



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLW
Title : Diethylphosphorylated Butyrylcholinesterase (Nonaged) Obtained By
Reaction With Echothiophate
Authors : Nachon, F.; Asojo, O.A.; Borgstahl, G.E.O.; Masson, P.; Lockridge, O.
Deposited on : 2004-09-30
Resolution : 2.10 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 ⓘ symbol.

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

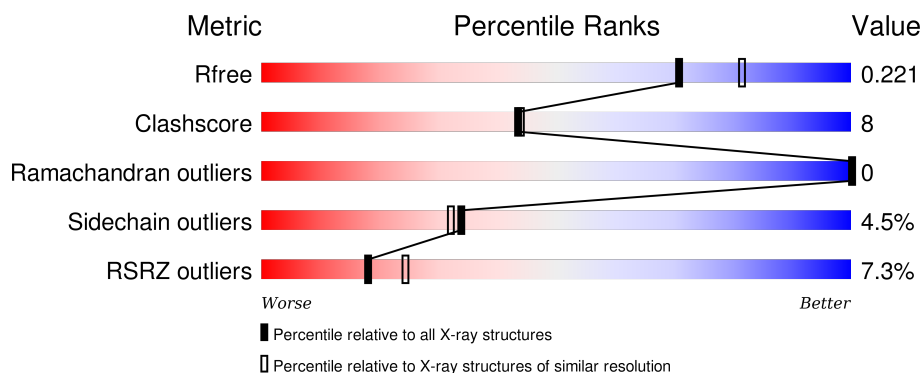
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	

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
3	FUC	A	535	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	A	537	X	-	-	X
5	NAG	A	539	-	-	-	X
6	SO4	A	601	-	-	-	X
6	SO4	A	604	-	-	X	-
7	CL	A	701	-	-	X	-
9	GOL	A	605	-	-	-	X
9	GOL	A	607	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4706 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 BUTYRYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	11	0
			4226	2724	714	771	17			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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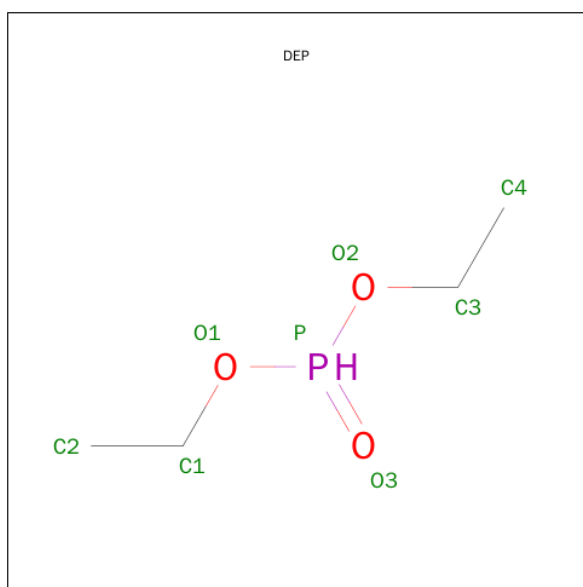
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is DIETHYL PHOSPHONATE (three-letter code: DEP) (formula: C₄H₁₁O₃P).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

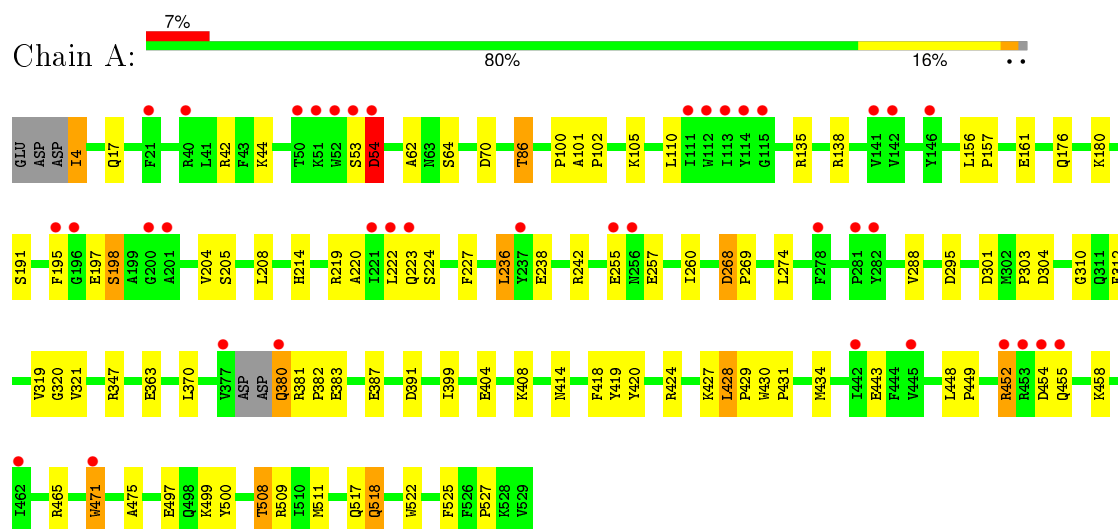
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	290	Total	O	0	0
			290	290		

