



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 10:08 PM EST

PDB ID : 2JGF  
Title : Crystal structure of mouse acetylcholinesterase inhibited by non-aged fenamiphos  
Authors : Hornberg, A.; Tunemalm, A.-K.; Ekstrom, F.  
Deposited on : 2007-02-13  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

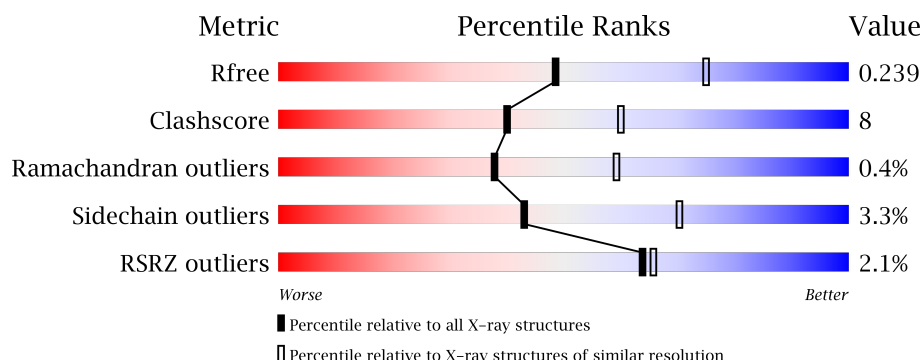
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	548	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>

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
4	PGE	A	1546	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8580 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.

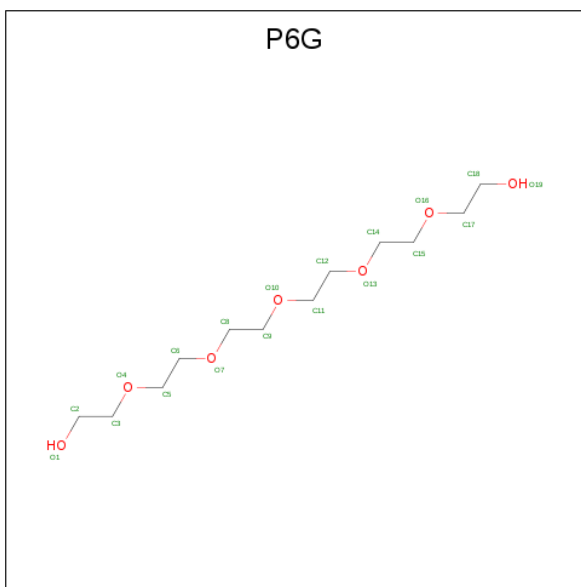
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	P	S	0	0	0
			4190	2687	727	761	1	14			
1	B	534	Total	C	N	O	P	S	0	0	1
			4174	2678	723	758	1	14			

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



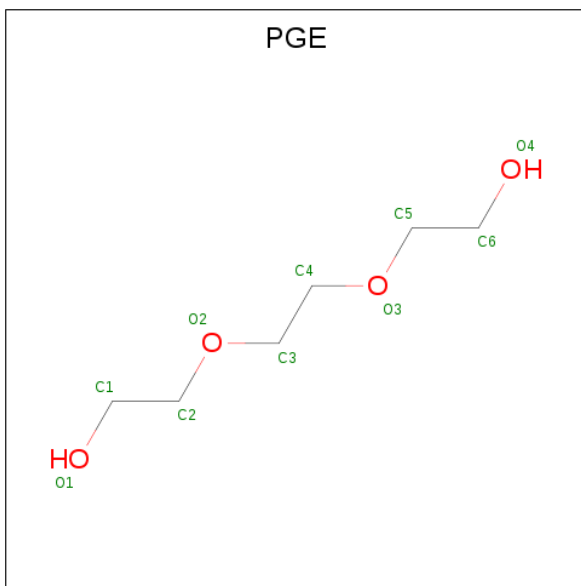
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

