



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:05 AM EDT

PDB ID : 2JGI / pdb_00002jgi
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

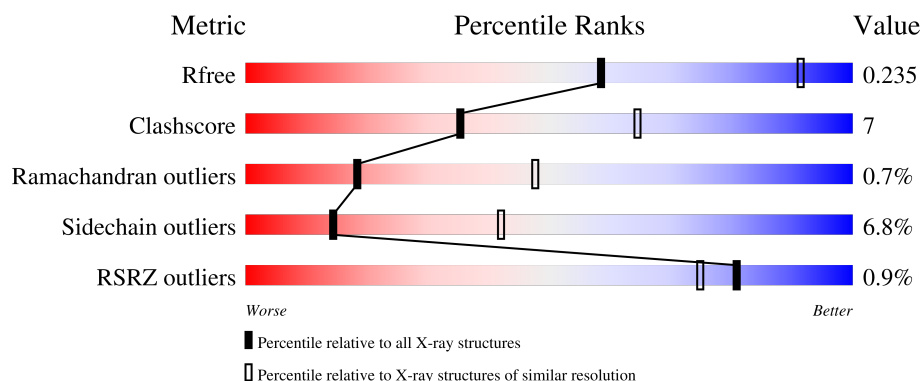
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	% 79% 17% ..
1	B	548	% 75% 19% ...

2 Entry composition [i](#)

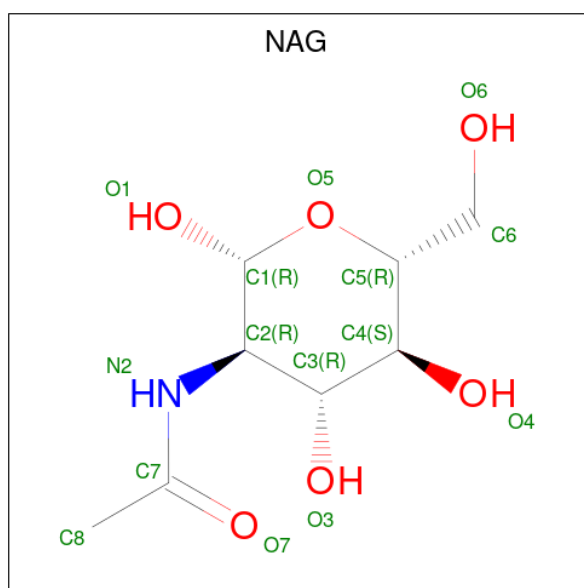
There are 4 unique types of molecules in this entry. The entry contains 8441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

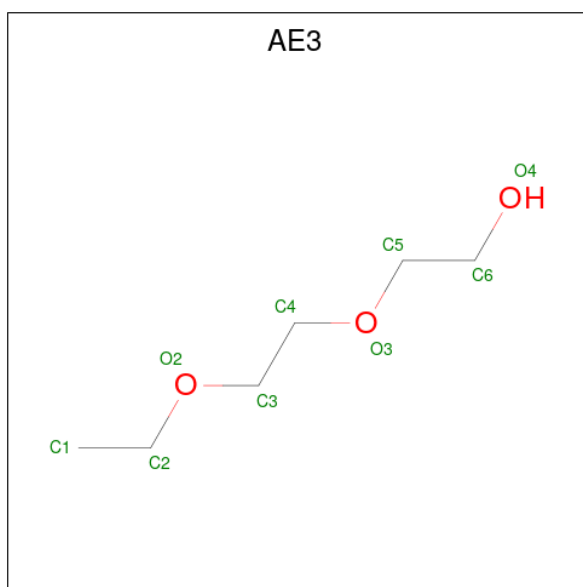
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	P	S	0	0	0
			4191	2688	726	762	1	14			
1	B	532	Total	C	N	O	P	S	0	0	0
			4167	2675	720	757	1	14			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: $C_6H_{14}O_3$).



