



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XLU
Title : X-Ray Structure Of Di-Isopropyl-Phosphoro-Fluoridate (Dfp) Inhibited Butyrylcholinesterase after Aging
Authors : Nachon, F.; Asojo, O.A.; Borgstahl, G.E.O.; Masson, P.; Lockridge, O.
Deposited on : 2004-09-30
Resolution : 2.20 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

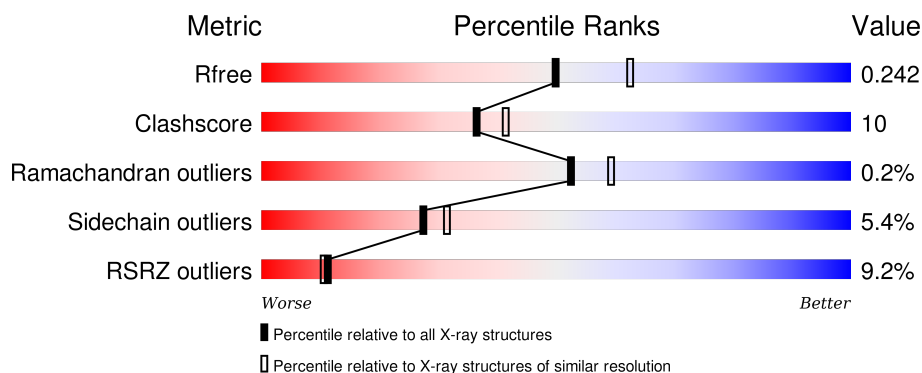
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	<div> <div>9%</div> <div>79%</div> <div>17%</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
4	NAG	A	537	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	A	701	-	-	X	-
8	GOL	A	604	-	-	-	X
8	GOL	A	607	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4685 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	10	0
			4274	2756	722	779	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 (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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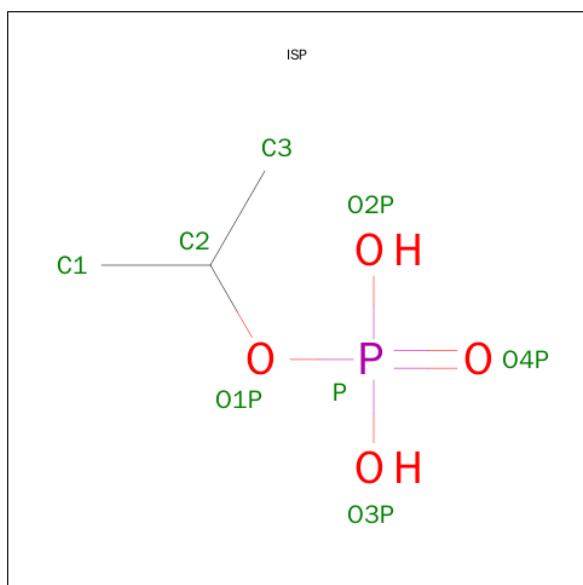
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is PHOSPHORYLISOPROPANE (three-letter code: ISP) (formula: C₃H₉O₄P).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	255	Total	O	0	0
			255	255		

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.50 Å 154.50 Å 127.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 30.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.3 (40.00-2.20) 90.3 (30.36-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.193 , 0.242 0.191 , 0.242	Depositor DCC
R_{free} test set	1911 reflections (5.67%)	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37851 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, ISP, SO4, FUL, CSS

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	0.84	1/4387 (0.0%)	0.82	11/5950 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	PHE	CE2-CZ	5.18	1.47	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	87[A]	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	87[B]	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	295	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	391	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	324	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	268	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	301	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	297	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	54	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	465	ARG	NE-CZ-NH2	-5.03	117.78	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	4156	83	0
2	A	38	0	34	1	0
3	A	28	0	25	0	0
4	A	42	0	39	0	0
5	A	15	0	0	0	0
6	A	2	0	0	2	0
7	A	7	0	7	0	0
8	A	24	0	32	5	0
9	A	255	0	0	16	0
All	All	4685	0	4293	83	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 10.