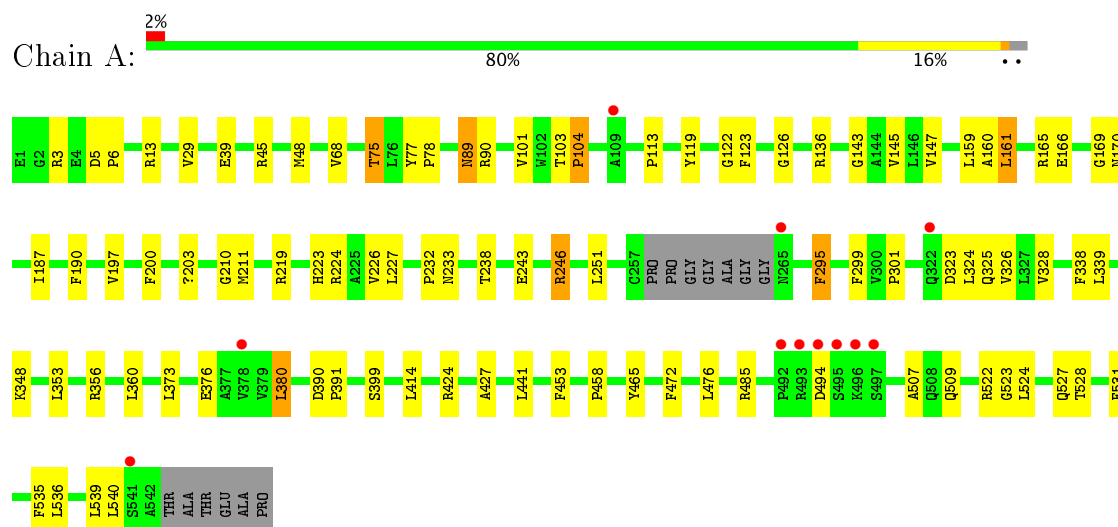
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total 102	O 102	0	0
5	B	72	Total 72	O 72	0	0

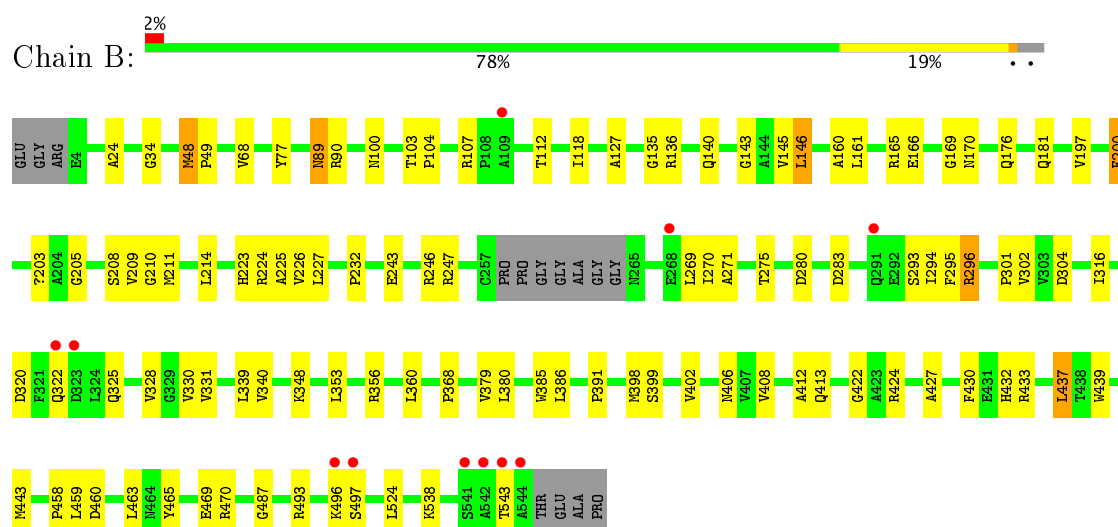
### 3 Residue-property plots

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

#### • 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, $\alpha$ , $\beta$ , $\gamma$	79.06Å 111.73Å 224.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.50 19.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.73-2.50) 99.9 (19.73-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.253 0.206 , 0.239	Depositor DCC
$R_{free}$ test set	1384 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: PGE, SXE, P6G, NAG

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	0.53	0/4297	0.64	1/5868 (0.0%)
1	B	0.52	0/4281	0.64	0/5849
All	All	0.53	0/8578	0.64	1/11717 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	CA-CB-CG	-6.24	100.95	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4190	0	4086	64	0
1	B	4174	0	4069	75	0
2	A	14	0	13	0	0
3	A	19	0	24	5	0
4	A	9	0	11	0	0
5	A	102	0	0	2	0
5	B	72	0	0	0	0
All	All	8580	0	8203	137	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 8.

