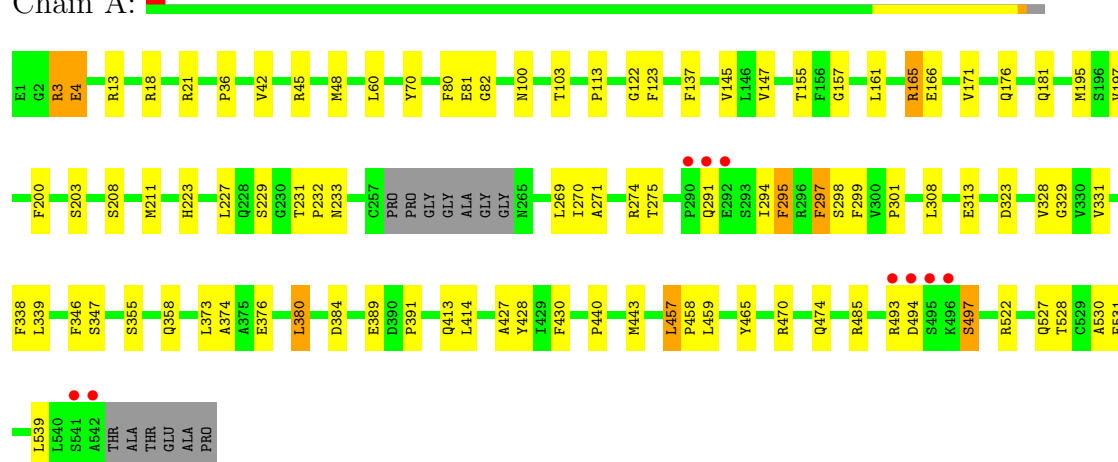
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	20	Total	O	0	0
			20	20		

### 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 errors 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.

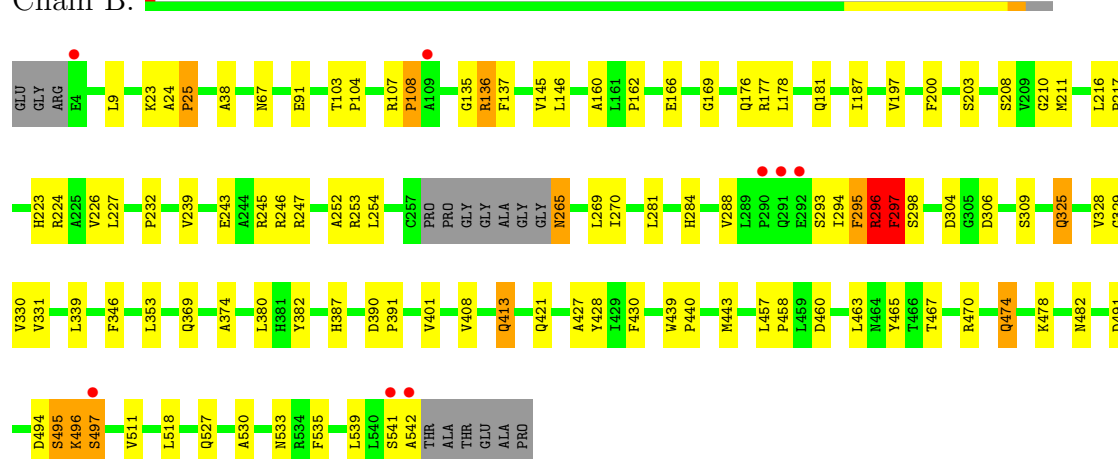
#### • Molecule 1: ACETYLCHOLINESTERASE

Chain A:



#### • Molecule 1: ACETYLCHOLINESTERASE

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.72Å 109.88Å 226.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.90) 100.0 (19.97-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.242 0.198 , 0.234	Depositor DCC
$R_{free}$ test set	869 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 9.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 44326 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AE3, NAG, SVY