All (83) 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:518:GLN:H	1:A:518:GLN:HE21	1.05	0.91
1:A:176[A]:GLN:NE2	1:A:180:LYS:HD2	1.92	0.85
1:A:452:ARG:HH22	1:A:458:LYS:HA	1.51	0.75
1:A:427:LYS:HB2	8:A:607:GOL:H32	1.72	0.72
1:A:87[B]:ASP:OD1	9:A:1317:HOH:O	2.08	0.71
1:A:62:ALA:O	1:A:86:THR:HG21	1.91	0.71
1:A:518:GLN:H	1:A:518:GLN:NE2	1.86	0.70
1:A:176[A]:GLN:HE22	1:A:180:LYS:HD2	1.55	0.70
1:A:367[B]:GLU:OE1	9:A:1350:HOH:O	2.12	0.68
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.77	0.67
1:A:383:GLU:O	1:A:387:GLU:HG3	1.94	0.66
1:A:506:GLU:HG3	1:A:507:SER:H	1.61	0.66
1:A:452:ARG:NH2	1:A:458:LYS:HA	2.15	0.62
1:A:209:LEU:HD11	1:A:227[A]:PHE:CZ	2.36	0.61
1:A:198:SER:HA	1:A:224:SER:O	2.02	0.60
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.38	0.59
1:A:4:ILE:N	1:A:4:ILE:HD12	2.17	0.58
1:A:304:ASP:HB3	9:A:1246:HOH:O	2.03	0.58
1:A:238:GLU:O	1:A:242:ARG:HG3	2.05	0.57
1:A:408:LYS:HE3	9:A:1270:HOH:O	2.04	0.57
1:A:77:HIS:ND1	9:A:1337:HOH:O	2.33	0.56
1:A:518:GLN:HE21	1:A:518:GLN:N	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.89	0.54
1:A:323:LYS:HE2	9:A:1322:HOH:O	2.07	0.54
1:A:227[B]:PHE:CE2	1:A:303:PRO:HB2	2.42	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.43	0.53
1:A:508:THR:HG23	6:A:701:CL:CL	2.45	0.53
1:A:399:ILE:HD11	9:A:1309:HOH:O	2.08	0.52
1:A:319:VAL:O	1:A:418:PHE:HA	2.10	0.52
1:A:443:GLU:OE2	8:A:607:GOL:O3	2.28	0.51
1:A:508:THR:HB	9:A:1173:HOH:O	2.10	0.51
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.92	0.51
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.93	0.51
1:A:427:LYS:CB	8:A:607:GOL:H32	2.39	0.51
1:A:427:LYS:C	8:A:607:GOL:H32	2.31	0.51
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.42	0.50
1:A:257:GLU:HA	1:A:260:ILE:HD12	1.93	0.50
1:A:456:TYR:HB2	9:A:1335:HOH:O	2.13	0.49
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.42	0.49
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.78	0.49
1:A:256:ASN:ND2	9:A:1282:HOH:O	2.39	0.48
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.66	0.47
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.96	0.47
1:A:348:LYS:HD2	1:A:351:GLN:OE1	2.14	0.47
1:A:227[B]:PHE:O	1:A:232:ALA:HB3	2.14	0.47
1:A:227[B]:PHE:CD2	1:A:303:PRO:HB2	2.49	0.47
1:A:255:GLU:CD	1:A:255:GLU:H	2.17	0.47
1:A:227[B]:PHE:C	1:A:227[B]:PHE:CD2	2.89	0.46
1:A:64:SER:OG	1:A:86:THR:HG22	2.16	0.46
1:A:157:PRO:HD2	9:A:1344:HOH:O	2.15	0.46
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.98	0.46
1:A:339:LYS:O	1:A:431:PRO:HG3	2.17	0.45
1:A:157:PRO:CD	9:A:1344:HOH:O	2.64	0.45
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.52	0.44
1:A:508:THR:CG2	9:A:1173:HOH:O	2.65	0.44
1:A:508:THR:CG2	6:A:701:CL:CL	3.03	0.44
1:A:156:LEU:CD1	1:A:243:THR:HG21	2.46	0.44
1:A:253:SER:O	1:A:254:ARG:HD3	2.18	0.44
1:A:176[A]:GLN:NE2	1:A:180:LYS:CD	2.74	0.43
1:A:4:ILE:HD11	1:A:17:GLN:HG2	1.99	0.43
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.34	0.43
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.99	0.43
1:A:522:TRP:O	1:A:527:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:HB2	9:A:1340:HOH:O	2.18	0.43
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.91	0.43
1:A:236:LEU:HD12	9:A:1284:HOH:O	2.18	0.43
1:A:448:LEU:N	1:A:449:PRO:CD	2.82	0.43
1:A:321:VAL:HG11	1:A:399:ILE:HA	2.00	0.42
1:A:14:ARG:HB2	1:A:55:ILE:HG21	2.01	0.42
1:A:255:GLU:CD	1:A:255:GLU:N	2.73	0.42
1:A:454:ASP:O	1:A:455:GLN:HB2	2.20	0.42
1:A:99:ILE:HA	1:A:100:PRO:HD3	1.94	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.55	0.41
1:A:249:LEU:HG	2:A:532:FUL:H62	2.02	0.41
1:A:508:THR:CB	9:A:1173:HOH:O	2.68	0.41
1:A:428:LEU:HA	8:A:607:GOL:H31	2.03	0.41
1:A:176[A]:GLN:HE21	1:A:180:LYS:HD2	1.80	0.41
1:A:282:TYR:HD1	1:A:359:PRO:HB3	1.86	0.41
1:A:221:ILE:C	1:A:222:LEU:HD12	2.41	0.41
1:A:381:ARG:HA	1:A:382:PRO:HD3	1.96	0.41
1:A:62:ALA:O	1:A:86:THR:CG2	2.65	0.40
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.83	0.40
1:A:161:GLU:HB3	1:A:261:ILE:HG21	2.03	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	529/529 (100%)	507 (96%)	21 (4%)	1 (0%)	52 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	GLU