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

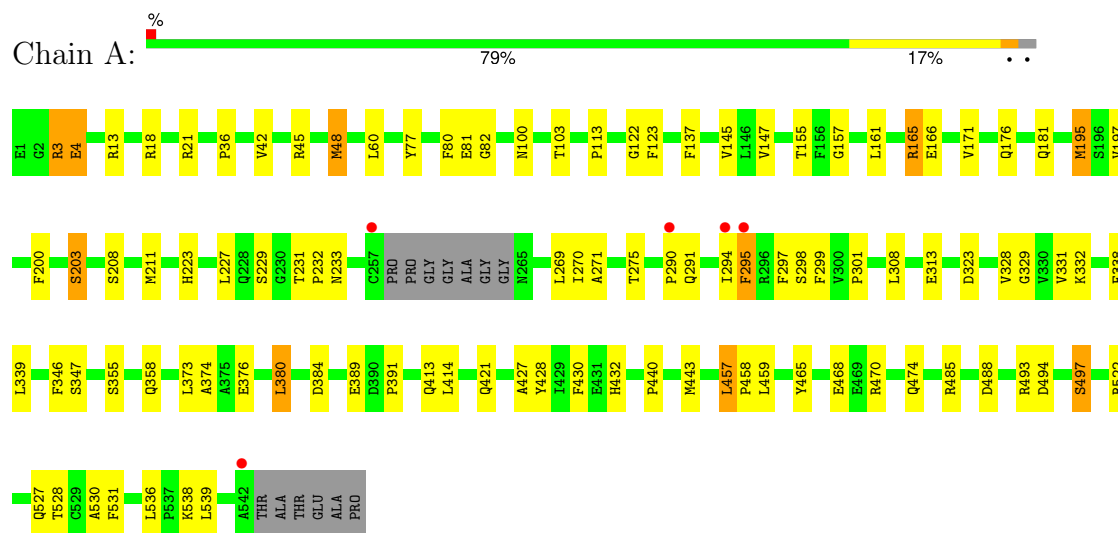
- Molecule 4 is water.

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

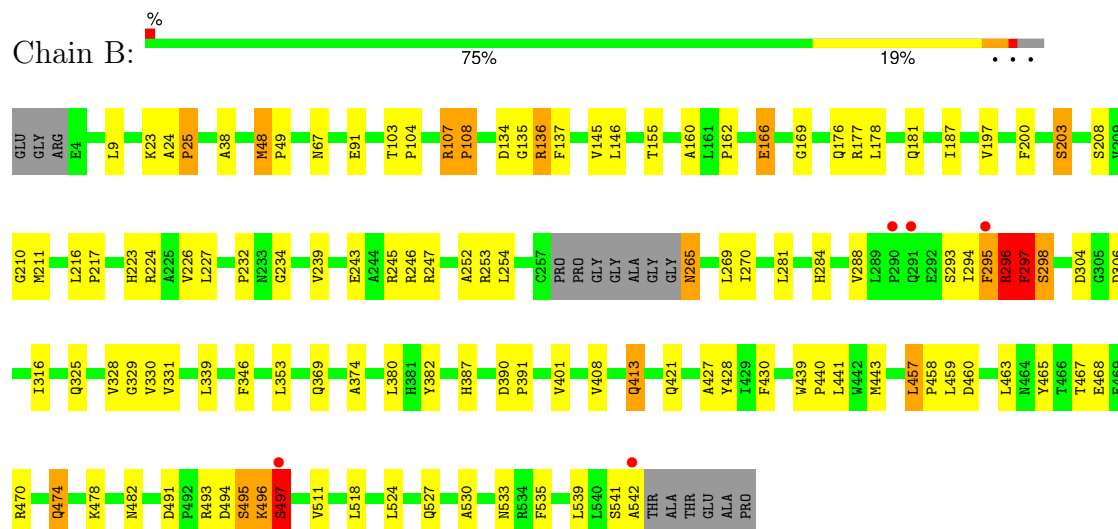
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (19.97-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.242 0.198 , 0.235	Depositor DCC
R_{free} test set	869 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.61	0/4297	0.91	6/5868 (0.1%)
1	B	0.61	0/4273	0.91	5/5837 (0.1%)
All	All	0.61	0/8570	0.91	11/11705 (0.1%)

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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	234	GLY	CA-C-N	6.80	126.76	119.28
1	B	234	GLY	C-N-CA	6.80	126.76	119.28
1	B	107	ARG	CA-C-N	5.76	127.04	119.84
1	B	107	ARG	C-N-CA	5.76	127.04	119.84
1	A	432	HIS	N-CA-C	5.75	118.10	108.96
1	B	497	SER	N-CA-C	-5.49	103.25	110.39
1	A	77	TYR	CA-C-N	5.46	125.47	119.90
1	A	77	TYR	C-N-CA	5.46	125.47	119.90
1	A	290	PRO	N-CA-C	-5.26	106.22	113.53
1	A	488	ASP	CA-C-N	5.25	124.86	119.56
1	A	488	ASP	C-N-CA	5.25	124.86	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	LYS	Peptide