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: BUTYRYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.46 Å 154.46 Å 127.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 30.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.4 (40.00-2.10) 90.4 (30.34-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.184 , 0.223 0.183 , 0.221	Depositor DCC
R_{free} test set	2222 reflections (5.76%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43695 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, NAG, CL, DEP, FUC, FUL, CSS, 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	0.89	1/4392 (0.0%)	0.85	9/5957 (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
3	A	1	0
4	A	1	0
All	All	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TRP	CB-CG	6.38	1.61	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	295	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	70	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	465	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	198	SER	CA-CB-OG	5.79	126.82	111.20
1	A	391	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	301	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	219	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	54	ASP	CB-CG-OD2	5.61	123.35	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	535	FUC	C1
4	A	537	FUC	C1

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	4226	0	4113	70	0
2	A	38	0	34	0	0
3	A	38	0	34	0	0
4	A	24	0	22	1	0
5	A	42	0	39	0	0
6	A	20	0	0	2	0
7	A	2	0	0	3	0
8	A	8	0	10	0	0
9	A	18	0	24	2	0
10	A	290	0	0	11	2
All	All	4706	0	4276	71	2

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 (71) 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:138[B]:ARG:NH1	10:A:1366:HOH:O	1.89	1.04
1:A:176[B]:GLN:OE1	1:A:180:LYS:HD2	1.60	1.01
1:A:518:GLN:H	1:A:518:GLN:HE21	1.05	0.96
1:A:508:THR:HB	10:A:1170:HOH:O	1.84	0.77
1:A:304:ASP:HB3	10:A:1243:HOH:O	1.91	0.70
1:A:508:THR:CG2	7:A:701:CL:CL	2.79	0.67
1:A:420:TYR:OH	6:A:604:SO4:O2	2.08	0.64
1:A:383:GLU:O	1:A:387:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	10:A:1284:HOH:O	1.99	0.63
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.52	0.63
1:A:62:ALA:O	1:A:86:THR:HG21	2.00	0.62
1:A:508:THR:HG21	7:A:701:CL:CL	2.38	0.61
1:A:238:GLU:O	1:A:242:ARG:HG3	2.00	0.61
1:A:135:ARG:HA	1:A:138[B]:ARG:HH21	1.66	0.60
1:A:135:ARG:O	1:A:138[B]:ARG:NE	2.34	0.60
1:A:508:THR:HG23	7:A:701:CL:CL	2.41	0.58
1:A:227:PHE:CD2	1:A:227:PHE:C	2.76	0.58
1:A:452:ARG:HH21	1:A:458:LYS:HD2	1.67	0.58
6:A:604:SO4:O4	10:A:1325:HOH:O	2.17	0.58
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.38	0.58
1:A:518:GLN:H	1:A:518:GLN:NE2	1.88	0.57
1:A:518:GLN:HE21	1:A:518:GLN:N	1.88	0.56
1:A:191:SER:HB2	4:A:537:FUC:H3	1.88	0.55
1:A:138[A]:ARG:NH2	10:A:1365:HOH:O	1.73	0.55
1:A:138[B]:ARG:NH2	10:A:1334:HOH:O	2.41	0.53
1:A:138[A]:ARG:NH2	10:A:1366:HOH:O	2.31	0.53
1:A:4:ILE:N	1:A:4:ILE:HD12	2.24	0.52
1:A:347:ARG:NH1	1:A:370:LEU:HD21	2.25	0.52