All (137) 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:B:197:VAL:H	1:B:223:HIS:HD2	1.09	0.94
1:B:197:VAL:H	1:B:223:HIS:CD2	1.92	0.87
1:A:48:MET:HE1	1:A:166:GLU:HA	1.64	0.79
1:B:170:ASN:HD21	1:B:302:VAL:H	1.30	0.79
1:A:89:ASN:H	1:A:89:ASN:HD22	1.40	0.70
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.75	0.69
1:A:527:GLN:HE21	3:A:1545:P6G:H171	1.58	0.69
1:A:197:VAL:H	1:A:223:HIS:HD2	1.42	0.68
1:A:203:SXE:HB	1:A:203:SXE:H4C1	1.77	0.65
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.80	0.64
1:B:170:ASN:ND2	1:B:302:VAL:H	1.96	0.62
1:B:48:MET:CE	1:B:165:ARG:O	2.49	0.61
1:A:380:LEU:HB3	3:A:1545:P6G:C5	2.31	0.60
1:B:48:MET:HE1	1:B:165:ARG:O	2.01	0.60
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.84	0.59
1:A:203:SXE:C1	1:A:203:SXE:H4C1	2.32	0.59
1:A:48:MET:HE1	1:A:166:GLU:CA	2.32	0.59
1:B:170:ASN:HD21	1:B:302:VAL:N	2.00	0.58
1:A:75:THR:O	1:A:78:PRO:HD3	2.04	0.58
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.86	0.58
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.86	0.58
1:B:103:THR:HG22	1:B:145:VAL:HG22	1.85	0.57
1:B:320:ASP:OD1	1:B:322:GLN:HG3	2.05	0.56
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.38	0.56
1:B:68:VAL:HG13	1:B:127:ALA:HB2	1.88	0.55
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.42	0.55
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.88	0.55
1:A:200:PHE:CB	1:A:226:VAL:HB	2.37	0.55
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.88	0.55
1:B:412:ALA:HB2	1:B:524:LEU:HD23	1.89	0.55
1:A:233:ASN:H	1:A:233:ASN:ND2	2.05	0.54
1:B:34:GLY:H	1:B:100:ASN:HD22	1.53	0.54
1:B:328:VAL:O	1:B:427:ALA:HA	2.08	0.54
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.89	0.54
1:A:380:LEU:HB3	3:A:1545:P6G:H51	1.90	0.53
1:A:509:GLN:HB2	5:A:2094:HOH:O	2.08	0.53
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:HE2	1:B:49:PRO:HD2	1.91	0.52
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.91	0.52
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.91	0.52
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.40	0.51
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.92	0.51
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.92	0.51
1:B:224:ARG:HD3	1:B:325:GLN:HE21	1.75	0.51
1:A:373:LEU:HD23	1:A:539:LEU:HD11	1.93	0.51
1:B:118:ILE:O	1:B:205:GLY:HA3	2.11	0.50
1:B:433:ARG:NH2	1:B:439:TRP:O	2.42	0.50
1:B:203:SXE:HB	1:B:203:SXE:H4C1	1.94	0.50
1:B:89:ASN:HD22	1:B:89:ASN:H	1.60	0.49
