Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:33 AM GMT

PDB ID	:	2XI4
Title	:	TORPEDO CALIFORNICA ACETYLCHOLINESTERASE IN COMPLEX WITH AFLATOXIN B1 (ORTHORHOMBIC SPACE GROUP)
Authors	:	Sanson, B.; Colletier, J.P.; Xu, Y.; Lang, P.T.; Jiang, H.; Silman, I.; Sussman, J.L.; Weik, M.
Deposited on	:	2010-06-28
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

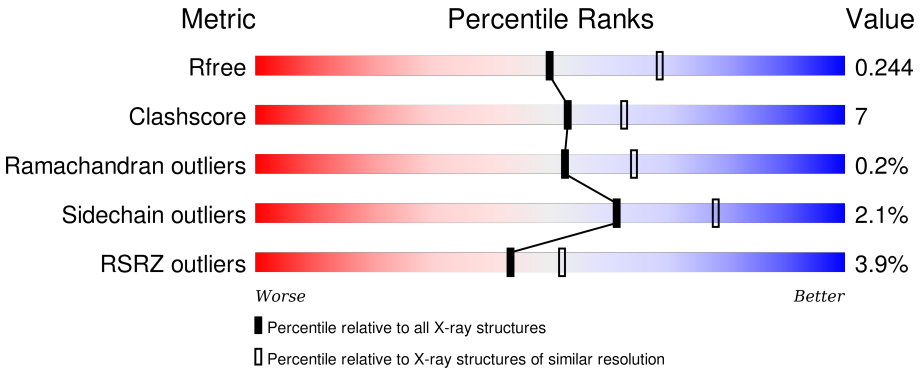
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 >=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 <=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	537	3% 85% 13%
1	B	537	5% 88% 11%

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	AFT	A	1000	-	-	-	X
2	AFT	B	1000	-	-	-	X
4	PEG	A	1004	-	-	X	X
4	PEG	A	1005	-	-	-	X
4	PEG	B	1003	-	-	-	X
4	PEG	B	1005	-	-	-	X
5	PGE	A	1006	-	-	-	X
5	PGE	B	1004	-	-	-	X

2 Entry composition

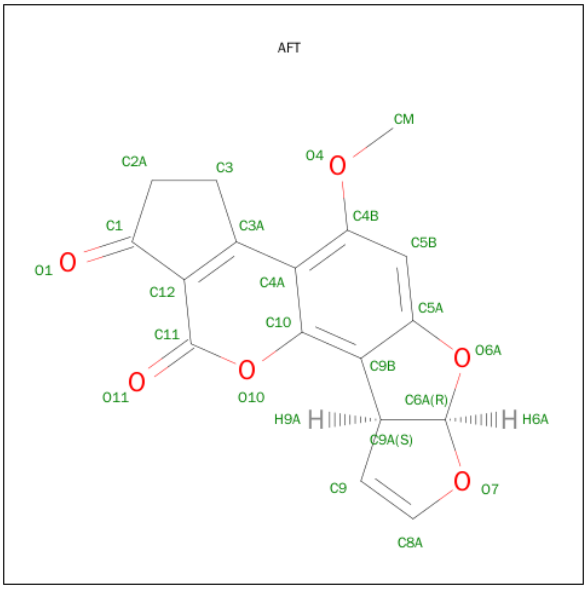
There are 8 unique types of molecules in this entry. The entry contains 9496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	530	Total	C	N	O	S	0	11	0
			4274	2747	720	783	24			
1	B	532	Total	C	N	O	S	0	11	0
			4295	2758	721	791	25			

- Molecule 2 is AFLATOXIN B1 (three-letter code: AFT) (formula: $C_{17}H_{12}O_6$).

