



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 AM GMT

PDB ID : 2XMD  
Title : G117H MUTANT OF HUMAN BUTYRYLCHOLINESTERASE IN COMPLEX WITH ECHOTHIOPHATE  
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Deposited on : 2010-07-27  
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](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

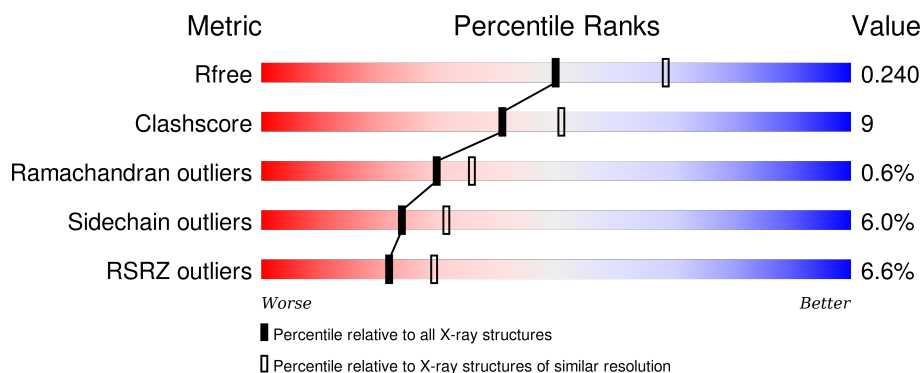
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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  $\geq 3$ , 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	529	<div> <div>7%</div> <div>82%</div> <div>14%</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
10	FUL	A	1558	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	1539	-	-	-	X
2	UNX	A	1545	-	-	-	X
2	UNX	A	1546	-	-	-	X
2	UNX	A	1551	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 4705 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
			Total	C	N	O	S			
1	A	527	4222	2724	711	772	15	0	2	0

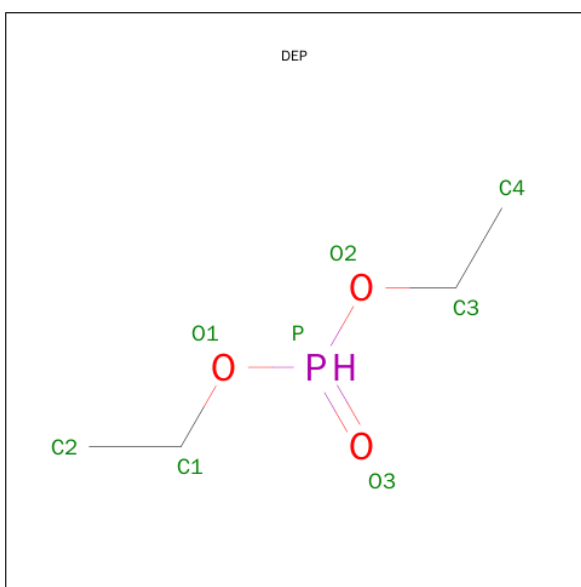
There are 5 discrepancies between the modelled and reference sequences:

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	21	Total	X	0	0
			21	21		

- Molecule 3 is DIETHYL PHOSPHONATE (three-letter code: DEP) (formula: C<sub>4</sub>H<sub>11</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	4	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Cl 4 4	0	0

- Molecule 6 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

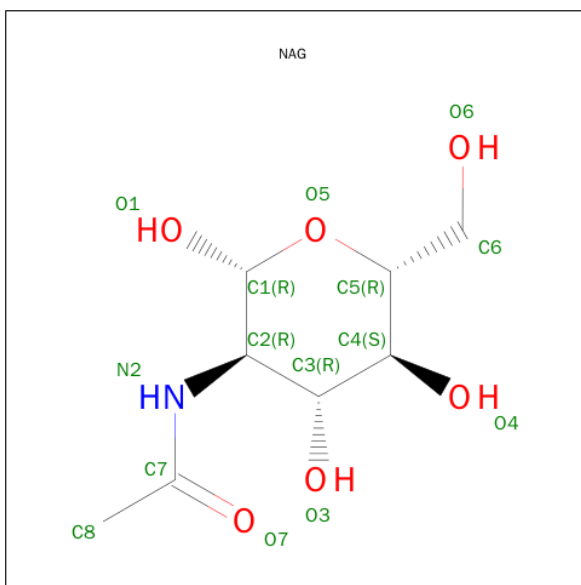
- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