1:A:48:MET:HE1	1:A:165:ARG:O	2.11	0.49
1:A:376:GLU:HG2	1:B:538:LYS:HD3	1.95	0.49
1:B:203:SXE:H4C1	1:B:203:SXE:C1	2.43	0.48
1:A:77:TYR:CZ	1:A:348:LYS:HG2	2.48	0.48
1:B:34:GLY:H	1:B:100:ASN:ND2	2.11	0.48
1:A:380:LEU:HB3	3:A:1545:P6G:H52	1.95	0.48
1:A:48:MET:HA	1:A:48:MET:CE	2.44	0.48
1:A:323:ASP:OD1	1:A:323:ASP:N	2.46	0.48
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.96	0.48
1:A:233:ASN:H	1:A:233:ASN:HD22	1.62	0.47
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.97	0.47
1:B:459:LEU:HD22	1:B:470:ARG:HG2	1.97	0.47
1:A:507:ALA:HA	1:A:522:ARG:HH21	1.79	0.47
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.97	0.47
1:B:459:LEU:CD2	1:B:470:ARG:HG2	2.45	0.47
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.97	0.46
1:B:224:ARG:CG	1:B:325:GLN:HE21	2.29	0.46
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.69	0.46
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.97	0.46
1:B:48:MET:HE3	1:B:165:ARG:O	2.15	0.46
1:B:322:GLN:HG2	1:B:422:GLY:HA3	1.97	0.46
1:A:45:ARG:O	1:A:48:MET:HB2	2.15	0.46
1:B:112:THR:HG21	1:B:143:GLY:O	2.15	0.46
1:B:104:PRO:HG3	1:B:143:GLY:HA2	1.97	0.45
1:A:324:LEU:HG	1:A:326:VAL:HG23	1.97	0.45
1:B:271:ALA:O	1:B:275:THR:HG23	2.16	0.45
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.46	0.45
1:A:101:VAL:HG22	1:A:147:VAL:HG22	1.98	0.45
1:A:535:PHE:CE2	3:A:1545:P6G:H91	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE2	1:A:246:ARG:HD3	2.17	0.45
1:B:214:LEU:HD21	1:B:316:ILE:HG22	1.99	0.45
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.99	0.44
1:A:227:LEU:HD22	1:A:414:LEU:HD21	1.99	0.44
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.98	0.44
1:A:339:LEU:HD11	1:A:399:SER:HA	2.00	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.44
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.98	0.44
1:B:339:LEU:HD11	1:B:399:SER:HA	2.00	0.44
1:B:340:VAL:HG11	1:B:443:MET:CE	2.47	0.44
1:A:122:GLY:O	1:A:123:PHE:HB2	2.18	0.43
1:A:528:THR:O	1:A:531:PHE:HB3	2.19	0.43
1:A:238:THR:HA	1:A:301:PRO:O	2.18	0.43
1:B:360:LEU:HD22	1:B:379:VAL:HG11	2.01	0.43
1:B:160:ALA:HB2	1:B:169:GLY:HA3	2.00	0.42
1:B:437:LEU:HD23	1:B:439:TRP:HB2	2.01	0.42
1:A:160:ALA:HB2	1:A:169:GLY:HA3	2.01	0.42
1:B:77:TYR:CZ	1:B:348:LYS:HG2	2.55	0.42
1:A:295:PHE:CE2	1:A:338:PHE:CE1	3.08	0.42
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.02	0.42
1:B:331:VAL:HG12	1:B:430:PHE:HB3	2.01	0.42
1:A:360:LEU:HD11	5:A:2075:HOH:O	2.18	0.42
1:B:48:MET:HE2	1:B:49:PRO:CD	2.49	0.42