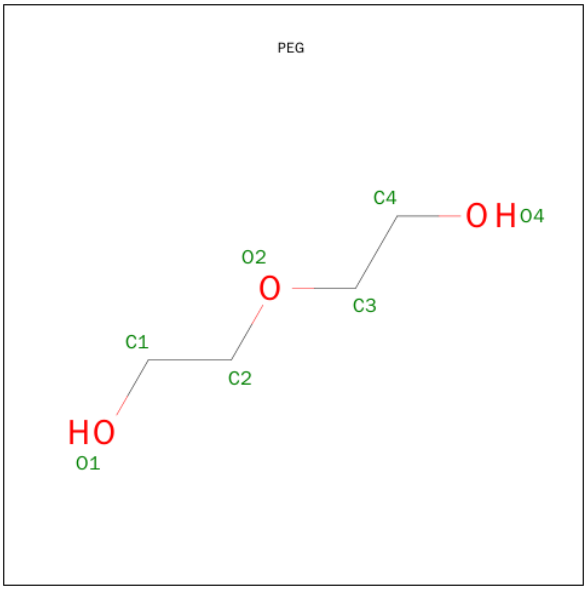


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			23	17	6			
2	B	1	Total	C	O		0	0
			23	17	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

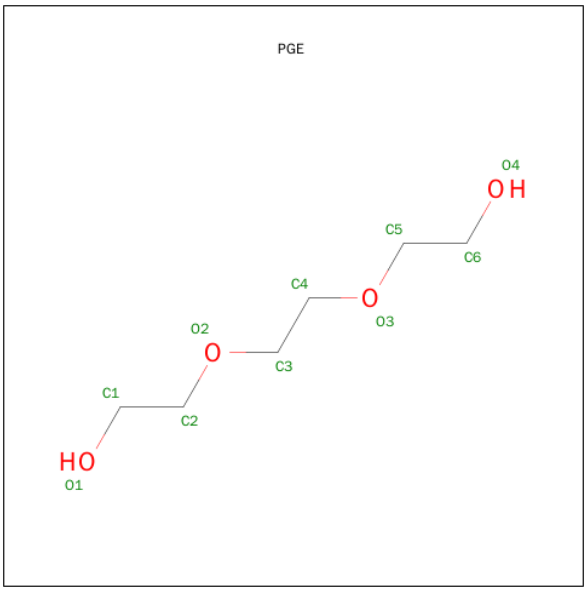
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



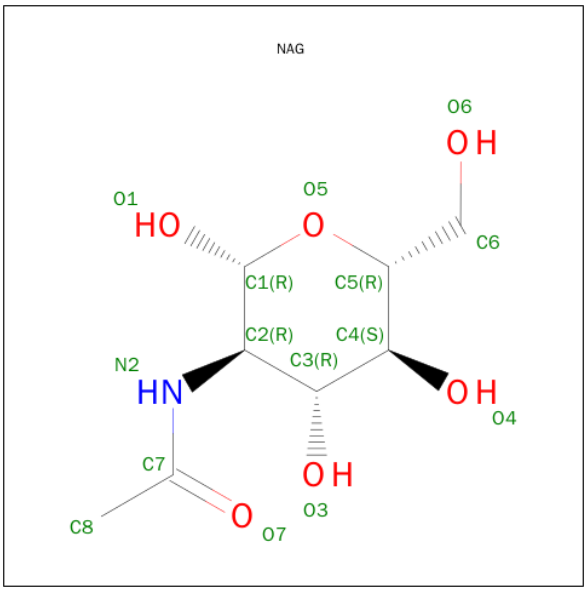
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is water.

