Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:35 AM GMT

PDB ID	:	2XMG
Title	:	G117H mutant of human butyrylcholinesterase in complex with VX
Authors	:	Nachon, F.; Carletti, E.; Wandhammer, M.; Nicolet, Y.; Schopfer, L.M.; Masson, P.; Lockridge, O.
Deposited on	:	2010-07-27
Resolution	:	2.70 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:

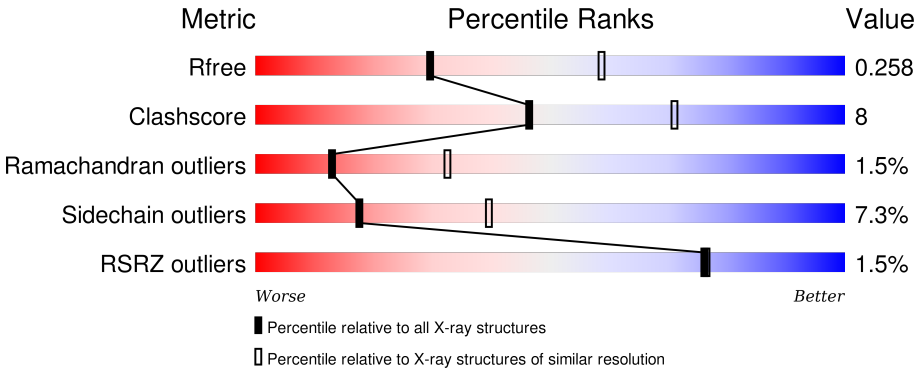
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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 >=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	529	2% 81% 15%

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	UNX	A	1536	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	1539	-	-	-	X
7	FUL	A	1554	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4544 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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	2	0
			4226	2727	713	771	15			

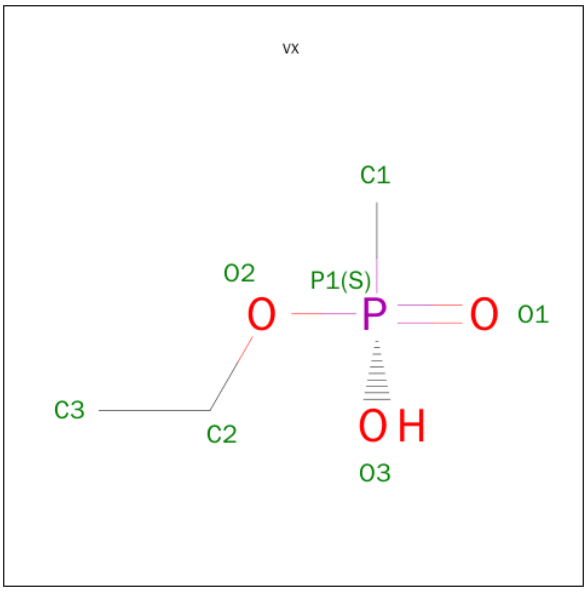
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

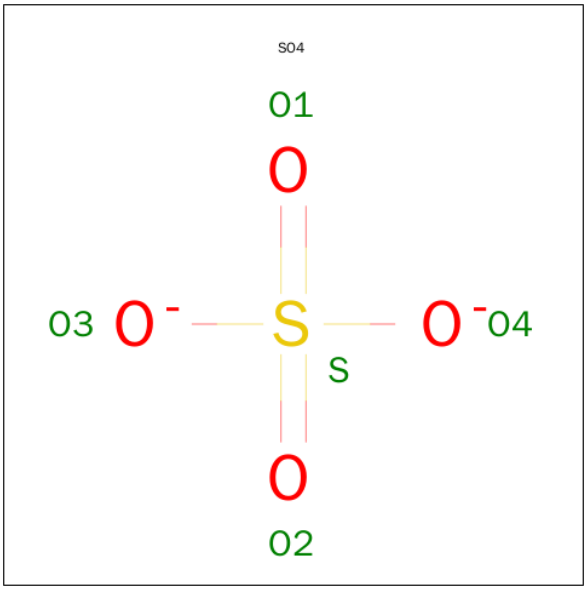
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	X	0	0
			7	7		