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	0.51	0/4297	0.64	1/5868 (0.0%)
1	B	0.51	0/4273	0.64	0/5837
All	All	0.51	0/8570	0.64	1/11705 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	274	ARG	NE-CZ-NH2	-5.26	117.67	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	LYS	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4191	0	4087	56	0
1	B	4167	0	4063	64	0
2	A	14	0	13	1	0
3	B	9	0	14	0	0
4	A	40	0	0	1	0
4	B	20	0	0	1	0
All	All	8441	0	8177	119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:SVY:H3'3	1:A:297:PHE:CZ	2.05	0.91
1:B:197:VAL:H	1:B:223:HIS:HD2	1.22	0.88
1:A:48:MET:HE3	1:A:165:ARG:O	1.80	0.82
1:B:203:SVY:H2'3	1:B:295:PHE:CE2	2.15	0.82
1:B:203:SVY:H2'3	1:B:295:PHE:HE2	1.43	0.81
1:A:203:SVY:H3'3	1:A:297:PHE:HZ	1.45	0.79
1:B:197:VAL:H	1:B:223:HIS:CD2	2.01	0.77
1:A:203:SVY:H2'3	1:A:295:PHE:CE2	2.26	0.70
1:A:203:SVY:H2'3	1:A:295:PHE:HE2	1.57	0.70
1:A:295:PHE:N	1:A:295:PHE:CD1	2.60	0.69
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.27	0.69
1:A:459:LEU:HD23	1:A:470:ARG:HG2	1.76	0.68
1:A:197:VAL:H	1:A:223:HIS:HD2	1.43	0.66
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.78	0.66
1:A:295:PHE:N	1:A:295:PHE:HD1	1.95	0.64
1:B:243:GLU:O	1:B:247:ARG:HG3	1.99	0.63
1:A:203:SVY:C3'	1:A:297:PHE:HZ	2.10	0.62
1:B:295:PHE:CD1	1:B:295:PHE:N	2.67	0.61
1:B:295:PHE:HD1	1:B:295:PHE:N	1.98	0.61
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.83	0.61
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.83	0.60
1:A:494:ASP:OD1	1:A:497:SER:HB2	2.01	0.59
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.03	0.59
1:B:374:ALA:HA	1:B:539:LEU:HD21	1.84	0.59
1:B:470:ARG:O	1:B:474:GLN:HG3	2.06	0.55
1:A:295:PHE:H	1:A:295:PHE:HD1	1.54	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.89	0.54
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.90	0.53
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.44	0.53
1:B:328:VAL:O	1:B:427:ALA:HA	2.08	0.53
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.44	0.53
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.91	0.52
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.90	0.52
1:A:294:ILE:HG21	1:A:338:PHE:HB3	1.91	0.52
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.90	0.52
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.92	0.52
1:B:295:PHE:HD1	1:B:295:PHE:H	1.58	0.51
1:A:48:MET:HE3	1:A:166:GLU:HA	1.92	0.51
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.40	0.50
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.93	0.50
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.93	0.50
1:B:478:LYS:O	1:B:482:ASN:HB2	2.11	0.50
1:A:45:ARG:O	1:A:48:MET:HB2	2.12	0.50
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.92	0.50
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.93	0.50
1:B:413:GLN:HB2	1:B:533:ASN:ND2	2.26	0.50
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.94	0.50
1:B:331:VAL:HG12	1:B:430:PHE:HB3	1.95	0.49
1:B:440:PRO:HG2	1:B:443:MET:HG3	1.94	0.49
1:B:160:ALA:HB2	1:B:169:GLY:HA3	1.94	0.48
1:A:380:LEU:HD13	1:B:535:PHE:HB2	1.95	0.48
1:A:36:PRO:HD3	1:A:60:LEU:HD21	1.95	0.48
1:B:103:THR:HG22	1:B:145:VAL:HG22	1.95	0.48
1:A:295:PHE:HZ	1:A:338:PHE:CD1	2.32	0.47
1:A:3:ARG:HD3	4:A:2001:HOH:O	2.13	0.47
1:A:176:GLN:OE1	1:A:208:SER:HB3	2.14	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.49	0.47