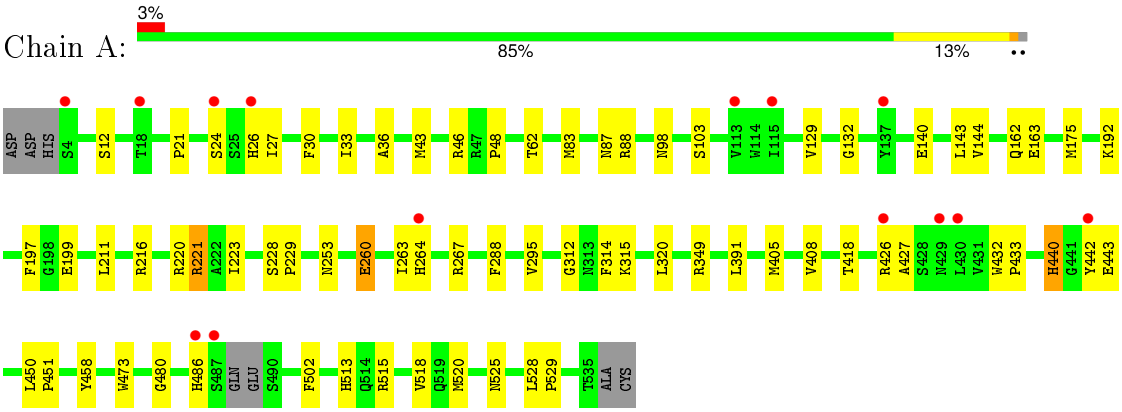
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	351	Total O 351 351	0	0
8	B	393	Total O 393 393	0	0

3 Residue-property plots (i)

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.

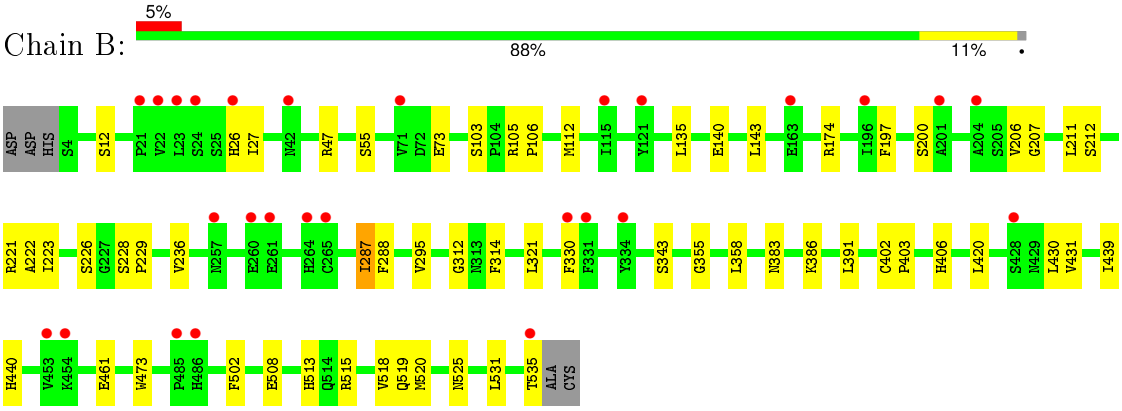
- Molecule 1: ACETYLCHOLINESTERASE

Chain A:



- Molecule 1: ACETYLCHOLINESTERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.73Å 107.03Å 150.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 2.30 46.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.22-2.30) 98.1 (46.22-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.234 0.193 , 0.244	Depositor DCC
R_{free} test set	3156 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 65334 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9496	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.73 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7755e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, NAG, CL, K, AFT, PEG

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	0.71	0/4428	0.72	1/6009 (0.0%)
1	B	0.70	0/4451	0.70	2/6041 (0.0%)
All	All	0.70	0/8879	0.71	3/12050 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	221	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	221	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	221	ARG	NE-CZ-NH1	5.86	123.23	120.30

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	4274	0	4148	55	1
1	B	4295	0	4158	45	1
2	A	23	0	12	1	0
2	B	23	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	21	0	30	11	0
4	B	21	0	30	3	0
5	A	10	0	14	5	0
5	B	10	0	14	5	0
6	A	42	0	39	0	0
6	B	28	0	26	0	0
7	A	1	0	0	0	0
8	A	351	0	0	8	0
8	B	393	0	0	7	0
All	All	9496	0	8483	114	1