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

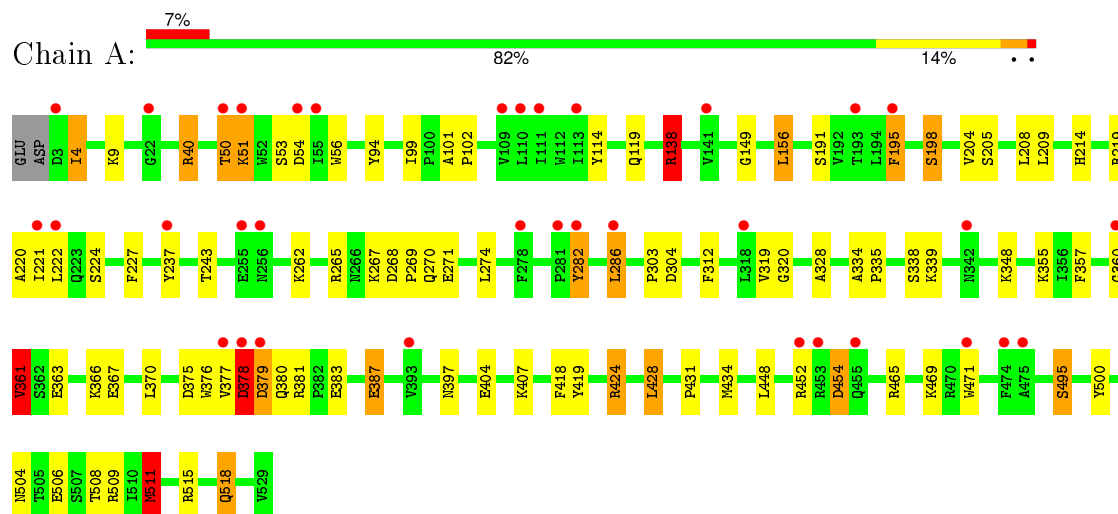
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	285	Total	O	0	0
			285	285		

### 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.88Å 154.88Å 127.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.15 – 2.30 28.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.15-2.30) 96.0 (28.15-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.53 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.170 , 0.214 0.194 , 0.240	Depositor DCC
$R_{free}$ test set	1090 reflections (3.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33216 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: NAG, CL, DEP, NA, CA, UNX, FUC, BR, FUL, SO4

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	1.10	4/4346 (0.1%)	0.97	14/5900 (0.2%)

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	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CG-CD	6.25	1.61	1.51
1	A	515	ARG	CZ-NH1	5.88	1.40	1.33
1	A	114	TYR	CD1-CE1	5.37	1.47	1.39
1	A	94	TYR	CD1-CE1	5.23	1.47	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	515	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	465	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	424	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	424	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	219	ARG	CG-CD-NE	-6.00	99.19	111.80
1	A	448	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	515	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	511	MET	CG-SD-CE	-5.83	90.87	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	VAL	N-CA-C	5.82	126.70	111.00
1	A	219	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	286	LEU	CA-CB-CG	-5.36	102.96	115.30
1	A	375	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	138	ARG	NE-CZ-NH2	-5.22	117.69	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	377	VAL	Peptide
1	A	378	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4222	0	4115	71	0
2	A	21	0	0	2	0
3	A	8	0	10	1	0
4	A	5	0	0	0	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	1
9	A	38	0	34	1	0
10	A	38	0	34	1	0
11	A	42	0	39	1	0
12	A	38	0	34	0	0
13	A	285	0	0	10	0
All	All	4705	0	4266	75	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 9.