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	4191	0	4087	58	0
1	B	4167	0	4063	66	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	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (123) 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: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: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:48:MET:HE1	1:A:165:ARG:O	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:CD1	1:B:295:PHE:N	2.67	0.61
1:B:295:PHE:N	1:B:295:PHE:HD1	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:HD1	1:A:295:PHE:H	1.54	0.54
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:B:48:MET:HE2	1:B:49:PRO:HD2	1.91	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:A:211:MET:HG3	1:A:232:PRO:HB3	1.92	0.52
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.90	0.52
1:B:295:PHE:HD1	1:B:295:PHE:H	1.58	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:A:195:MET:HA	1:A:195:MET:HE2	1.94	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:3:ARG:HD3	4:A:2001:HOH:O	2.13	0.47
1:A:295:PHE:HZ	1:A:338:PHE:CD1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:OD1	1:B:91:GLU:HB2	2.15	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CE1	2.50	0.47
1:A:347:SER:HB2	2:A:1544:NAG:H62	1.97	0.47
1:A:527:GLN:O	1:A:530:ALA:HB3	2.14	0.47
1:B:382:TYR:CD1	1:B:401:VAL:HG22	2.50	0.47
1:B:457:LEU:N	1:B:458:PRO:CD	2.77	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:374:ALA:HA	1:A:539:LEU:HD23	1.97	0.46
1:A:528:THR:O	1:A:531:PHE:HB3	2.15	0.46
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.96	0.46
1:A:470:ARG:O	1:A:474:GLN:HG3	2.16	0.46
1:B:162:PRO:HD2	1:B:245:ARG:HB2	1.96	0.46
1:B:203:SVY:C3'	1:B:297:PHE:CZ	2.99	0.46
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.98	0.46
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.50	0.46
1:B:252:ALA:HB2	1:B:269:LEU:HD21	1.97	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:458:PRO:HA	1:B:465:TYR:HD2	1.80	0.46
1:A:48:MET:HE3	1:A:166:GLU:C	2.41	0.45
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.99	0.45
1:B:497:SER:HB3	4:B:2017:HOH:O	2.17	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:24:ALA:O	1:B:25:PRO:C	2.59	0.45
1:B:294:ILE:HB	1:B:295:PHE:HD1	1.82	0.45
1:A:137:PHE:HE2	1:A:457:LEU:HD22	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: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:HB3	1:A:165:ARG:HH11	1.82	0.43
1:A:271:ALA:O	1:A:275:THR:HG23	2.18	0.43
1:B:247:ARG:HH11	1:B:298:SER:HA	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:134:ASP:CG	1:B:136:ARG:HD2	2.45	0.42
1:A:211:MET:HG2	1:A:308:LEU:HD21	2.02	0.41
1:A:157:GLY:O	1:A:171:VAL:HG22	2.19	0.41
1:B:470:ARG:HE	1:B:470:ARG:HB3	1.68	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:A:468:GLU:H	1:A:468:GLU:CD	2.29	0.41
1:B:254:LEU:HD13	1:B:284:HIS:HB3	2.03	0.41
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: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: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
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/548 (97%)	497 (94%)	31 (6%)	2 (0%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	527/548 (96%)	489 (93%)	33 (6%)	5 (1%)	14	41
All	All	1057/1096 (96%)	986 (93%)	64 (6%)	7 (1%)	18	48

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%)	413 (94%)	26 (6%)	18	48
1	B	437/445 (98%)	403 (92%)	34 (8%)	11	35
All	All	876/890 (98%)	816 (93%)	60 (7%)	14	42

All (60) 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	48	MET
1	A	81	GLU
1	A	165	ARG
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	195	MET
1	A	200	PHE
1	A	229	SER
1	A	295	PHE
1	A	298	SER
1	A	301	PRO
1	A	313	GLU
1	A	332	LYS
1	A	380	LEU
1	A	384	ASP
1	A	413	GLN
1	A	421	GLN
1	A	457	LEU
1	A	497	SER
1	A	522	ARG
1	A	536	LEU
1	A	538	LYS
1	B	9	LEU
1	B	23	LYS
1	B	48	MET
1	B	107	ARG
1	B	136	ARG
1	B	155	THR
1	B	166	GLU
1	B	181	GLN
1	B	216	LEU
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	298	SER
1	B	316	ILE
1	B	369	GLN
1	B	380	LEU
1	B	387	HIS
1	B	413	GLN
1	B	421	GLN