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

All (114) 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)
4:A:1004:PEG:O1	4:A:1004:PEG:H41	1.36	1.25
1:A:520[A]:MET:SD	8:A:2237:HOH:O	1.99	1.20
4:A:1004:PEG:H41	4:A:1004:PEG:C1	1.68	1.19
1:B:520[A]:MET:SD	8:B:2274:HOH:O	2.13	1.05
4:A:1004:PEG:C4	4:A:1004:PEG:C1	2.30	1.04
4:A:1004:PEG:C4	4:A:1004:PEG:H12	1.91	0.99
1:B:520[B]:MET:CE	1:B:520[B]:MET:H	1.77	0.97
1:B:520[B]:MET:SD	8:B:2168:HOH:O	2.32	0.87
1:B:430:LEU:HD21	1:B:439:ILE:HD12	1.59	0.83
1:B:520[B]:MET:HE2	1:B:520[B]:MET:H	1.44	0.81
1:A:43[A]:MET:HE2	8:A:2030:HOH:O	1.82	0.78
1:A:26:HIS:O	1:A:27:ILE:HG23	1.84	0.76
1:A:426:ARG:HA	8:A:2270:HOH:O	1.87	0.75
1:B:520[B]:MET:H	1:B:520[B]:MET:HE3	1.51	0.74
1:A:163:GLU:HG3	1:A:267:ARG:HH22	1.53	0.74
1:A:132:GLY:HA3	1:A:143:LEU:HD23	1.72	0.72
1:A:260:GLU:O	1:A:264:HIS:ND1	2.30	0.65
1:A:427:ALA:HA	1:A:442:TYR:OH	1.99	0.62
1:A:163:GLU:HG3	1:A:267:ARG:NH2	2.15	0.62
1:B:406:HIS:HA	4:B:1005:PEG:H42	1.81	0.62
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.82	0.61
4:A:1005:PEG:O4	4:A:1005:PEG:H21	1.99	0.61
1:B:519:GLN:HB3	1:B:520[B]:MET:HE2	1.81	0.61
1:A:26:HIS:O	1:A:27:ILE:CG2	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:HIS:CD2	5:A:1006:PGE:HO1	2.17	0.60
1:A:163:GLU:HB3	1:A:263:ILE:HD13	1.83	0.60
1:A:36:ALA:HB2	1:A:175:MET:CE	2.31	0.60
1:B:525:ASN:HD22	4:B:1005:PEG:H31	1.67	0.60
1:B:228:SER:HB2	1:B:229:PRO:HD2	1.86	0.58
1:A:62:THR:HG23	1:A:88[B]:ARG:NH2	2.19	0.58
4:A:1004:PEG:O1	4:A:1004:PEG:C4	2.30	0.57
1:A:30:PHE:HB3	1:A:33:ILE:HD11	1.86	0.57
1:A:46:ARG:NH1	1:A:163:GLU:OE2	2.37	0.57
5:A:1006:PGE:H4	8:A:2095:HOH:O	2.06	0.55
1:A:62:THR:HG23	1:A:88[B]:ARG:HH22	1.71	0.55
1:A:132:GLY:CA	1:A:143:LEU:HD23	2.36	0.54
1:B:26:HIS:O	1:B:27:ILE:HG23	2.07	0.54
1:B:531:LEU:HD23	1:B:531:LEU:C	2.27	0.54
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.90	0.52
1:A:432:TRP:HE1	4:A:1004:PEG:H32	1.74	0.52
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.92	0.52
1:B:27:ILE:CG2	8:B:2103:HOH:O	2.57	0.52
1:B:27:ILE:HG22	8:B:2103:HOH:O	2.10	0.51
1:A:162:GLN:NE2	8:A:2124:HOH:O	2.43	0.51
2:A:1000:AFT:H6A	8:A:2001:HOH:O	2.10	0.51
1:B:383:ASN:HB3	1:B:386:LYS:HB2	1.91	0.51
1:A:432:TRP:HB3	1:A:433:PRO:HD2	1.93	0.51
1:B:73:GLU:HB3	8:B:2064:HOH:O	2.10	0.50
4:B:1005:PEG:H32	8:B:2377:HOH:O	2.12	0.50
1:A:440:HIS:CD2	5:A:1006:PGE:O1	2.64	0.50
1:B:27:ILE:HG22	1:B:103:SER:H	1.76	0.49
1:A:450:LEU:N	1:A:451:PRO:CD	2.75	0.49
1:B:206:VAL:CG1	1:B:222:ALA:HB1	2.42	0.49
1:B:211:LEU:HD23	1:B:314:PHE:HB3	1.94	0.48
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.48	0.48