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.40	0.51
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.46	0.51
1:A:404:GLU:HG2	10:A:1241:HOH:O	2.11	0.50
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.47	0.50
1:A:257:GLU:HA	1:A:260:ILE:HD12	1.94	0.50
1:A:44:LYS:NZ	1:A:161:GLU:OE1	2.45	0.49
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.94	0.49
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.95	0.48
1:A:198:SER:HA	1:A:224:SER:O	2.12	0.48
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.48	0.48
1:A:157:PRO:HG3	1:A:236:LEU:HG	1.93	0.48
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.48	0.48
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.47
1:A:431:PRO:HG2	1:A:434:MET:HG3	1.96	0.47
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.30	0.46
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.98	0.46
1:A:522:TRP:O	1:A:527:PRO:HD3	2.16	0.46
1:A:227:PHE:CD2	1:A:303:PRO:HB2	2.51	0.45
1:A:452:ARG:NH2	1:A:458:LYS:HA	2.31	0.45
1:A:176[B]:GLN:OE1	1:A:180:LYS:CD	2.49	0.44
1:A:214[A]:HIS:HE1	10:A:1306:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:O	1:A:54:ASP:HB2	2.17	0.44
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.48	0.44
1:A:135:ARG:HD2	1:A:138[B]:ARG:NH2	2.33	0.44
1:A:64:SER:OG	1:A:86:THR:HG22	2.17	0.44
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.82	0.44
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.82	0.43
1:A:4:ILE:HD11	1:A:17:GLN:HG2	2.00	0.43
1:A:380:GLN:HB3	1:A:381:ARG:H	1.61	0.43
1:A:497:GLU:OE1	1:A:499:LYS:HE3	2.19	0.43
1:A:101:ALA:HA	1:A:102:PRO:C	2.38	0.42
1:A:381:ARG:HA	1:A:382:PRO:HD3	1.92	0.42
1:A:380:GLN:HB2	10:A:1333:HOH:O	2.20	0.42
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.93	0.42
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.02	0.42
1:A:321:VAL:HG11	1:A:399:ILE:HA	2.02	0.42
1:A:404:GLU:OE2	1:A:408:LYS:HE2	2.20	0.41
1:A:443:GLU:OE2	9:A:607:GOL:O3	2.34	0.41
1:A:197:GLU:HA	1:A:223:GLN:O	2.21	0.40
1:A:448:LEU:N	1:A:449:PRO:CD	2.84	0.40
1:A:525:PHE:C	1:A:527:PRO:HD2	2.41	0.40
1:A:288:VAL:HB	9:A:605:GOL:H32	2.03	0.40

All (2) 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)
10:A:1288:HOH:O	10:A:1288:HOH:O[6_556]	1.70	0.50
10:A:1354:HOH:O	10:A:1354:HOH:O[15_545]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/529 (100%)	515 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	459/453 (101%)	437 (95%)	22 (5%)	31	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	54	ASP
1	A	86	THR
1	A	100	PRO
1	A	105	LYS
1	A	156	LEU
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	274	LEU
1	A	363[A]	GLU
1	A	363[B]	GLU
1	A	380	GLN
1	A	428	LEU
1	A	452	ARG
1	A	454	ASP
1	A	455	GLN
1	A	471	TRP
1	A	508	THR
1	A	517[A]	GLN
1	A	517[B]	GLN
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	119	GLN
1	A	172	GLN
1	A	270	GLN
1	A	275	ASN
1	A	455	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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	CSS	A	66	1	4,6,7	0.73	0	3,6,8	2.63	1 (33%)

