



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:22 AM GMT

PDB ID : 2WU3  
Title : CRYSTAL STRUCTURE OF MOUSE ACETYLCHOLINESTERASE IN  
COMPLEX WITH FENAMIPHOS AND HI-6  
Authors : Hornberg, A.; Artursson, E.; Warne, R.; Pang, Y.-P.; Ekstrom, F.  
Deposited on : 2009-09-28  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

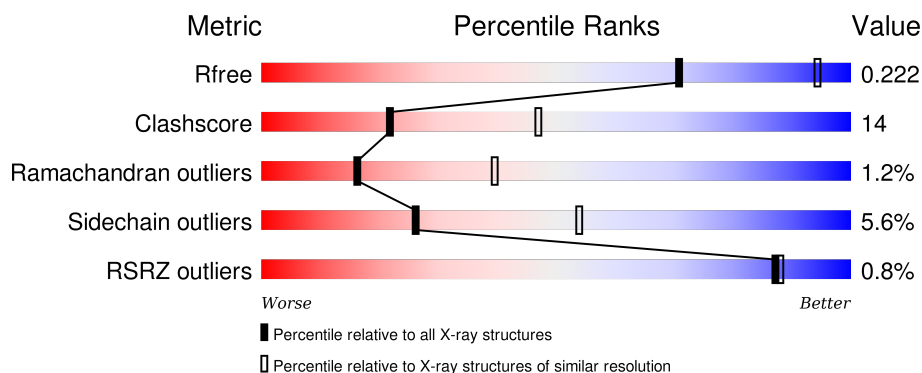
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>74%</div> <div>22%</div> <div>• •</div> </div>
1	B	548	<div> <div>68%</div> <div>26%</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
2	HI6	A	601	-	-	X	X
2	HI6	B	601	-	-	X	X
3	NAG	C	601	-	-	-	X
3	NAG	C	701	X	-	-	-
4	P6G	C	901	-	-	-	X

## 2 Entry composition [i](#)

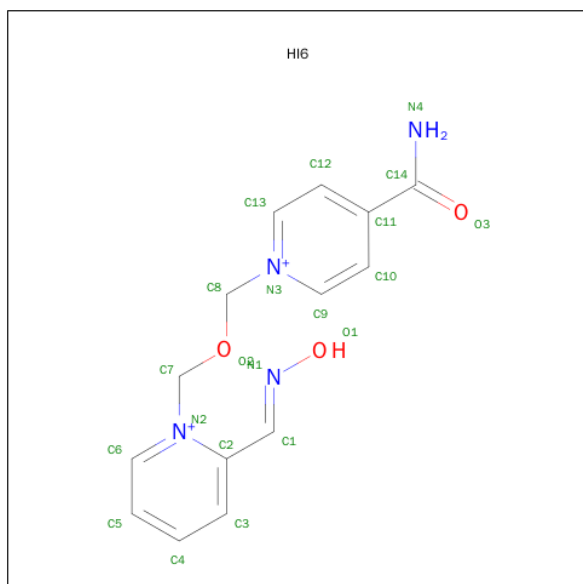
There are 6 unique types of molecules in this entry. The entry contains 8805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	539	Total	C	N	O	P	S	0	2	0
			4239	2715	733	775	2	14			
1	B	533	Total	C	N	O	P	S	0	1	0
			4184	2684	724	760	2	14			

- Molecule 2 is 4-(AMINOCARBONYL)-1-[(2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]PYRIDINIUM (three-letter code: HI6) (formula:  $C_{14}H_{16}N_4O_3$ ).



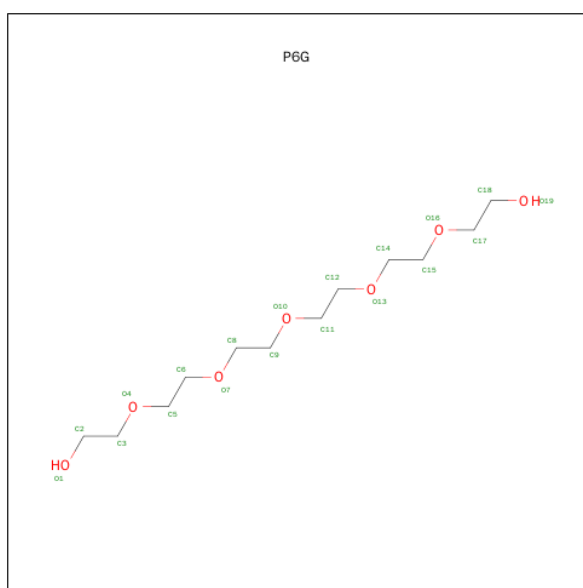
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



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

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula:  $CO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	160	Total	O	0	0
			160	160		
6	B	125	Total	O	0	0
			125	125		
6	C	4	Total	O	0	0
			4	4		
6	D	2	Total	O	0	0
			2	2		

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A: ■ ■ ■

Chain B:

Amino Acid	Frequency (%)
GLU	68%
THR	68%
GLY	68%
ARG	68%
P4	68%
Q7	68%
L8	68%
L9	68%
V10	68%
R11	68%
G19	68%
K23	68%
A24	68%
F32	68%
P36	68%
E39	68%
P40	68%
P41	68%
V42	68%
G43	68%
S44	68%
M48	68%
P49	68%
K53	68%
R54	68%
Q66	68%
M67	68%
Q71	68%
Y77	68%
F80	68%
E84	68%
E94	68%
Y98	68%
L99	68%
M100	68%
W101	68%
W102	68%
T103	68%
P104	68%
Y105	68%
P106	68%
R107	68%
P108	68%
P111	68%
T112	68%
P113	26%
L114	26%
L115	26%
G121	26%
G122	26%
Y123	26%
Y124	26%
G125	26%
G126	26%
A127	26%
A128	26%
D134	26%
G135	26%
R136	26%
Q140	26%
G143	26%
V147	26%
N150	26%
L161	26%
E166	26%
Q181	26%
I187	26%
G191	26%
V197	26%
T198	26%
L199	26%
F200	26%
G201	26%
E202	26%
F203	26%
V209	26%
G210	26%
M211	26%
H212	26%
T213	26%
L216	26%
L339	26%
V340	26%
Y341	26%
G342	26%
K348	26%
D349	26%
N350	26%
E351	26%
C352	26%
E243	68%
R246	68%
R247	68%
C257	68%
PRO	68%
GLY	68%
GLY	68%
ALA	68%
GLY	68%
GLY	68%
N265	68%
L269	68%
I270	68%
R274	68%
W286	68%
Q291	68%
F295	68%
R296	68%
V300	68%
P301	68%
D304	68%
G305	68%
D306	68%
F307	68%
L308	68%
S309	68%
I316	68%
L324	68%
G325	68%
V326	68%
L327	68%
V328	68%
G329	68%
G335	68%
S336	68%
Y337	68%
F338	68%
L339	68%
V340	68%
Y341	68%
G342	68%
K348	68%
D349	68%
N350	68%
E351	68%
C352	68%
S355	68%
R356	68%
A357	68%
Q358	68%
F359	68%
L360	68%
R364	68%
V367	68%
P368	68%
Q369	68%
A370	68%
A375	68%
E376	68%
V379	68%
L380	68%
L386	68%
R395	68%
S399	68%
Q421	68%
A427	68%
Y428	68%
I429	68%
F430	68%
R433	68%
L437	68%
T438	68%
W439	68%
P440	68%
L441	68%
W442	68%
W443	68%
L457	68%
P458	68%
L459	68%
D460	68%
L463	68%
Y464	68%
Y465	68%
R470	68%
Q474	68%
R475	68%
L476	68%
W480	68%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.76Å 111.23Å 227.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.02 – 2.70 29.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.02-2.70) 100.0 (29.02-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.171 , 0.226 0.170 , 0.222	Depositor DCC
$R_{free}$ test set	1098 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55785 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CO3, P6G, NAG, HI6, SXE

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	0.56	1/4334 (0.0%)	0.69	2/5919 (0.0%)
1	B	0.51	0/4276	0.66	0/5842
All	All	0.53	1/8610 (0.0%)	0.68	2/11761 (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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	CYS	CB-SG	-8.67	1.67	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	SER	N-CA-C	-5.57	95.95	111.00
1	A	540	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	540	LEU	Peptide
1	A	95	ASP	Peptide

## 5.2 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	4239	0	4131	110	0
1	B	4184	0	4080	128	0
2	A	18	0	14	11	0
2	B	18	0	14	9	0
3	C	28	0	26	1	0
4	C	19	0	24	5	0
5	D	8	0	0	0	0
6	A	160	0	0	3	0
6	B	125	0	0	4	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
All	All	8805	0	8289	235	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 14.

The worst 5 of 235 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:350:ASN:HD22	1:A:352:SER:H	1.09	0.96
1:B:7:GLN:HE22	1:B:107:ARG:H	0.96	0.95
1:A:350:ASN:ND2	1:A:352:SER:H	1.67	0.91
1:B:7:GLN:NE2	1:B:107:ARG:H	1.71	0.88
1:A:350:ASN:OD1	3:C:601:NAG:C1	2.22	0.87

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	535/548 (98%)	505 (94%)	24 (4%)	6 (1%)	17	42
1	B	528/548 (96%)	500 (95%)	21 (4%)	7 (1%)	15	37
All	All	1063/1096 (97%)	1005 (94%)	45 (4%)	13 (1%)	16	39

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	541	SER
1	A	544	ALA
1	A	545	THR
1	B	494	ASP

### 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	443/445 (100%)	421 (95%)	22 (5%)	30	60
1	B	437/445 (98%)	410 (94%)	27 (6%)	23	49
All	All	880/890 (99%)	831 (94%)	49 (6%)	26	54