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.49	0.48
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.49	0.48
1:B:135:LEU:HD23	1:B:143:LEU:HD13	1.96	0.47
1:A:27:ILE:HG22	1:A:103:SER:H	1.78	0.47
1:A:36:ALA:CB	1:A:175:MET:CE	2.93	0.47
1:B:112:MET:HB2	1:B:143:LEU:HD12	1.96	0.47
1:B:461:GLU:N	1:B:461:GLU:OE1	2.45	0.47
1:B:430:LEU:HD21	1:B:439:ILE:CD1	2.38	0.47
1:A:62:THR:CG2	1:A:88[B]:ARG:NH2	2.78	0.47
1:B:440:HIS:HD2	5:B:1004:PGE:H4	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASN:HD22	4:A:1005:PEG:H21	1.79	0.46
1:B:200:SER:HA	1:B:226:SER:O	2.14	0.46
1:B:174[A]:ARG:NH2	1:B:212:SER:OG	2.49	0.46
1:A:432:TRP:NE1	4:A:1004:PEG:H32	2.31	0.46
4:A:1005:PEG:C2	4:A:1005:PEG:O4	2.64	0.46
1:A:48:PRO:HB2	1:A:175:MET:HE1	1.97	0.46
1:A:216:ARG:HG2	1:A:315:LYS:HB2	1.99	0.45
1:B:355:GLY:HA3	1:B:391:LEU:HD21	1.98	0.45
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.74	0.45
1:A:199:GLU:HG3	1:A:443:GLU:OE2	2.16	0.45
1:A:43[B]:MET:HG2	8:A:2030:HOH:O	2.16	0.45
1:B:330:PHE:CE2	5:B:1004:PGE:H22	2.51	0.45
1:A:220:ARG:HG3	1:A:221:ARG:HG3	1.99	0.45
5:B:1004:PGE:O2	5:B:1004:PGE:C5	2.65	0.44
1:B:287:ILE:HG12	1:B:358:LEU:HB3	2.00	0.44
1:A:83:MET:SD	4:A:1004:PEG:H42	2.57	0.44
1:A:36:ALA:HB2	1:A:175:MET:HE2	1.99	0.44
1:B:312:GLY:HA2	1:B:314:PHE:CE2	2.52	0.44
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.82	0.44
1:A:98:ASN:O	1:A:144:VAL:HA	2.17	0.44
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.53	0.44
1:B:515:ARG:HB3	1:B:518:VAL:HB	1.99	0.43
1:A:440:HIS:NE2	5:A:1006:PGE:O1	2.44	0.43
5:B:1004:PGE:C2	5:B:1004:PGE:H5	2.48	0.43
1:A:405:MET:HA	1:A:408:VAL:HG12	2.01	0.43
1:A:408:VAL:CG2	1:A:418:THR:HG21	2.49	0.43
1:B:105:ARG:HA	1:B:106:PRO:HD2	1.90	0.42
5:A:1006:PGE:O1	5:A:1006:PGE:H32	2.20	0.42
5:B:1004:PGE:O2	5:B:1004:PGE:H5	2.19	0.42
1:A:211:LEU:HD23	1:A:314:PHE:HB3	2.02	0.42
1:A:132:GLY:CA	1:A:143:LEU:CD2	2.98	0.42
1:B:26:HIS:O	1:B:27:ILE:CG2	2.67	0.41
1:B:47[B]:ARG:HB2	1:B:47[B]:ARG:NH1	2.35	0.41
1:B:197:PHE:HB2	1:B:223:ILE:HB	2.02	0.41
1:A:440:HIS:ND1	8:A:2279:HOH:O	2.30	0.41
1:A:405:MET:O	1:A:408:VAL:HG12	2.21	0.41
1:B:321:LEU:O	1:B:420:LEU:HA	2.20	0.41
1:A:221:ARG:HD3	1:A:480:GLY:HA2	2.03	0.41
1:A:223:ILE:HA	1:A:320:LEU:O	2.19	0.41
1:B:431:VAL:HG22	8:B:2310:HOH:O	2.21	0.41
1:A:87:ASN:O	1:A:88[A]:ARG:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:CG2	1:A:88[B]:ARG:HH22	2.33	0.40
1:B:402:CYS:N	1:B:403:PRO:CD	2.85	0.40
1:A:528:LEU:HB3	1:A:529:PRO:HD3	2.04	0.40
1:B:236:VAL:HG23	1:B:295:VAL:HG12	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:NE2	1:B:508:GLU:OE2[3_755]	2.19	0.01