1:B:67:ASN:OD1	1:B:91:GLU:HB2	2.15	0.47
1:B:457:LEU:N	1:B:458:PRO:CD	2.77	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CE1	2.50	0.47
1:B:382:TYR:CD1	1:B:401:VAL:HG22	2.50	0.47
1:A:527:GLN:O	1:A:530:ALA:HB3	2.14	0.47
1:A:347:SER:HB2	2:A:1544:NAG:H62	1.97	0.47
1:B:495:SER:OG	1:B:496:LYS:N	2.46	0.47
1:B:527:GLN:O	1:B:530:ALA:HB3	2.15	0.47
1:A:528:THR:O	1:A:531:PHE:HB3	2.15	0.46
1:A:374:ALA:HA	1:A:539:LEU:HD23	1.97	0.46
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:470:ARG:O	1:A:474:GLN:HG3	2.16	0.46
1:B:203:SVY:C3'	1:B:297:PHE:CZ	2.99	0.46
1:B:162:PRO:HD2	1:B:245:ARG:HB2	1.96	0.46
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.98	0.46
1:B:252:ALA:HB2	1:B:269:LEU:HD21	1.97	0.46
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.50	0.46
1:B:458:PRO:HA	1:B:465:TYR:HD2	1.80	0.46
1:A:100:ASN:O	1:A:147:VAL:HA	2.16	0.46
1:A:323:ASP:OD1	1:A:323:ASP:N	2.43	0.46
1:B:497:SER:HB3	4:B:2017:HOH:O	2.17	0.45
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.99	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.16	0.45
1:A:389:GLU:O	1:A:391:PRO:HD3	2.17	0.45
1:B:294:ILE:HB	1:B:295:PHE:HD1	1.82	0.45
1:A:294:ILE:HB	1:A:295:PHE:HD1	1.81	0.45
1:B:136:ARG:HG2	1:B:137:PHE:N	2.32	0.45
1:A:137:PHE:HE2	1:A:457:LEU:HD22	1.82	0.45
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.17	0.45
1:A:122:GLY:O	1:A:123:PHE:HB2	2.17	0.45
1:B:330:VAL:HG11	1:B:408:VAL:HA	1.98	0.45
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.44
1:A:373:LEU:O	1:A:376:GLU:HB3	2.18	0.44
1:A:231:THR:HG22	1:A:414:LEU:HD22	1.98	0.44
1:A:165:ARG:HH11	1:A:165:ARG:HB3	1.82	0.43
1:B:247:ARG:HH11	1:B:298:SER:HA	1.82	0.43
1:A:271:ALA:O	1:A:275:THR:HG23	2.18	0.43
1:A:355:SER:OG	1:A:358:GLN:HG3	2.18	0.43
1:B:247:ARG:HB3	1:B:288:VAL:HG11	2.00	0.43
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.18	0.43
1:B:265:ASN:HD22	1:B:265:ASN:HA	1.69	0.43
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.00	0.43
1:A:155:THR:HG22	1:A:299:PHE:CE2	2.53	0.43
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.54	0.42
1:A:137:PHE:CE2	1:A:457:LEU:HD22	2.54	0.42
1:A:211:MET:HG2	1:A:308:LEU:HD21	2.02	0.41
1:B:470:ARG:HE	1:B:470:ARG:HB3	1.68	0.41
1:A:157:GLY:O	1:A:171:VAL:HG22	2.19	0.41
1:B:203:SVY:C3'	1:B:297:PHE:HZ	2.33	0.41
1:B:104:PRO:HB2	1:B:108:PRO:HD3	2.02	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.56	0.41
1:B:511:VAL:HG11	1:B:518:LEU:HD13	2.03	0.41
1:B:24:ALA:O	1:B:25:PRO:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:ARG:O	1:B:297:PHE:O	2.38	0.41
1:B:390:ASP:HA	1:B:391:PRO:HD2	1.89	0.41
1:B:254:LEU:HD13	1:B:284:HIS:HB3	2.03	0.41
1:A:231:THR:HB	1:A:233:ASN:OD1	2.21	0.40
1:B:210:GLY:HA3	1:B:232:PRO:HG3	2.02	0.40
1:B:541:SER:O	1:B:542:ALA:HB3	2.21	0.40
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.02	0.40
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.56	0.40
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.99	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/548 (97%)	497 (94%)	31 (6%)	2 (0%)	43	82
1	B	527/548 (96%)	489 (93%)	33 (6%)	5 (1%)	25	66
All	All	1057/1096 (96%)	986 (93%)	64 (6%)	7 (1%)	30	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	PHE
1	A	291	GLN
1	A	493	ARG
1	B	495	SER
1	B	296	ARG
1	B	25	PRO
1	B	108	PRO