1:A:89:ASN:N	1:A:89:ASN:HD22	2.08	0.42
1:B:166:GLU:HB2	1:B:270:ILE:HG21	2.02	0.42
1:B:135:GLY:HA3	1:B:146:LEU:HD22	2.01	0.41
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.02	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.84	0.41
1:B:170:ASN:ND2	1:B:301:PRO:HA	2.35	0.41
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.54	0.41
1:B:209:VAL:CG1	1:B:225:ALA:HB1	2.50	0.41
1:B:224:ARG:HD3	1:B:487:GLY:CA	2.51	0.41
1:B:280:ASP:O	1:B:283:ASP:HB2	2.20	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.20	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.41
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.02	0.41
1:A:29:VAL:HG21	1:A:136:ARG:HB2	2.03	0.41
1:B:205:GLY:O	1:B:209:VAL:HG23	2.20	0.41
1:B:294:ILE:HD11	1:B:402:VAL:HG21	2.01	0.41
1:B:340:VAL:CG1	1:B:443:MET:CE	2.99	0.41
1:A:104:PRO:HG3	1:A:143:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HB3	1:A:45:ARG:HH21	1.86	0.41
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.20	0.41
1:A:119:TYR:CD1	1:A:126:GLY:HA3	2.56	0.41
1:B:197:VAL:N	1:B:223:HIS:HD2	1.93	0.41
1:B:224:ARG:CD	1:B:487:GLY:HA2	2.50	0.41
1:B:302:VAL:HG13	1:B:304:ASP:HB3	2.03	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD2	1.97	0.40
1:B:330:VAL:HG11	1:B:408:VAL:HA	2.02	0.40
1:A:159:LEU:HA	1:A:299:PHE:CD1	2.56	0.40
1:A:187:ILE:HA	1:A:187:ILE:HD12	1.93	0.40
1:A:251:LEU:O	1:A:251:LEU:HG	2.21	0.40
1:A:356:ARG:O	1:A:360:LEU:HG	2.21	0.40
1:B:380:LEU:HD22	1:B:385:TRP:HZ2	1.87	0.40
1:B:432:HIS:HE2	1:B:469:GLU:HG2	1.86	0.40
1:A:523:GLY:HA3	1:B:386:LEU:CD2	2.51	0.40
1:B:339:LEU:HD22	1:B:398:MET:HG3	2.03	0.40
1:B:243:GLU:O	1:B:247:ARG:HG3	2.21	0.40
1:B:293:SER:HB3	1:B:368:PRO:HB3	2.04	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%)	498 (94%)	29 (6%)	3 (1%)	28	48
1	B	529/548 (96%)	506 (96%)	22 (4%)	1 (0%)	51	73
All	All	1059/1096 (97%)	1004 (95%)	51 (5%)	4 (0%)	38	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	ASP
1	A	540	LEU
1	B	497	SER
1	A	104	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%)	427 (97%)	12 (3%)	50	77
1	B	438/445 (98%)	421 (96%)	17 (4%)	37	63
All	All	877/890 (98%)	848 (97%)	29 (3%)	43	70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	13	ARG
1	A	75	THR
1	A	89	ASN
1	A	161	LEU
1	A	246	ARG
1	A	295	PHE
1	A	380	LEU
1	A	424	ARG
1	A	441	LEU
1	A	524	LEU
1	A	536	LEU
1	B	48	MET
1	B	89	ASN
1	B	107	ARG
1	B	136	ARG
1	B	146	LEU
1	B	181	GLN
1	B	200	PHE
1	B	246	ARG