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	537/537 (100%)	510 (95%)	25 (5%)	2 (0%)	39 48
1	B	541/537 (101%)	519 (96%)	22 (4%)	0	100 100
All	All	1078/1074 (100%)	1029 (96%)	47 (4%)	2 (0%)	52 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	HIS
1	A	440	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	470/469 (100%)	458 (97%)	12 (3%)	54 71
1	B	473/469 (101%)	466 (98%)	7 (2%)	72 85
All	All	943/938 (100%)	924 (98%)	19 (2%)	61 79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	21	PRO
1	A	24	SER
1	A	129	VAL
1	A	192	LYS
1	A	197	PHE
1	A	253	ASN
1	A	260	GLU
1	A	288	PHE
1	A	295	VAL
1	A	349	ARG
1	A	473	TRP
1	B	12	SER
1	B	55	SER
1	B	287	ILE
1	B	288	PHE
1	B	343	SER
1	B	473	TRP
1	B	535	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	533	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 for Mogul analysis.

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	AFT	A	1000	-	22,27,27	1.58	3 (13%)	21,42,42	2.71	10 (47%)
4	PEG	A	1003	-	6,6,6	0.49	0	5,5,5	0.71	0
4	PEG	A	1004	-	6,6,6	0.43	0	5,5,5	0.53	0
4	PEG	A	1005	-	6,6,6	0.66	0	5,5,5	0.30	0
5	PGE	A	1006	-	9,9,9	0.76	0	8,8,8	0.74	0
6	NAG	A	1007	1	14,14,15	0.52	0	15,19,21	1.95	5 (33%)
6	NAG	A	1008	1	14,14,15	0.67	0	15,19,21	1.68	4 (26%)
6	NAG	A	1009	1	14,14,15	0.69	0	15,19,21	1.49	2 (13%)
2	AFT	B	1000	-	22,27,27	1.75	4 (18%)	21,42,42	2.56	8 (38%)
4	PEG	B	1003	-	6,6,6	0.85	0	5,5,5	0.44	0
5	PGE	B	1004	-	9,9,9	1.07	0	8,8,8	0.71	0
4	PEG	B	1005	-	6,6,6	0.80	0	5,5,5	1.58	1 (20%)
4	PEG	B	1006	-	6,6,6	0.73	0	5,5,5	0.55	0
6	NAG	B	1008	1	14,14,15	0.50	0	15,19,21	1.32	2 (13%)
6	NAG	B	1009	1	14,14,15	0.52	0	15,19,21	1.28	2 (13%)