All (75) 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:99:ILE:HD11	13:A:2010:HOH:O	1.25	1.33
1:A:379:ASP:H	1:A:380:GLN:HA	1.00	1.16
1:A:379:ASP:N	1:A:380:GLN:HA	1.80	0.95
1:A:518:GLN:H	1:A:518:GLN:HE21	1.14	0.92
1:A:508:THR:OG1	13:A:2263:HOH:O	1.80	0.89
1:A:378:ASP:HB3	1:A:379:ASP:HA	1.62	0.81
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.64	0.80
1:A:379:ASP:H	1:A:380:GLN:CA	1.89	0.80
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.48	0.78
1:A:282:TYR:O	1:A:282:TYR:HD2	1.76	0.69
1:A:138:ARG:NE	13:A:2091:HOH:O	2.28	0.66
1:A:156:LEU:CD1	1:A:243:THR:HG21	2.26	0.66
1:A:4:ILE:H	1:A:4:ILE:HD12	1.62	0.64
1:A:227:PHE:CD2	1:A:227:PHE:C	2.71	0.64
2:A:1569:UNX:UNK	2:A:1570:UNX:UNK	1.45	0.61
1:A:500:TYR:CZ	1:A:511:MET:HB3	2.37	0.59
1:A:40:ARG:H	1:A:40:ARG:HE	1.49	0.59
1:A:518:GLN:H	1:A:518:GLN:NE2	1.94	0.59
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.38	0.58
1:A:4:ILE:N	1:A:4:ILE:HD12	2.18	0.57
1:A:370:LEU:C	1:A:370:LEU:HD23	2.25	0.56
1:A:53:SER:O	1:A:54:ASP:CG	2.45	0.55
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.43	0.55
1:A:407:LYS:HG3	1:A:495:SER:OG	2.07	0.54
3:A:1530:DEP:H31	13:A:2113:HOH:O	2.07	0.54
1:A:361:VAL:O	1:A:366:LYS:NZ	2.41	0.54
1:A:56:TRP:C	1:A:56:TRP:CD1	2.82	0.53
1:A:376:TRP:O	1:A:378:ASP:OD1	2.27	0.53
1:A:500:TYR:CE1	1:A:511:MET:HB3	2.44	0.53
1:A:101:ALA:HA	1:A:102:PRO:C	2.29	0.53
1:A:319:VAL:O	1:A:418:PHE:HA	2.09	0.52
1:A:338:SER:HB2	9:A:1554:NAG:H62	1.91	0.51
1:A:191:SER:HB2	10:A:1558:FUL:H3	1.92	0.51
2:A:1540:UNX:UNK	2:A:1542:UNX:UNK	1.55	0.51
1:A:214[A]:HIS:HE1	13:A:2156:HOH:O	1.93	0.50
1:A:518:GLN:HE21	1:A:518:GLN:N	1.97	0.50
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.48	0.49
1:A:379:ASP:N	1:A:380:GLN:CA	2.62	0.48
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.67	0.48
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.97	0.48
1:A:407:LYS:HE2	1:A:407:LYS:HB2	1.23	0.48
1:A:328:ALA:HA	1:A:434:MET:CE	2.44	0.47
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.97	0.47
1:A:495:SER:HB2	13:A:2199:HOH:O	2.14	0.45
1:A:267:LYS:HD2	1:A:271:GLU:OE2	2.17	0.45
1:A:50:THR:O	1:A:51:LYS:HB3	2.17	0.45
1:A:265:ARG:NE	13:A:2134:HOH:O	2.28	0.44
1:A:383:GLU:O	1:A:387:GLU:HG2	2.17	0.44
1:A:265:ARG:NH2	13:A:2133:HOH:O	2.50	0.44
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.32	0.44
1:A:195:PHE:CB	1:A:221:ILE:HB	2.48	0.44
1:A:198:SER:HA	1:A:224:SER:O	2.18	0.44
1:A:379:ASP:OD1	1:A:381:ARG:HG3	2.18	0.44
1:A:119:GLN:OE1	1:A:149:GLY:HA2	2.17	0.44
1:A:282:TYR:O	1:A:282:TYR:CD2	2.63	0.43
1:A:328:ALA:HA	1:A:434:MET:HE3	2.00	0.43
1:A:452:ARG:C	1:A:454:ASP:H	2.23	0.42
1:A:267:LYS:HA	1:A:267:LYS:HD3	1.86	0.42
1:A:304:ASP:HB3	13:A:2017:HOH:O	2.19	0.42
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.50	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.55	0.41
11:A:1562:NAG:C8	13:A:2283:HOH:O	2.68	0.41
1:A:286:LEU:HD22	1:A:397:ASN:CG	2.40	0.41
1:A:508:THR:HG22	1:A:508:THR:O	2.20	0.41
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.94	0.41
1:A:40:ARG:NE	1:A:40:ARG:H	2.15	0.41
1:A:504:ASN:OD1	1:A:506:GLU:HG3	2.21	0.41
1:A:209:LEU:HD22	1:A:312:PHE:HB3	2.01	0.41
1:A:334:ALA:HB2	1:A:357:PHE:HE2	1.86	0.41
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.89	0.41
1:A:268:ASP:O	1:A:269:PRO:C	2.57	0.41
1:A:50:THR:O	1:A:51:LYS:CB	2.68	0.41
1:A:339:LYS:O	1:A:431:PRO:HG3	2.20	0.40
1:A:268:ASP:HB2	1:A:269:PRO:CD	2.51	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)
8:A:1537:CA:CA	8:A:1537:CA:CA[5_556]	1.55	0.65