- Molecule 3 is O-ETHYLMETHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VX) (formula: $C_3H_9O_3P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 6 3 2 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

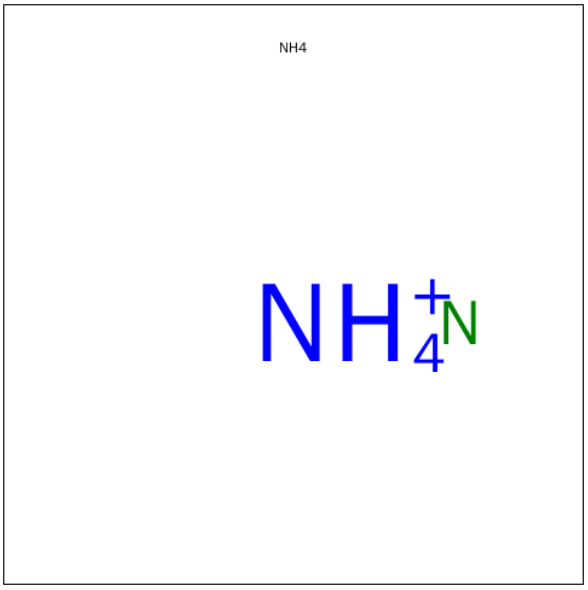


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Cl 5 5	0	0

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N 1 1	0	0
6	A	1	Total N 1 1	0	0

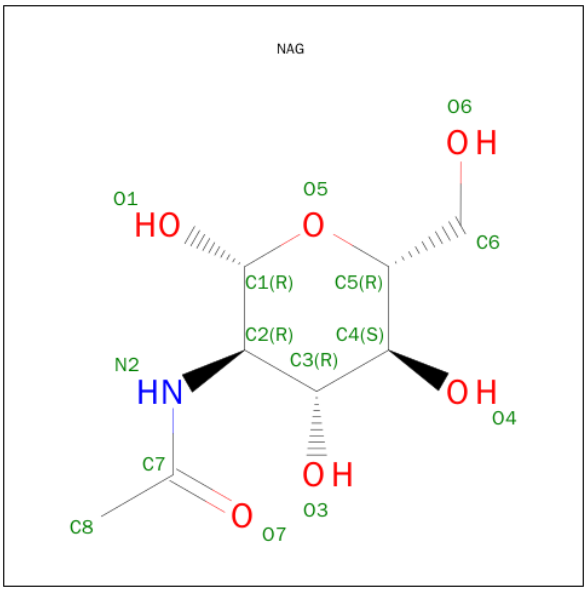
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total C N O 38 22 2 14	0	0
7	A	3	Total C N O 38 22 2 14	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total C N O 24 14 1 9	0	0

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

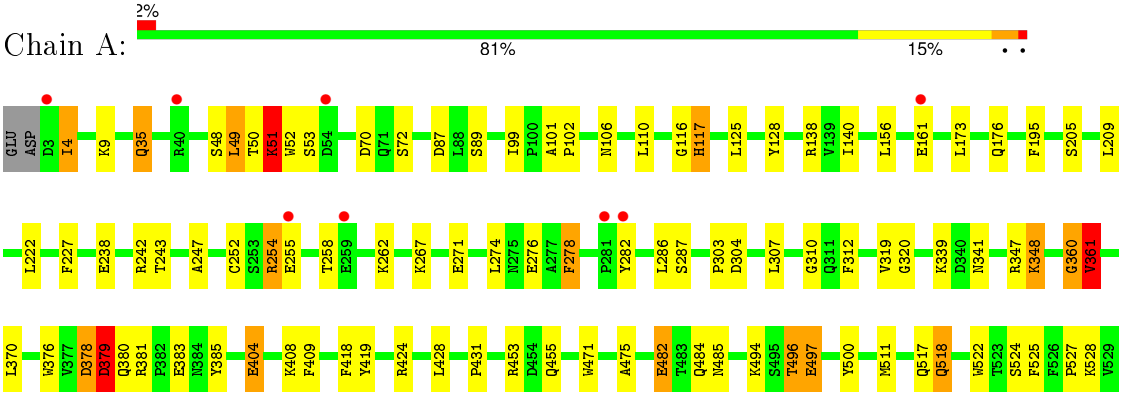
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	151	Total O 151 151	0	0