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	AFT	A	1000	-	-	0/2/29/29	0/5/5/5
4	PEG	A	1003	-	-	0/4/4/4	0/0/0/0
4	PEG	A	1004	-	-	0/4/4/4	0/0/0/0
4	PEG	A	1005	-	-	0/4/4/4	0/0/0/0
5	PGE	A	1006	-	-	0/7/7/7	0/0/0/0
6	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
2	AFT	B	1000	-	-	0/2/29/29	0/5/5/5
4	PEG	B	1003	-	-	0/4/4/4	0/0/0/0
5	PGE	B	1004	-	-	0/7/7/7	0/0/0/0
4	PEG	B	1005	-	-	0/4/4/4	0/0/0/0
4	PEG	B	1006	-	-	0/4/4/4	0/0/0/0
6	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1009	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	AFT	C3-C3A	2.38	1.54	1.51
2	A	1000	AFT	C3-C3A	2.70	1.55	1.51
2	B	1000	AFT	O7-C6A	3.01	1.46	1.43
2	B	1000	AFT	C2A-C1	3.94	1.54	1.51
2	A	1000	AFT	C5A-C9B	3.99	1.39	1.36
2	A	1000	AFT	C2A-C1	4.12	1.54	1.51
2	B	1000	AFT	C5A-C9B	4.48	1.40	1.36

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	AFT	C5B-C5A-C9B	-6.41	118.44	124.26
2	B	1000	AFT	C5B-C5A-C9B	-5.76	119.03	124.26
2	B	1000	AFT	C3-C2A-C1	-5.63	104.14	106.42
2	A	1000	AFT	C3-C2A-C1	-4.59	104.56	106.42
6	A	1008	NAG	C2-N2-C7	-3.84	118.11	123.04
2	B	1000	AFT	O7-C6A-C9A	-3.64	104.62	107.60
6	A	1007	NAG	C4-C3-C2	-3.56	105.69	111.23
2	A	1000	AFT	O4-C4B-C5B	-3.27	118.43	123.60
2	A	1000	AFT	O7-C6A-C9A	-3.24	104.95	107.60
4	B	1005	PEG	O2-C3-C4	-3.15	95.91	110.43
2	A	1000	AFT	CM-O4-C4B	-2.73	113.78	117.77
2	B	1000	AFT	O1-C1-C2A	-2.32	123.81	125.83
6	A	1008	NAG	O3-C3-C4	-2.27	105.23	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1009	NAG	C3-C2-N2	-2.22	105.24	110.56
2	B	1000	AFT	O4-C4B-C5B	-2.13	120.23	123.60
2	A	1000	AFT	O1-C1-C12	-2.12	124.26	127.55
6	A	1007	NAG	O7-C7-C8	-2.10	118.21	122.06
6	A	1008	NAG	C1-O5-C5	-2.00	109.71	112.25
6	A	1007	NAG	C8-C7-N2	2.04	120.00	116.11
2	A	1000	AFT	C5A-C9B-C10	2.21	121.45	119.75
2	B	1000	AFT	O10-C10-C4A	2.31	123.54	121.15
2	A	1000	AFT	O10-C10-C4A	2.62	123.86	121.15
6	A	1007	NAG	O5-C5-C6	2.66	113.12	107.35
6	B	1008	NAG	O5-C5-C6	2.92	113.66	107.35
6	A	1009	NAG	C4-C3-C2	2.95	115.81	111.23
6	A	1008	NAG	C4-C3-C2	2.95	115.82	111.23
6	B	1008	NAG	C1-O5-C5	2.99	116.05	112.25
6	B	1009	NAG	C1-O5-C5	3.09	116.16	112.25
6	A	1009	NAG	C2-N2-C7	3.11	127.03	123.04
2	B	1000	AFT	O4-C4B-C4A	3.17	120.89	115.89
2	A	1000	AFT	O4-C4B-C4A	3.65	121.65	115.89
6	A	1007	NAG	C1-O5-C5	4.36	117.78	112.25
2	B	1000	AFT	O6A-C5A-C5B	4.75	129.81	123.40
2	A	1000	AFT	O6A-C5A-C5B	4.95	130.09	123.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	AFT	1	0
4	A	1004	PEG	8	0
4	A	1005	PEG	3	0
5	A	1006	PGE	5	0
5	B	1004	PGE	5	0
4	B	1005	PEG	3	0