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Mol	Chain	Res	Type
1	B	295	PHE
1	B	296	ARG
1	B	356	ARG
1	B	413	GLN
1	B	424	ARG
1	B	437	LEU
1	B	493	ARG
1	B	496	LYS
1	B	543	THR

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

Mol	Chain	Res	Type
1	A	89	ASN
1	A	223	HIS
1	A	233	ASN
1	A	287	HIS
1	A	509	GLN
1	B	89	ASN
1	B	100	ASN
1	B	170	ASN
1	B	223	HIS
1	B	325	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	SXE	A	203	1	14,14,15	5.37	3 (21%)	13,18,20	3.17	6 (46%)
1	SXE	B	203	1	14,14,15	5.24	3 (21%)	13,18,20	3.22	6 (46%)

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	SXE	A	203	1	-	0/14/17/19	0/0/0/0
1	SXE	B	203	1	-	0/14/17/19	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SXE	CA-C	2.74	1.53	1.50
1	B	203	SXE	CA-C	3.56	1.54	1.50
1	A	203	SXE	P1-O1	5.49	1.60	1.47
1	B	203	SXE	P1-O1	5.53	1.60	1.47
1	B	203	SXE	P1-N1	18.25	1.80	1.61
1	A	203	SXE	P1-N1	18.88	1.81	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	SXE	OG-P1-O1	-5.95	88.71	113.96
1	A	203	SXE	P1-OG-CB	-5.47	102.60	120.83
1	A	203	SXE	OG-P1-O1	-4.51	94.81	113.96
1	B	203	SXE	P1-OG-CB	-4.43	106.07	120.83
1	A	203	SXE	O-C-CA	-2.25	118.80	125.02
1	B	203	SXE	O-C-CA	-2.06	119.33	125.02
1	A	203	SXE	P1-N1-C1	2.71	130.34	124.56
1	B	203	SXE	P1-N1-C1	2.87	130.69	124.56
1	B	203	SXE	O2-P1-OG	4.70	122.78	101.45
1	A	203	SXE	OG-CB-CA	4.99	113.09	108.17
1	A	203	SXE	O2-P1-OG	5.46	126.22	101.45
1	B	203	SXE	OG-CB-CA	5.79	113.88	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	SXE	2	0
1	B	203	SXE	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	0.58	0	15,19,21	1.16	1 (6%)
3	P6G	A	1545	-	18,18,18	1.76	5 (27%)	17,17,17	2.12	9 (52%)
4	PGE	A	1546	-	8,8,9	0.79	0	7,7,8	0.34	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	P6G	A	1545	-	-	0/16/16/16	0/0/0/0
4	PGE	A	1546	-	-	0/6/6/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1545	P6G	C9-C8	-2.94	1.33	1.49
3	A	1545	P6G	C15-C14	-2.92	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1545	P6G	C3-C2	-2.91	1.34	1.49
3	A	1545	P6G	C17-C18	-2.90	1.34	1.49
3	A	1545	P6G	C6-C5	-2.70	1.35	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1545	P6G	C5-O4-C3	2.06	122.24	113.30
3	A	1545	P6G	O16-C17-C18	2.09	119.79	110.15
3	A	1545	P6G	O4-C3-C2	2.14	120.01	110.15
3	A	1545	P6G	O10-C9-C8	2.34	121.14	110.41
3	A	1545	P6G	O16-C15-C14	2.40	121.45	110.41
3	A	1545	P6G	O13-C14-C15	2.66	122.60	110.41
3	A	1545	P6G	O7-C8-C9	2.74	123.00	110.41
3	A	1545	P6G	O7-C6-C5	3.09	124.60	110.41
3	A	1545	P6G	O4-C5-C6	3.18	124.99	110.41
2	A	1544	NAG	C1-O5-C5	4.04	117.74	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1545	P6G	5	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 ⓘ

### 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	534/548 (97%)	-0.35	11 (2%) 64 66	24, 40, 58, 81	0
1	B	533/548 (97%)	-0.23	11 (2%) 64 66	27, 43, 62, 91	0
All	All	1067/1096 (97%)	-0.29	22 (2%) 64 66	24, 41, 61, 91	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	9.7
1	B	497	SER	6.1
1	B	541	SER	5.5
1	B	542	ALA	5.0
1	A	496	LYS	4.9
1	A	493	ARG	4.2
1	B	496	LYS	3.9
1	B	109	ALA	3.7
1	B	543	THR	3.6
1	A	495	SER	3.1
1	B	323	ASP	2.9
1	B	268	GLU	2.7
1	A	109	ALA	2.5
1	A	494	ASP	2.4
1	A	541	SER	2.4
1	B	322	GLN	2.4
1	A	322	GLN	2.3
1	B	291	GLN	2.2
1	A	378	VAL	2.1
1	A	265	ASN	2.1
1	A	492	PRO	2.1
1	A	497	SER	2.0

## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SXE	B	203	15/16	0.87	0.22	-	32,68,72,73	0
1	SXE	A	203	15/16	0.89	0.18	-	29,60,65,65	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PGE	A	1546	9/10	0.87	0.23	3.20	80,83,83,83	0
3	P6G	A	1545	19/19	0.83	0.21	1.98	52,57,64,66	0
2	NAG	A	1544	14/15	0.84	0.40	-	76,84,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.