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: CHOLINESTERASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	156.57Å 156.57Å 128.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.43 – 2.70 61.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (110.43-2.70) 94.3 (61.47-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.250 0.185 , 0.258	Depositor DCC
R_{free} test set	927 reflections (4.62%)	DCC
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 20940 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4544	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAG, CL, UNX, NH4, SO4, VX, FUL

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	0.87	1/4351 (0.0%)	0.83	2/5907 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CG-CD	6.07	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	424	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	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	4226	0	4117	65	0
2	A	7	0	0	0	0
3	A	6	0	8	2	0
4	A	5	0	0	0	0
5	A	5	0	0	0	0
6	A	2	0	0	0	0
7	A	76	0	68	3	0
8	A	24	0	22	1	0
9	A	42	0	39	1	0
10	A	151	0	0	4	0
All	All	4544	0	4254	66	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 (66) 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:156:LEU:HD13	1:A:243:THR:HG21	1.47	0.97
1:A:518:GLN:HE21	1:A:518:GLN:N	1.62	0.96
1:A:50:THR:O	1:A:51:LYS:HB3	1.67	0.94
1:A:518:GLN:H	1:A:518:GLN:NE2	1.72	0.87
1:A:518:GLN:H	1:A:518:GLN:HE21	0.86	0.82
1:A:117:HIS:HB3	3:A:1530:VX:H33	1.62	0.79
9:A:1550:NAG:H5	10:A:2151:HOH:O	1.82	0.79
1:A:341:ASN:HD22	7:A:1544:NAG:H83	1.52	0.74
1:A:380:GLN:N	1:A:381:ARG:HB2	2.03	0.74
1:A:341:ASN:ND2	7:A:1544:NAG:H83	2.03	0.73
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.30	0.66
1:A:380:GLN:H	1:A:381:ARG:HB2	1.61	0.65
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.98	0.64
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.82	0.62
1:A:524:SER:O	1:A:528:LYS:HE3	1.99	0.62
1:A:4:ILE:N	1:A:4:ILE:HD12	2.14	0.62
1:A:482:GLU:OE2	1:A:485:ASN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:O	1:A:418:PHE:HA	2.03	0.59
1:A:227:PHE:CD2	1:A:227:PHE:C	2.80	0.55
1:A:173:LEU:O	1:A:176:GLN:HB3	2.07	0.55
1:A:50:THR:HA	10:A:2011:HOH:O	2.08	0.54
1:A:4:ILE:H	1:A:4:ILE:HD12	1.73	0.54
1:A:496:THR:OG1	1:A:497:GLU:HG2	2.08	0.54
1:A:482:GLU:OE1	1:A:484:GLN:N	2.33	0.53
1:A:525:PHE:C	1:A:525:PHE:CD1	2.82	0.53
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.44	0.52
1:A:101:ALA:HA	1:A:102:PRO:C	2.29	0.51
1:A:35:GLN:NE2	1:A:48:SER:O	2.43	0.51
1:A:376:TRP:CE3	1:A:376:TRP:HA	2.45	0.51
1:A:278:PHE:CD2	1:A:278:PHE:N	2.77	0.51
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.46	0.50
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.46	0.50
1:A:347:ARG:HD2	1:A:385:TYR:OH	2.11	0.49
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.48	0.49
1:A:238:GLU:O	1:A:242:ARG:HG3	2.13	0.49
1:A:35:GLN:NE2	1:A:49:LEU:HA	2.29	0.47
1:A:116:GLY:C	1:A:117:HIS:CD2	2.87	0.47
1:A:361:VAL:HA	10:A:2090:HOH:O	2.14	0.47
1:A:404:GLU:OE2	1:A:408:LYS:HE2	2.14	0.47
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.96	0.47
1:A:125:LEU:HD12	1:A:128:TYR:CE2	2.50	0.47
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.51	0.46
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.98	0.46
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.46	0.45
1:A:49:LEU:HD12	1:A:50:THR:H	1.80	0.45
1:A:247:ALA:O	1:A:252:CYS:N	2.40	0.44
1:A:339:LYS:O	1:A:431:PRO:HG3	2.17	0.44
1:A:117:HIS:CB	3:A:1530:VX:H33	2.42	0.44
1:A:379:ASP:HB2	1:A:381:ARG:HG3	1.99	0.44
1:A:380:GLN:CA	1:A:381:ARG:HB2	2.47	0.44
1:A:376:TRP:HA	1:A:376:TRP:HE3	1.81	0.44
1:A:381:ARG:NE	1:A:383:GLU:OE1	2.51	0.43
1:A:278:PHE:O	7:A:1554:FUL:H4	2.18	0.42
1:A:378:ASP:O	1:A:380:GLN:NE2	2.53	0.42
1:A:4:ILE:N	1:A:4:ILE:CD1	2.80	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.82	0.42
1:A:376:TRP:O	1:A:378:ASP:OD1	2.37	0.42
1:A:209:LEU:HD11	1:A:227:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.55	0.41
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.85	0.41
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.02	0.41
1:A:51:LYS:HG3	1:A:52:TRP:N	2.34	0.41
1:A:522:TRP:O	1:A:527:PRO:HD3	2.21	0.40
1:A:106:ASN:ND2	8:A:1547:NAG:H83	2.35	0.40
1:A:312:PHE:CD1	1:A:409:PHE:CE1	3.10	0.40
1:A:348:LYS:HB2	10:A:2088:HOH:O	2.21	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	527/529 (100%)	483 (92%)	36 (7%)	8 (2%)	13 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	379	ASP
1	A	51	LYS
1	A	496	THR
1	A	87	ASP
1	A	378	ASP
1	A	276	GLU
1	A	360	GLY