## 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%)	499 (95%)	25 (5%)	3 (1%)	30 36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	361	VAL
1	A	379	ASP

### 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%)	428 (94%)	27 (6%)	24 32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	40	ARG

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Mol	Chain	Res	Type
1	A	50	THR
1	A	138	ARG
1	A	156	LEU
1	A	195	PHE
1	A	198	SER
1	A	237	TYR
1	A	262	LYS
1	A	270	GLN
1	A	274	LEU
1	A	282	TYR
1	A	348	LYS
1	A	355	LYS
1	A	361	VAL
1	A	363	GLU
1	A	367	GLU
1	A	378	ASP
1	A	387	GLU
1	A	428	LEU
1	A	454	ASP
1	A	471	TRP
1	A	495	SER
1	A	509	ARG
1	A	511	MET
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	289	ASN
1	A	517	GLN
1	A	518	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

9 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	$\# Z  > 2$
9	NAG	A	1554	1,9	14,14,15	0.89	1 (7%)	15,19,21	2.17	4 (26%)
9	NAG	A	1555	9	14,14,15	0.68	0	15,19,21	2.09	3 (20%)
9	FUL	A	1556	9	10,10,11	1.27	1 (10%)	14,14,16	3.40	8 (57%)
10	NAG	A	1557	1,10	14,14,15	0.95	0	15,19,21	1.82	4 (26%)
10	FUL	A	1558	10	10,10,11	1.01	1 (10%)	14,14,16	3.81	7 (50%)
10	NAG	A	1559	10	14,14,15	0.76	0	15,19,21	2.38	6 (40%)
12	NAG	A	1563	1,12	14,14,15	0.77	0	15,19,21	2.76	5 (33%)
12	NAG	A	1564	12	14,14,15	1.11	1 (7%)	15,19,21	1.16	2 (13%)
12	FUC	A	1565	12	10,10,11	0.85	0	14,14,16	1.80	5 (35%)

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
9	NAG	A	1554	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1555	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1556	9	-	0/0/17/20	0/1/1/1
10	NAG	A	1557	1,10	-	0/6/23/26	0/1/1/1
10	FUL	A	1558	10	-	0/0/17/20	0/1/1/1
10	NAG	A	1559	10	-	0/6/23/26	0/1/1/1
12	NAG	A	1563	1,12	-	0/6/23/26	0/1/1/1
12	NAG	A	1564	12	-	0/6/23/26	0/1/1/1
12	FUC	A	1565	12	-	0/0/17/20	0/1/1/1