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	458/453 (101%)	432 (94%)	26 (6%)	25	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	50	THR
1	A	54	ASP
1	A	86	THR
1	A	105	LYS
1	A	156	LEU
1	A	176[A]	GLN
1	A	176[B]	GLN
1	A	195	PHE
1	A	236	LEU
1	A	240	ARG
1	A	254	ARG
1	A	255	GLU
1	A	282	TYR
1	A	287	SER
1	A	299	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	471	TRP
1	A	496	THR
1	A	508	THR
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	119	GLN
1	A	172	GLN
1	A	311	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	0.58	0	3,6,8	3.03	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	-5.00	94.14	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

5 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	0.52	0	15,19,21	1.04	1 (6%)
2	NAG	A	531	2	14,14,15	0.51	0	15,19,21	1.41	2 (13%)
2	FUL	A	532	2	10,10,11	0.70	0	14,14,16	2.30	5 (35%)
3	NAG	A	533	1,3	14,14,15	0.77	0	15,19,21	1.97	4 (26%)
3	NAG	A	534	3	14,14,15	0.51	0	15,19,21	2.41	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	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
3	NAG	A	534	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	532	FUL	C1-C2-C3	-6.39	101.99	109.54
3	A	533	NAG	C3-C2-N2	-3.04	103.27	110.56
2	A	532	FUL	C1-O5-C5	-2.77	108.10	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	531	NAG	C4-C3-C2	-2.31	107.64	111.23
2	A	532	FUL	O5-C1-C2	-2.01	107.59	110.86
2	A	532	FUL	O2-C2-C1	2.27	113.76	109.21
3	A	533	NAG	C8-C7-N2	2.37	120.64	116.11
2	A	532	FUL	O5-C5-C6	2.48	110.22	106.13
3	A	533	NAG	C1-O5-C5	2.88	115.91	112.25
2	A	530	NAG	C1-O5-C5	2.89	115.92	112.25
2	A	531	NAG	C1-O5-C5	3.11	116.20	112.25
3	A	534	NAG	C3-C4-C5	4.80	118.56	110.20
3	A	533	NAG	C2-N2-C7	4.81	129.22	123.04
3	A	534	NAG	C1-O5-C5	6.83	120.91	112.25

There are no chirality outliers.