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	CSS	A	66	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CSS	CB-SG-SD	-4.21	95.68	103.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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
2	NAG	A	530	1,2	14,14,15	0.64	0	15,19,21	1.05	2 (13%)
2	NAG	A	531	2	14,14,15	0.64	0	15,19,21	1.29	1 (6%)
2	FUL	A	532	2	10,10,11	0.81	0	14,14,16	2.55	5 (35%)
3	NAG	A	533	1,3	14,14,15	0.93	1 (7%)	15,19,21	1.80	4 (26%)
3	NAG	A	534	3	14,14,15	0.52	0	15,19,21	2.49	3 (20%)
3	FUC	A	535	3	10,10,11	0.97	0	14,14,16	2.50	5 (35%)
4	NAG	A	536	1,4	14,14,15	0.86	1 (7%)	15,19,21	1.63	5 (33%)
4	FUC	A	537	4	10,10,11	0.96	0	14,14,16	1.96	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
2	NAG	A	530	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	531	2	-	0/6/23/26	0/1/1/1
2	FUL	A	532	2	-	0/0/17/20	0/1/1/1
3	NAG	A	533	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	534	3	-	0/6/23/26	0/1/1/1
3	FUC	A	535	3	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	A	536	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	537	4	1/1/4/5	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)
3	A	533	NAG	O5-C1	-2.11	1.40	1.43
4	A	536	NAG	C1-C2	2.32	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	532	FUL	C1-C2-C3	-6.79	101.51	109.54
3	A	535	FUC	C1-C2-C3	-6.58	101.76	109.54
4	A	537	FUC	C1-C2-C3	-4.06	104.74	109.54
2	A	532	FUL	C1-O5-C5	-3.93	106.30	112.38
3	A	535	FUC	C1-O5-C5	-3.60	106.82	112.38
3	A	535	FUC	O5-C1-C2	-3.27	105.55	110.86
4	A	537	FUC	O5-C1-C2	-2.78	106.35	110.86
4	A	536	NAG	O7-C7-C8	-2.76	116.99	122.06
3	A	534	NAG	O3-C3-C2	-2.17	104.82	109.11
3	A	533	NAG	C3-C2-N2	-2.10	105.53	110.56
4	A	536	NAG	O3-C3-C2	2.00	113.08	109.11
2	A	530	NAG	C1-O5-C5	2.06	114.86	112.25
4	A	536	NAG	O5-C5-C6	2.15	112.00	107.35
3	A	535	FUC	O5-C5-C6	2.19	109.74	106.13
3	A	535	FUC	O2-C2-C1	2.28	113.77	109.21
4	A	537	FUC	O2-C2-C3	2.34	114.83	110.12
2	A	530	NAG	C4-C3-C2	2.35	114.88	111.23
2	A	532	FUL	O2-C2-C1	2.48	114.17	109.21
2	A	532	FUL	O5-C5-C6	2.55	110.35	106.13
2	A	532	FUL	C3-C4-C5	2.63	114.15	109.72
3	A	533	NAG	C2-N2-C7	2.67	126.47	123.04
4	A	536	NAG	C2-N2-C7	2.77	126.60	123.04
4	A	537	FUC	O3-C3-C2	2.80	115.06	110.00
4	A	536	NAG	C8-C7-N2	2.95	121.76	116.11
2	A	531	NAG	C4-C3-C2	3.13	116.09	111.23
3	A	533	NAG	C6-C5-C4	3.70	122.15	113.02
3	A	533	NAG	O6-C6-C5	3.75	123.73	111.33
3	A	534	NAG	C3-C4-C5	4.64	118.28	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	534	NAG	C1-O5-C5	7.36	121.59	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	537	FUC	C1
3	A	535	FUC	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	537	FUC	1	0

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
8	DEP	A	1001	1	2,7,7	0.65	0	2,7,7	0.87	0
5	NAG	A	538	1	14,14,15	0.69	0	15,19,21	1.31	2 (13%)
5	NAG	A	539	1	14,14,15	0.79	0	15,19,21	1.13	1 (6%)
5	NAG	A	540	1	14,14,15	0.55	0	15,19,21	1.04	1 (6%)
6	SO4	A	601	-	4,4,4	0.37	0	6,6,6	0.27	0
6	SO4	A	602	-	4,4,4	0.28	0	6,6,6	0.40	0
6	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.24	0
6	SO4	A	604	-	4,4,4	0.28	0	6,6,6	0.55	0
9	GOL	A	605	-	5,5,5	0.85	0	5,5,5	0.71	0
9	GOL	A	606	-	5,5,5	0.35	0	5,5,5	0.55	0
9	GOL	A	607	-	5,5,5	0.42	0	5,5,5	1.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	DEP	A	1001	1	-	0/2/6/6	0/0/0/0
5	NAG	A	538	1	-	0/6/23/26	0/1/1/1
5	NAG	A	539	1	-	0/6/23/26	0/1/1/1
5	NAG	A	540	1	-	0/6/23/26	0/1/1/1
6	SO4	A	601	-	-	0/0/0/0	0/0/0/0
6	SO4	A	602	-	-	0/0/0/0	0/0/0/0
6	SO4	A	603	-	-	0/0/0/0	0/0/0/0
6	SO4	A	604	-	-	0/0/0/0	0/0/0/0
9	GOL	A	605	-	-	0/4/4/4	0/0/0/0
9	GOL	A	606	-	-	0/4/4/4	0/0/0/0
9	GOL	A	607	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	538	NAG	O7-C7-C8	-2.31	117.82	122.06
5	A	540	NAG	C1-O5-C5	2.09	114.90	112.25
5	A	539	NAG	O7-C7-N2	2.73	127.44	121.86
5	A	538	NAG	O5-C5-C6	3.33	114.56	107.35