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	455/455 (100%)	422 (93%)	33 (7%)	17 39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	35	GLN
1	A	49	LEU
1	A	51	LYS
1	A	53	SER
1	A	72	SER
1	A	89	SER
1	A	117	HIS
1	A	138	ARG
1	A	195	PHE
1	A	254	ARG
1	A	255	GLU
1	A	262	LYS
1	A	274	LEU
1	A	278	PHE
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	304	ASP
1	A	348	LYS
1	A	361	VAL
1	A	370	LEU
1	A	379	ASP
1	A	428	LEU
1	A	453	ARG
1	A	455	GLN
1	A	471	TRP
1	A	482	GLU
1	A	494	LYS

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Mol	Chain	Res	Type
1	A	497	GLU
1	A	517	GLN
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	35	GLN
1	A	117	HIS
1	A	380	GLN
1	A	517	GLN
1	A	518	GLN

5.3.3 RNA (i)

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)

8 carbohydrates 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	$\#\|Z\| > 2$
7	NAG	A	1544	1,7	14,14,15	0.70	0	15,19,21	1.87	6 (40%)
7	NAG	A	1545	7	14,14,15	0.79	0	15,19,21	2.46	6 (40%)
7	FUL	A	1546	7	10,10,11	0.95	0	14,14,16	3.44	4 (28%)
8	NAG	A	1547	1,8	14,14,15	1.26	1 (7%)	15,19,21	2.03	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FUL	A	1548	8	10,10,11	0.78	0	14,14,16	2.78	7 (50%)
7	NAG	A	1552	1,7	14,14,15	0.74	0	15,19,21	2.78	3 (20%)
7	NAG	A	1553	7	14,14,15	0.77	1 (7%)	15,19,21	1.87	5 (33%)
7	FUL	A	1554	7	10,10,11	0.88	0	14,14,16	2.50	4 (28%)