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1558	FUL	O5-C1	-2.52	1.39	1.43
9	A	1554	NAG	O5-C1	-2.29	1.39	1.43
9	A	1556	FUL	C2-C3	2.18	1.55	1.52
12	A	1564	NAG	C1-C2	3.31	1.57	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1558	FUL	C1-O5-C5	-8.53	99.20	112.38
9	A	1556	FUL	C1-C2-C3	-8.38	99.63	109.54
10	A	1558	FUL	C1-C2-C3	-8.18	99.87	109.54
9	A	1556	FUL	C1-O5-C5	-5.47	103.93	112.38
9	A	1555	NAG	C3-C2-N2	-5.12	98.31	110.56
9	A	1556	FUL	O5-C1-C2	-3.94	104.47	110.86
9	A	1554	NAG	C3-C4-C5	-3.88	103.43	110.20
10	A	1558	FUL	C2-C3-C4	-3.40	105.27	111.04
12	A	1563	NAG	O7-C7-N2	-2.77	116.21	121.86
10	A	1558	FUL	O4-C4-C5	-2.63	103.66	109.84
10	A	1557	NAG	C1-O5-C5	-2.59	108.96	112.25
12	A	1563	NAG	O7-C7-C8	-2.41	117.63	122.06
10	A	1559	NAG	C4-C3-C2	-2.40	107.50	111.23
10	A	1559	NAG	C2-N2-C7	-2.35	120.03	123.04
10	A	1559	NAG	O7-C7-C8	-2.04	118.32	122.06
12	A	1564	NAG	O5-C5-C6	2.04	111.76	107.35
10	A	1559	NAG	C6-C5-C4	2.10	118.19	113.02
9	A	1556	FUL	C6-C5-C4	2.13	117.28	113.08
10	A	1557	NAG	O3-C3-C4	2.18	115.24	110.34
12	A	1565	FUC	C1-C2-C3	2.20	112.15	109.54
12	A	1564	NAG	O4-C4-C3	2.24	115.39	110.34
9	A	1556	FUL	C2-C3-C4	2.35	115.04	111.04
10	A	1558	FUL	O2-C2-C3	2.40	114.95	110.12
12	A	1565	FUC	O5-C5-C4	2.42	113.72	109.53
12	A	1565	FUC	O4-C4-C5	2.43	115.55	109.84
12	A	1565	FUC	C6-C5-C4	2.46	117.92	113.08
9	A	1554	NAG	C6-C5-C4	2.76	119.82	113.02
10	A	1557	NAG	C6-C5-C4	2.77	119.84	113.02
9	A	1556	FUL	C3-C4-C5	2.86	114.55	109.72
12	A	1565	FUC	O3-C3-C4	2.92	116.91	110.34
9	A	1554	NAG	O6-C6-C5	3.04	121.38	111.33
10	A	1557	NAG	O5-C5-C6	3.09	114.04	107.35
9	A	1556	FUL	O2-C2-C3	3.19	116.54	110.12
10	A	1558	FUL	O3-C3-C2	3.28	115.92	110.00
9	A	1555	NAG	C2-N2-C7	3.61	127.68	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1555	NAG	C4-C3-C2	3.70	116.98	111.23
9	A	1556	FUL	O5-C5-C6	3.89	112.56	106.13
10	A	1559	NAG	C3-C2-N2	4.42	121.14	110.56
9	A	1554	NAG	C2-N2-C7	4.45	128.76	123.04
10	A	1558	FUL	C3-C4-C5	4.49	117.28	109.72
12	A	1563	NAG	C1-O5-C5	4.49	117.95	112.25
12	A	1563	NAG	C8-C7-N2	5.24	126.14	116.11
10	A	1559	NAG	C1-O5-C5	6.07	119.95	112.25
12	A	1563	NAG	C2-N2-C7	6.35	131.19	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1554	NAG	1	0
10	A	1558	FUL	1	0

## 5.6 Ligand geometry

Of 34 ligands modelled in this entry, 21 are unknown and 8 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	DEP	A	1530	1	2,7,7	0.97	0	2,7,7	1.06	0
4	SO4	A	1531	-	4,4,4	0.46	0	6,6,6	0.66	0
11	NAG	A	1560	1	14,14,15	0.88	0	15,19,21	1.78	3 (20%)
11	NAG	A	1561	1	14,14,15	0.86	0	15,19,21	1.41	3 (20%)
11	NAG	A	1562	1	14,14,15	0.56	0	15,19,21	2.46	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
3	DEP	A	1530	1	-	0/2/6/6	0/0/0/0
4	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
11	NAG	A	1560	1	-	0/6/23/26	0/1/1/1
11	NAG	A	1561	1	-	0/6/23/26	0/1/1/1
11	NAG	A	1562	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1561	NAG	O7-C7-C8	-2.32	117.81	122.06
11	A	1560	NAG	C8-C7-N2	2.22	120.35	116.11
11	A	1562	NAG	C2-N2-C7	2.36	126.08	123.04
11	A	1560	NAG	C1-O5-C5	2.49	115.41	112.25
11	A	1561	NAG	C4-C3-C2	2.56	115.21	111.23
11	A	1561	NAG	C1-O5-C5	2.67	115.64	112.25
11	A	1560	NAG	O5-C5-C6	4.74	117.60	107.35
11	A	1562	NAG	C1-O5-C5	8.36	122.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1530	DEP	1	0
11	A	1562	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	527/529 (99%)	0.15	35 (6%)	22 29	22, 37, 68, 95	3 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	5.7
1	A	378	ASP	4.9
1	A	282	TYR	4.8
1	A	379	ASP	4.2
1	A	453	ARG	3.8
1	A	50	THR	3.7
1	A	3	ASP	3.6
1	A	255	GLU	3.5
1	A	452	ARG	3.4
1	A	377	VAL	3.1
1	A	393	VAL	3.0
1	A	110	LEU	3.0
1	A	455	GLN	3.0
1	A	281	PRO	2.8
1	A	141	VAL	2.7
1	A	54	ASP	2.6
1	A	318	LEU	2.6
1	A	342	ASN	2.6
1	A	221	ILE	2.5
1	A	51	LYS	2.4
1	A	286	LEU	2.4
1	A	55	ILE	2.4
1	A	193	THR	2.4
1	A	360	GLY	2.3
1	A	195	PHE	2.3
1	A	109	VAL	2.3
1	A	256	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	475	ALA	2.2
1	A	222	LEU	2.2
1	A	111	ILE	2.1
1	A	113	ILE	2.0
1	A	22	GLY	2.0
1	A	278	PHE	2.0
1	A	474	PHE	2.0
1	A	471	TRP	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](#)