5.7 Other polymers (i)

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^{th} 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	530/537 (98%)	0.05	14 (2%)	59	68	21, 36, 55, 82	3 (0%)
1	B	532/537 (99%)	0.20	27 (5%)	32	41	22, 36, 56, 79	1 (0%)
All	All	1062/1074 (98%)	0.13	41 (3%)	43	52	21, 36, 56, 82	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535	THR	6.2
1	B	257	ASN	4.1
1	A	429[A]	ASN	3.4
1	B	261	GLU	3.3
1	B	264	HIS	3.1
1	A	487	SER	3.0
1	B	24	SER	3.0
1	B	260	GLU	3.0
1	B	454	LYS	3.0
1	A	426	ARG	2.9
1	A	486	HIS	2.9
1	A	430	LEU	2.8
1	B	42	ASN	2.8
1	B	115	ILE	2.8
1	B	23	LEU	2.7
1	B	453	VAL	2.7
1	B	163	GLU	2.6
1	B	428	SER	2.6
1	A	18	THR	2.6
1	B	21	PRO	2.4
1	A	113	VAL	2.4
1	B	71	VAL	2.4
1	B	486	HIS	2.4
1	A	137	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	SER	2.3
1	B	331	PHE	2.2
1	B	485	PRO	2.2
1	B	265	CYS	2.2
1	B	204	ALA	2.2
1	B	201	ALA	2.2
1	B	196	ILE	2.1
1	A	264	HIS	2.1
1	A	4	SER	2.1
1	A	442	TYR	2.1
1	B	334	TYR	2.1
1	B	26	HIS	2.1
1	B	121	TYR	2.0
1	A	115	ILE	2.0
1	B	22	VAL	2.0
1	A	26	HIS	2.0
1	B	330	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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^{th} 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^2)	Q<0.9
5	PGE	A	1006	10/10	0.86	0.30	8.18	56,59,63,64	0
5	PGE	B	1004	10/10	0.84	0.46	7.08	57,63,64,65	0
2	AFT	A	1000	23/23	0.74	0.34	7.05	47,50,51,52	23
4	PEG	B	1005	7/7	0.88	0.23	5.75	46,47,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	AFT	B	1000	23/23	0.68	0.38	4.83	46,52,55,56	23
4	PEG	A	1004	7/7	0.77	0.23	2.53	54,59,61,62	0
4	PEG	B	1003	7/7	0.55	0.29	2.30	64,68,74,74	0
4	PEG	A	1005	7/7	0.89	0.16	2.19	55,59,67,68	0
7	K	A	1010	1/1	0.97	0.10	-2.26	36,36,36,36	0
3	CL	B	1002	1/1	0.94	0.05	-3.70	67,67,67,67	0
4	PEG	B	1006	7/7	0.81	0.23	-	55,64,68,68	0
3	CL	B	1001	1/1	0.93	0.07	-	61,61,61,61	0
6	NAG	B	1008	14/15	0.87	0.24	-	54,63,65,65	0
3	CL	A	1001	1/1	0.95	0.11	-	66,66,66,66	0
4	PEG	A	1003	7/7	0.90	0.26	-	64,66,68,68	0
3	CL	A	1002	1/1	0.93	0.10	-	63,63,63,63	0
6	NAG	A	1009	14/15	0.78	0.27	-	60,69,74,75	0
6	NAG	B	1009	14/15	0.90	0.11	-	38,43,48,49	0
6	NAG	A	1007	14/15	0.89	0.30	-	54,62,66,66	0
6	NAG	A	1008	14/15	0.86	0.10	-	47,52,58,59	0

6.5 Other polymers

There are no such residues in this entry.