### 5.3.2 Protein sidechains ⓘ

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	439/445 (99%)	416 (95%)	23 (5%)	32	71
1	B	437/445 (98%)	412 (94%)	25 (6%)	29	66
All	All	876/890 (98%)	828 (94%)	48 (6%)	30	68

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	13	ARG
1	A	21	ARG
1	A	42	VAL
1	A	70	TYR
1	A	81	GLU
1	A	165	ARG
1	A	181	GLN
1	A	195	MET
1	A	200	PHE
1	A	229	SER
1	A	295	PHE
1	A	297	PHE
1	A	298	SER
1	A	301	PRO
1	A	313	GLU
1	A	380	LEU
1	A	384	ASP
1	A	413	GLN
1	A	457	LEU
1	A	497	SER
1	A	522	ARG
1	B	9	LEU
1	B	23	LYS
1	B	107	ARG
1	B	136	ARG
1	B	181	GLN
1	B	216	LEU

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Mol	Chain	Res	Type
1	B	239	VAL
1	B	246	ARG
1	B	253	ARG
1	B	265	ASN
1	B	281	LEU
1	B	293	SER
1	B	295	PHE
1	B	296	ARG
1	B	297	PHE
1	B	309	SER
1	B	325	GLN
1	B	369	GLN
1	B	380	LEU
1	B	387	HIS
1	B	413	GLN
1	B	421	GLN
1	B	467	THR
1	B	474	GLN
1	B	497	SER

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

Mol	Chain	Res	Type
1	A	223	HIS
1	B	223	HIS
1	B	265	ASN
1	B	474	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SVY	A	203	1	15,15,16	5.08	5 (33%)	18,20,22	4.78	7 (38%)
1	SVY	B	203	1	15,15,16	5.35	5 (33%)	18,20,22	7.14	9 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SVY	A	203	1	-	0/16/18/20	0/0/0/0
1	SVY	B	203	1	-	0/16/18/20	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	SVY	O-C	19.45	1.24	1.11
1	A	203	SVY	O-C	18.28	1.24	1.11
1	A	203	SVY	P-O1P	4.10	1.64	1.57
1	B	203	SVY	P-O1P	3.63	1.63	1.57
1	A	203	SVY	CA-C	3.59	1.55	1.48
1	B	203	SVY	P-O3P	3.44	1.60	1.48
1	B	203	SVY	CA-C	3.40	1.54	1.48
1	A	203	SVY	P-O3P	3.32	1.60	1.48
1	B	203	SVY	P-O2P	2.77	1.62	1.57
1	A	203	SVY	P-O2P	2.45	1.61	1.57

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	SVY	OG-P-O1P	23.67	167.65	103.12
1	A	203	SVY	OG-P-O1P	15.56	145.53	103.12
1	B	203	SVY	OG-P-O2P	-14.70	63.07	103.12
1	A	203	SVY	OG-P-O2P	-9.56	77.08	103.12
1	B	203	SVY	OG-P-O3P	-8.37	80.50	113.93
1	A	203	SVY	O2P-P-O3P	-6.08	102.54	115.21
1	B	203	SVY	O2P-P-O3P	-4.61	105.61	115.21
1	B	203	SVY	C-CA-N	-3.95	109.88	113.83
1	B	203	SVY	OG-CB-CA	3.62	113.81	108.69
1	A	203	SVY	C-CA-N	-3.47	110.36	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	SVY	OG-P-O3P	-3.00	101.94	113.93
1	A	203	SVY	OG-CB-CA	2.34	112.00	108.69
1	B	203	SVY	P-OG-CB	2.33	129.04	120.64
1	B	203	SVY	O1P-C1-C3	2.27	115.93	107.74
1	A	203	SVY	O1P-P-O3P	-2.07	110.89	115.21
1	B	203	SVY	O2P-P-O1P	2.04	108.58	103.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1544	1	12,14,15	0.63	0	15,19,21	1.66	1 (6%)
3	AE3	B	1544	-	8,8,8	0.61	0	7,7,7	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1544	1	-	0/6/23/26	0/1/1/1
3	AE3	B	1544	-	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1544	NAG	O5-C5-C6	5.44	112.69	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	535/548 (97%)	-0.55	9 (1%) 67 76	27, 44, 65, 87	0
1	B	532/548 (97%)	-0.46	8 (1%) 70 79	31, 48, 71, 95	0
All	All	1067/1096 (97%)	-0.50	17 (1%) 67 78	27, 46, 71, 95	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	PRO	4.5
1	A	290	PRO	3.8
1	A	495	SER	3.6
1	A	541	SER	3.5
1	A	542	ALA	3.4
1	B	541	SER	3.2
1	A	496	LYS	3.2
1	B	542	ALA	3.0
1	B	109	ALA	2.9
1	A	493	ARG	2.9
1	A	292	GLU	2.8
1	A	494	ASP	2.6
1	A	291	GLN	2.4
1	B	292	GLU	2.4
1	B	497	SER	2.3
1	B	4	GLU	2.1
1	B	291	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SVY	A	203	16/17	0.17	1.06	34,58,63,63	0
1	SVY	B	203	16/17	0.16	0.71	38,60,64,64	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1544	14/15	0.55	9.37	74,79,81,81	0
3	AE3	B	1544	9/9	0.21	0.50	79,82,84,85	0

### 6.5 Other polymers

There are no such residues in this entry.