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
7	NAG	A	1544	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1545	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1546	7	-	0/0/17/20	0/1/1/1
8	NAG	A	1547	1,8	-	0/6/23/26	0/1/1/1
8	FUL	A	1548	8	-	0/0/17/20	0/1/1/1
7	NAG	A	1552	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1553	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1554	7	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1553	NAG	C1-C2	2.52	1.56	1.52
8	A	1547	NAG	C1-C2	3.72	1.57	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1546	FUL	C1-C2-C3	-10.27	97.40	109.54
8	A	1548	FUL	C1-C2-C3	-6.54	101.80	109.54
7	A	1554	FUL	C1-C2-C3	-6.22	102.19	109.54
7	A	1546	FUL	C1-O5-C5	-4.85	104.88	112.38
8	A	1548	FUL	O5-C1-C2	-3.51	105.17	110.86
7	A	1545	NAG	C3-C2-N2	-3.50	102.17	110.56
7	A	1544	NAG	O7-C7-C8	-3.44	115.74	122.06
7	A	1554	FUL	O5-C1-C2	-3.05	105.92	110.86
8	A	1548	FUL	C2-C3-C4	-2.87	106.16	111.04
8	A	1547	NAG	C3-C4-C5	-2.70	105.50	110.20
7	A	1544	NAG	C3-C4-C5	-2.67	105.54	110.20
7	A	1552	NAG	O7-C7-C8	-2.58	117.33	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1553	NAG	C4-C3-C2	-2.48	107.38	111.23
8	A	1548	FUL	C1-O5-C5	-2.33	108.77	112.38
7	A	1553	NAG	C3-C4-C5	-2.32	106.16	110.20
8	A	1547	NAG	O3-C3-C2	2.06	113.19	109.11
8	A	1547	NAG	O4-C4-C5	2.08	114.75	109.24
7	A	1553	NAG	O3-C3-C2	2.09	113.24	109.11
7	A	1545	NAG	O7-C7-N2	2.09	126.12	121.86
7	A	1546	FUL	C6-C5-C4	2.10	117.21	113.08
7	A	1554	FUL	C3-C4-C5	2.17	113.38	109.72
7	A	1552	NAG	O7-C7-N2	2.23	126.42	121.86
7	A	1544	NAG	C8-C7-N2	2.27	120.45	116.11
8	A	1548	FUL	O5-C5-C6	2.33	109.99	106.13
7	A	1544	NAG	O6-C6-C5	2.38	119.20	111.33
7	A	1544	NAG	O5-C5-C6	2.50	112.75	107.35
7	A	1544	NAG	C6-C5-C4	2.51	119.20	113.02
7	A	1553	NAG	O4-C4-C5	2.51	115.90	109.24
7	A	1545	NAG	C4-C3-C2	2.56	115.20	111.23
8	A	1548	FUL	O3-C3-C2	2.81	115.07	110.00
7	A	1545	NAG	C1-O5-C5	2.84	115.86	112.25
8	A	1547	NAG	O5-C5-C6	2.90	113.62	107.35
8	A	1547	NAG	C8-C7-N2	2.96	121.77	116.11
7	A	1546	FUL	O5-C5-C6	3.77	112.37	106.13
8	A	1548	FUL	O2-C2-C1	3.93	117.09	109.21
7	A	1545	NAG	C3-C4-C5	4.32	117.73	110.20
7	A	1554	FUL	O2-C2-C1	4.45	118.12	109.21
8	A	1547	NAG	C2-N2-C7	4.56	128.89	123.04
7	A	1553	NAG	C1-O5-C5	4.82	118.37	112.25
7	A	1545	NAG	C2-N2-C7	5.88	130.59	123.04
7	A	1552	NAG	C1-O5-C5	9.55	124.37	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1544	NAG	2	0
8	A	1547	NAG	1	0
7	A	1554	FUL	1	0

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are unknown, 2 are modelled with single atom and 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	VX	A	1530	1	1,5,6	0.98	0	1,5,8	0.51	0
4	SO4	A	1531	-	4,4,4	0.50	0	6,6,6	0.21	0
9	NAG	A	1549	1	14,14,15	0.78	0	15,19,21	3.27	8 (53%)
9	NAG	A	1550	1	14,14,15	0.81	1 (7%)	15,19,21	2.14	2 (13%)
9	NAG	A	1551	1	14,14,15	0.94	0	15,19,21	1.74	4 (26%)