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Mol	Chain	Res	Type
1	B	441	LEU
1	B	457	LEU
1	B	459	LEU
1	B	467	THR
1	B	468	GLU
1	B	474	GLN
1	B	493	ARG
1	B	497	SER
1	B	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	265	ASN
1	A	393	HIS
1	B	16	GLN
1	B	223	HIS
1	B	265	ASN
1	B	287	HIS
1	B	369	GLN
1	B	387	HIS
1	B	474	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	14,15,16	1.86	3 (21%)	14,20,22	5.09	7 (50%)
1	SVY	B	203	1	14,15,16	1.83	3 (21%)	14,20,22	7.66	7 (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	-	3/16/18/20	-
1	SVY	B	203	1	-	6/16/18/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SVY	P-O1P	4.51	1.64	1.57
1	B	203	SVY	P-O1P	3.99	1.63	1.57
1	B	203	SVY	P-O3P	3.57	1.60	1.48
1	A	203	SVY	P-O3P	3.45	1.60	1.48
1	B	203	SVY	P-O2P	3.03	1.62	1.57
1	A	203	SVY	P-O2P	2.67	1.61	1.57

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	SVY	OG-P-O1P	21.88	167.65	103.41
1	A	203	SVY	OG-P-O1P	14.35	145.53	103.41
1	B	203	SVY	OG-P-O2P	-13.74	63.07	103.41
1	B	203	SVY	OG-P-O3P	-8.99	80.50	114.20
1	A	203	SVY	OG-P-O2P	-8.97	77.08	103.41
1	A	203	SVY	O2P-P-O3P	-5.99	102.54	115.03
1	B	203	SVY	OG-CB-CA	5.82	113.81	108.14
1	B	203	SVY	O2P-P-O3P	-4.52	105.61	115.03
1	A	203	SVY	OG-CB-CA	3.96	112.00	108.14
1	A	203	SVY	OG-P-O3P	-3.27	101.94	114.20
1	B	203	SVY	P-OG-CB	2.51	129.04	120.63
1	B	203	SVY	O1P-C1-C3	2.38	115.93	107.72
1	A	203	SVY	P-OG-CB	-2.14	113.44	120.63
1	A	203	SVY	O1P-C1-C3	2.02	114.67	107.72

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	SVY	C3-C1-O1P-P
1	B	203	SVY	N-CA-CB-OG
1	B	203	SVY	C3-C1-O1P-P
1	B	203	SVY	C1-O1P-P-O3P
1	B	203	SVY	CB-OG-P-O3P
1	A	203	SVY	C1-O1P-P-O3P
1	B	203	SVY	C1'-O2P-P-O3P
1	B	203	SVY	C1'-O2P-P-O1P
1	A	203	SVY	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	SVY	5	0
1	B	203	SVY	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	14,14,15	0.74	1 (7%)	17,19,21	1.18	2 (11%)
3	AE3	B	1544	-	8,8,8	0.61	0	7,7,7	0.18	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	-	2/6/23/26	0/1/1/1
3	AE3	B	1544	-	-	3/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1544	NAG	C1-C2	2.05	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1544	NAG	O5-C5-C6	2.58	112.69	107.66
2	A	1544	NAG	C1-O5-C5	2.41	115.41	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1544	NAG	C8-C7-N2-C2
2	A	1544	NAG	O7-C7-N2-C2
3	B	1544	AE3	O2-C3-C4-O3
3	B	1544	AE3	C1-C2-O2-C3
3	B	1544	AE3	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1544	NAG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	534/548 (97%)	-0.53	5 (0%) 81 75	27, 44, 65, 87	0
1	B	531/548 (96%)	-0.38	5 (0%) 81 75	31, 47, 71, 95	0
All	All	1065/1096 (97%)	-0.45	10 (0%) 81 75	27, 46, 71, 95	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	PHE	3.8
1	B	290	PRO	3.3
1	A	290	PRO	3.3
1	B	295	PHE	3.2
1	A	257	CYS	2.9
1	B	542	ALA	2.8
1	B	497	SER	2.8
1	B	291	GLN	2.3
1	A	294	ILE	2.2
1	A	542	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SVY	B	203	16/17	0.87	0.17	38,60,64,64	0
1	SVY	A	203	16/17	0.89	0.17	34,58,63,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AE3	B	1544	9/9	0.65	0.27	79,82,84,85	0
2	NAG	A	1544	14/15	0.75	0.14	74,79,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.