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
6	A	604	SO4	2	0
9	A	605	GOL	1	0
9	A	607	GOL	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, 95th 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	523/529 (98%)	0.10	38 (7%) 18 24	25, 38, 59, 77	18 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	7.1
1	A	281	PRO	4.9
1	A	452	ARG	3.8
1	A	54	ASP	3.8
1	A	282	TYR	3.8
1	A	278	PHE	3.8
1	A	237	TYR	3.7
1	A	453	ARG	3.4
1	A	221	ILE	3.3
1	A	255	GLU	3.1
1	A	52	TRP	2.9
1	A	113	ILE	2.9
1	A	454	ASP	2.9
1	A	40	ARG	2.8
1	A	445	VAL	2.7
1	A	115	GLY	2.6
1	A	112	TRP	2.6
1	A	222	LEU	2.6
1	A	195	PHE	2.5
1	A	455	GLN	2.5
1	A	462	ILE	2.4
1	A	196	GLY	2.4
1	A	442	ILE	2.4
1	A	21	PHE	2.3
1	A	201	ALA	2.3
1	A	111	ILE	2.3
1	A	53	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	VAL	2.2
1	A	256	ASN	2.2
1	A	50	THR	2.1
1	A	380	GLN	2.1
1	A	146	TYR	2.1
1	A	223	GLN	2.1
1	A	51	LYS	2.1
1	A	114	TYR	2.1
1	A	471	TRP	2.0
1	A	142	VAL	2.0
1	A	200	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
1	CSS	A	66	7/8	0.97	0.07	-	34,35,41,49	0

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, 95th 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
4	FUC	A	537	10/11	0.87	0.25	2.67	63,64,65,66	5
2	FUL	A	532	10/11	0.94	0.28	0.72	71,73,73,73	0
3	NAG	A	533	14/15	0.95	0.11	-0.46	48,56,62,67	0
4	NAG	A	536	14/15	0.81	0.21	-	59,66,69,70	0
3	NAG	A	534	14/15	0.85	0.19	-	68,73,76,76	0
3	FUC	A	535	10/11	0.91	0.20	-	67,70,71,73	0
2	NAG	A	530	14/15	0.90	0.34	-	72,78,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	531	14/15	0.82	0.43	-	83,85,86,87	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, 95th 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(\AA^2)	Q<0.9
5	NAG	A	539	14/15	0.69	0.28	12.44	58,70,71,72	3
9	GOL	A	607	6/6	0.88	0.20	2.89	50,55,56,57	0
6	SO4	A	601	5/5	0.99	0.13	2.31	52,53,55,56	0
9	GOL	A	605	6/6	0.87	0.15	2.11	49,51,51,52	0
8	DEP	A	1001	8/8	0.99	0.20	0.68	32,34,40,44	0
6	SO4	A	602	5/5	0.96	0.15	0.55	44,45,46,47	5
9	GOL	A	606	6/6	0.96	0.08	-1.01	43,51,54,59	0
6	SO4	A	604	5/5	0.93	0.25	-	40,41,47,47	5
5	NAG	A	540	14/15	0.80	0.37	-	91,95,97,97	0
7	CL	A	702	1/1	0.86	0.07	-	82,82,82,82	0
7	CL	A	701	1/1	0.95	0.12	-	64,64,64,64	0
5	NAG	A	538	14/15	0.81	0.36	-	73,78,79,80	0
6	SO4	A	603	5/5	0.88	0.17	-	50,51,53,53	5

6.5 Other polymers [i](#)

There are no such residues in this entry.