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
3	VX	A	1530	1	-	0/1/3/4	0/0/0/0
4	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
9	NAG	A	1549	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1550	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1551	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1550	NAG	O5-C1	2.03	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1549	NAG	C4-C3-C2	-3.81	105.30	111.23
9	A	1549	NAG	C3-C4-C5	-2.05	106.62	110.20
9	A	1549	NAG	O7-C7-C8	-2.01	118.37	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1550	NAG	O3-C3-C2	2.05	113.18	109.11
9	A	1551	NAG	O3-C3-C2	2.16	113.40	109.11
9	A	1549	NAG	O3-C3-C4	2.20	115.29	110.34
9	A	1549	NAG	O4-C4-C3	2.50	115.97	110.34
9	A	1551	NAG	C6-C5-C4	2.56	119.32	113.02
9	A	1549	NAG	C3-C2-N2	2.57	116.71	110.56
9	A	1551	NAG	O5-C5-C6	2.64	113.06	107.35
9	A	1551	NAG	C2-N2-C7	2.75	126.58	123.04
9	A	1549	NAG	C8-C7-N2	3.33	122.48	116.11
9	A	1550	NAG	C1-O5-C5	6.66	120.69	112.25
9	A	1549	NAG	C1-O5-C5	10.11	125.08	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1530	VX	2	0
9	A	1550	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	527/529 (99%)	-0.09	8 (1%)	76	76	31, 52, 90, 123	10 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.2
1	A	282	TYR	3.9
1	A	40	ARG	3.3
1	A	54	ASP	3.1
1	A	259	GLU	2.7
1	A	161	GLU	2.3
1	A	281	PRO	2.2
1	A	255	GLU	2.0

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

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

6.3 Carbohydrates

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
7	FUL	A	1554	10/11	0.88	0.33	2.18	90,92,94,96	0
7	NAG	A	1544	14/15	0.95	0.16	-0.14	51,59,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	A	1552	14/15	0.90	0.25	-	76,87,91,92	0
7	FUL	A	1546	10/11	0.93	0.26	-	73,75,78,78	0
8	FUL	A	1548	10/11	0.92	0.27	-	66,70,75,76	0
7	NAG	A	1545	14/15	0.87	0.30	-	79,85,88,88	0
7	NAG	A	1553	14/15	0.78	0.32	-	91,98,101,101	0
8	NAG	A	1547	14/15	0.79	0.20	-	63,67,68,68	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
2	UNX	A	1539	1/1	0.92	0.28	5.69	36,36,36,36	0
2	UNX	A	1536	1/1	0.94	0.19	3.11	31,31,31,31	0
9	NAG	A	1550	14/15	0.87	0.19	1.06	63,76,81,82	0
3	VX	A	1530	6/7	0.98	0.13	-0.88	53,55,56,57	0
2	UNX	A	1538	1/1	0.81	0.17	-	13,13,13,13	0
5	CL	A	1533	1/1	0.93	0.08	-	74,74,74,74	0
2	UNX	A	1542	1/1	0.91	0.18	-	23,23,23,23	0
2	UNX	A	1537	1/1	0.97	0.08	-	15,15,15,15	0
5	CL	A	1532	1/1	0.82	0.20	-	72,72,72,72	0
5	CL	A	1534	1/1	0.95	0.16	-	75,75,75,75	0
9	NAG	A	1551	14/15	0.89	0.25	-	72,79,84,86	0
5	CL	A	1535	1/1	0.96	0.24	-	67,67,67,67	0
2	UNX	A	1540	1/1	0.90	0.18	-	24,24,24,24	0
5	CL	A	1555	1/1	0.96	0.15	-	62,62,62,62	0
9	NAG	A	1549	14/15	0.83	0.17	-	76,82,84,84	0
6	NH4	A	1543	1/1	0.59	0.50	-	48,48,48,48	0
4	SO4	A	1531	5/5	0.97	0.10	-	67,68,69,71	0
6	NH4	A	1556	1/1	0.94	0.55	-	40,40,40,40	0
2	UNX	A	1541	1/1	0.93	0.32	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.