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	LEU
1	B	103	THR
1	B	491	ASP
1	B	23	LYS
1	B	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	B	7	GLN
1	B	350	ASN
1	A	350	ASN
1	A	421	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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[A]	1	13,14,15	1.69	1 (7%)	15,18,20	1.10	2 (13%)
1	SXE	A	203[B]	1	13,14,15	1.67	1 (7%)	15,18,20	1.01	1 (6%)
1	SXE	B	203[A]	1	13,14,15	1.68	1 (7%)	15,18,20	0.90	1 (6%)
1	SXE	B	203[B]	1	13,14,15	1.66	1 (7%)	15,18,20	1.03	1 (6%)

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[A]	1	-	0/15/17/19	0/0/0/0
1	SXE	A	203[B]	1	-	0/15/17/19	0/0/0/0
1	SXE	B	203[A]	1	-	0/15/17/19	0/0/0/0
1	SXE	B	203[B]	1	-	0/15/17/19	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203[A]	SXE	P1-N1	5.29	1.66	1.61
1	B	203[B]	SXE	P1-N1	5.30	1.66	1.61
1	A	203[B]	SXE	P1-N1	5.31	1.67	1.61
1	A	203[A]	SXE	P1-N1	5.35	1.67	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203[B]	SXE	O-C-CA	-2.67	118.53	125.49
1	A	203[A]	SXE	P1-N1-C1	-2.66	119.67	124.73
1	B	203[A]	SXE	O-C-CA	-2.59	118.73	125.49
1	A	203[B]	SXE	O-C-CA	-2.55	118.85	125.49
1	A	203[A]	SXE	O-C-CA	-2.49	119.00	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203[A]	SXE	5	0
1	A	203[B]	SXE	6	0
1	B	203[A]	SXE	1	0
1	B	203[B]	SXE	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	HI6	A	601	-	15,19,22	0.43	0	17,24,28	0.84	0
2	HI6	B	601	-	15,19,22	0.48	0	17,24,28	0.83	1 (5%)
3	NAG	C	601	-	14,14,15	0.50	0	15,19,21	1.36	2 (13%)
3	NAG	C	701	1	14,14,15	0.71	0	15,19,21	1.74	1 (6%)
4	P6G	C	901	-	18,18,18	1.73	5 (27%)	17,17,17	2.17	10 (58%)
5	CO3	D	951	-	0,3,3	0.00	-	0,3,3	0.00	-
5	CO3	D	952	-	0,3,3	0.00	-	0,3,3	0.00	-

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	HI6	A	601	-	-	0/10/10/13	0/2/2/2
2	HI6	B	601	-	-	0/10/10/13	0/2/2/2
3	NAG	C	601	-	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1	1/1/5/7	0/6/23/26	0/1/1/1
4	P6G	C	901	-	-	0/16/16/16	0/0/0/0
5	CO3	D	951	-	-	0/0/0/0	0/0/0/0
5	CO3	D	952	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	P6G	C15-C14	-2.82	1.34	1.48
4	C	901	P6G	C6-C5	-2.78	1.34	1.48
4	C	901	P6G	C9-C8	-2.76	1.34	1.48
4	C	901	P6G	C17-C18	-2.73	1.34	1.49
4	C	901	P6G	C3-C2	-2.72	1.34	1.49

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	O3-C3-C2	2.02	113.12	109.11
4	C	901	P6G	C17-O16-C15	2.05	122.13	113.31
4	C	901	P6G	C11-O10-C9	2.05	122.14	113.31
4	C	901	P6G	O4-C5-C6	2.11	119.74	110.36
2	B	601	HI6	C11-C14-N4	2.12	120.14	117.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	701	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HI6	11	0
2	B	601	HI6	9	0
3	C	601	NAG	1	0
4	C	901	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 [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, 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	538/548 (98%)	-0.60	8 (1%)	76 76	29, 45, 83, 159	0
1	B	532/548 (97%)	-0.53	1 (0%)	95 96	29, 52, 85, 145	0
All	All	1070/1096 (97%)	-0.56	9 (0%)	87 88	29, 48, 84, 159	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LYS	4.2
1	A	494	ASP	3.4
1	A	493	ARG	3.4
1	A	495	SER	2.9
1	A	542	ALA	2.6

### 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	A	203[B]	15/16	0.98	0.24	-	30,38,54,58	15
1	SXE	B	203[B]	15/16	0.98	0.17	-	37,52,64,66	15
1	SXE	B	203[A]	15/16	0.98	0.17	-	37,54,64,67	15
1	SXE	A	203[A]	15/16	0.98	0.24	-	32,39,55,58	15



### 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	P6G	C	901	19/19	0.94	0.20	4.97	46,81,100,100	0
3	NAG	C	601	14/15	0.83	0.28	3.84	87,110,117,118	0
2	HI6	A	601	18/21	0.94	0.17	3.45	56,71,88,89	0
2	HI6	B	601	18/21	0.93	0.17	2.80	78,93,106,108	0
5	CO3	D	952	4/4	0.87	0.19	-	87,87,94,98	0
3	NAG	C	701	14/15	0.81	0.34	-	106,119,126,126	0
5	CO3	D	951	4/4	0.83	0.17	-	78,82,82,86	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.