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
10	FUL	A	1558	10/11	0.80	0.28	2.51	31,34,40,41	10
12	FUC	A	1565	10/11	0.84	0.24	0.93	56,61,64,66	0
9	NAG	A	1554	14/15	0.95	0.14	-0.19	42,51,65,68	0
10	NAG	A	1559	14/15	0.85	0.38	-	81,86,88,88	0
9	NAG	A	1555	14/15	0.88	0.34	-	74,83,87,88	0
12	NAG	A	1563	14/15	0.88	0.32	-	49,61,71,76	0
9	FUL	A	1556	10/11	0.88	0.30	-	71,73,75,76	0
10	NAG	A	1557	14/15	0.91	0.21	-	48,60,65,72	0
12	NAG	A	1564	14/15	0.84	0.48	-	64,68,71,71	0

## 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( $\text{\AA}^2$ )	Q<0.9
2	UNX	A	1545	1/1	0.94	0.19	14.24	18,18,18,18	0
2	UNX	A	1551	1/1	0.91	0.25	3.23	43,43,43,43	0
2	UNX	A	1539	1/1	0.96	0.22	3.03	17,17,17,17	0
2	UNX	A	1546	1/1	0.95	0.16	2.35	26,26,26,26	0
2	UNX	A	1541	1/1	0.73	0.22	0.98	23,23,23,23	0
2	UNX	A	1538	1/1	0.96	0.15	0.59	14,14,14,14	0
3	DEP	A	1530	8/8	0.99	0.16	-0.74	26,29,31,34	0
5	CL	A	1534	1/1	0.97	0.22	-	62,62,62,62	0
2	UNX	A	1568	1/1	0.91	0.07	-	8,8,8,8	0
8	CA	A	1537	1/1	0.99	0.05	-	48,48,48,48	0
5	CL	A	1532	1/1	0.97	0.10	-	64,64,64,64	0
2	UNX	A	1571	1/1	0.93	0.14	-	37,37,37,37	0
2	UNX	A	1572	1/1	0.91	0.09	-	29,29,29,29	0
4	SO4	A	1531	5/5	0.97	0.18	-	38,44,47,48	5
2	UNX	A	1553	1/1	0.92	0.12	-	36,36,36,36	0
2	UNX	A	1540	1/1	0.99	0.11	-	21,21,21,21	0
2	UNX	A	1550	1/1	0.95	0.10	-	22,22,22,22	0
5	CL	A	1566	1/1	0.85	0.10	-	74,74,74,74	0
7	NA	A	1567	1/1	0.78	0.27	-	66,66,66,66	0
11	NAG	A	1562	14/15	0.84	0.44	-	61,66,76,77	9
2	UNX	A	1552	1/1	0.91	0.21	-	37,37,37,37	0
11	NAG	A	1560	14/15	0.75	0.42	-	64,75,77,77	0
11	NAG	A	1561	14/15	0.80	0.25	-	55,65,73,74	0
2	UNX	A	1548	1/1	0.91	0.15	-	16,16,16,16	0
6	BR	A	1535	1/1	1.00	0.09	-	42,42,42,42	0
5	CL	A	1533	1/1	0.99	0.10	-	37,37,37,37	0
2	UNX	A	1549	1/1	0.94	0.16	-	32,32,32,32	0
2	UNX	A	1569	1/1	0.99	0.06	-	37,37,37,37	0
2	UNX	A	1544	1/1	0.83	0.20	-	26,26,26,26	0
2	UNX	A	1547	1/1	0.86	0.18	-	33,33,33,33	0
2	UNX	A	1543	1/1	0.85	0.23	-	29,29,29,29	0
7	NA	A	1536	1/1	0.92	0.60	-	52,52,52,52	0
2	UNX	A	1570	1/1	0.97	0.10	-	2,2,2,2	0
2	UNX	A	1542	1/1	0.98	0.14	-	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.