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
2	A	532	FUL	1	0

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	ISP	A	1001	-	3,6,7	1.62	1 (33%)	3,7,10	0.90	0
4	NAG	A	535	1	14,14,15	0.74	1 (7%)	15,19,21	1.45	3 (20%)
4	NAG	A	536	1	14,14,15	0.58	0	15,19,21	1.31	2 (13%)
4	NAG	A	537	1	14,14,15	0.71	0	15,19,21	1.12	2 (13%)
5	SO4	A	601	-	4,4,4	0.34	0	6,6,6	0.10	0
5	SO4	A	602	-	4,4,4	0.28	0	6,6,6	0.15	0
5	SO4	A	603	-	4,4,4	0.18	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	604	-	5,5,5	0.40	0	5,5,5	0.55	0
8	GOL	A	605	-	5,5,5	0.37	0	5,5,5	0.51	0
8	GOL	A	606	-	5,5,5	0.31	0	5,5,5	0.60	0
8	GOL	A	607	-	5,5,5	0.40	0	5,5,5	1.19	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
7	ISP	A	1001	-	-	0/2/4/5	0/0/0/0
4	NAG	A	535	1	-	0/6/23/26	0/1/1/1
4	NAG	A	536	1	-	0/6/23/26	0/1/1/1
4	NAG	A	537	1	-	0/6/23/26	0/1/1/1
5	SO4	A	601	-	-	0/0/0/0	0/0/0/0
5	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	SO4	A	603	-	-	0/0/0/0	0/0/0/0
8	GOL	A	604	-	-	0/4/4/4	0/0/0/0
8	GOL	A	605	-	-	0/4/4/4	0/0/0/0
8	GOL	A	606	-	-	0/4/4/4	0/0/0/0
8	GOL	A	607	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	ISP	O1P-C2	-2.68	1.42	1.46
4	A	535	NAG	C1-C2	2.01	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	535	NAG	O7-C7-C8	-2.24	117.95	122.06
4	A	536	NAG	C4-C3-C2	-2.15	107.89	111.23
4	A	537	NAG	O7-C7-C8	-2.04	118.32	122.06
4	A	537	NAG	O7-C7-N2	2.01	125.96	121.86
4	A	535	NAG	C2-N2-C7	2.16	125.81	123.04
4	A	535	NAG	C8-C7-N2	2.74	121.36	116.11
4	A	536	NAG	O5-C5-C6	3.02	113.88	107.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	607	GOL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.30	48 (9%) 11 10	29, 42, 64, 78	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	5.8
1	A	377	VAL	5.2
1	A	281	PRO	4.6
1	A	282	TYR	4.5
1	A	278	PHE	4.4
1	A	51	LYS	4.4
1	A	452	ARG	4.4
1	A	453	ARG	4.3
1	A	221	ILE	3.8
1	A	40	ARG	3.7
1	A	113	ILE	3.7
1	A	4	ILE	3.4
1	A	52	TRP	3.3
1	A	462	ILE	3.2
1	A	112	TRP	3.1
1	A	255	GLU	3.1
1	A	222	LEU	3.0
1	A	442	ILE	3.0
1	A	458	LYS	3.0
1	A	223	GLN	3.0
1	A	224	SER	3.0
1	A	114	TYR	2.9
1	A	200	GLY	2.8
1	A	376	TRP	2.8
1	A	50	THR	2.7
1	A	471	TRP	2.7
1	A	196	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	2.7
1	A	258	THR	2.7
1	A	195	PHE	2.6
1	A	321	VAL	2.6
1	A	115	GLY	2.6
1	A	141	VAL	2.5
1	A	455	GLN	2.5
1	A	201	ALA	2.4
1	A	54	ASP	2.3
1	A	167	GLY	2.3
1	A	319	VAL	2.3
1	A	274	LEU	2.3
1	A	146	TYR	2.3
1	A	202	ALA	2.2
1	A	454	ASP	2.2
1	A	259	GLU	2.2
1	A	446	PHE	2.2
1	A	142	VAL	2.2
1	A	445	VAL	2.2
1	A	342	ASN	2.1
1	A	240	ARG	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	0.98	0.05	-	37,39,45,54	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(\AA^2)	Q<0.9
2	FUL	A	532	10/11	0.96	0.34	1.42	79,80,81,81	0
3	NAG	A	533	14/15	0.92	0.11	-0.35	56,61,66,67	0
2	NAG	A	531	14/15	0.87	0.43	-	79,86,88,88	0
3	NAG	A	534	14/15	0.84	0.22	-	73,77,81,82	0
2	NAG	A	530	14/15	0.86	0.35	-	77,81,86,87	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
4	NAG	A	537	14/15	0.73	0.27	9.08	63,75,80,80	0
8	GOL	A	607	6/6	0.92	0.29	4.55	55,59,60,61	0
8	GOL	A	604	6/6	0.84	0.18	3.89	57,62,63,68	0
8	GOL	A	605	6/6	0.92	0.22	0.26	54,56,58,59	0
7	ISP	A	1001	7/8	0.96	0.17	-0.34	47,55,56,58	0
5	SO4	A	602	5/5	0.97	0.10	-0.94	46,46,48,49	5
8	GOL	A	606	6/6	0.98	0.07	-1.54	49,54,57,62	0
4	NAG	A	536	14/15	0.81	0.33	-	72,76,79,79	0
5	SO4	A	603	5/5	0.92	0.12	-	52,55,57,57	5
6	CL	A	702	1/1	0.93	0.25	-	73,73,73,73	0
5	SO4	A	601	5/5	0.98	0.10	-	57,58,59,60	0
6	CL	A	701	1/1	0.98	0.21	-	63,63,63,63	0
4	NAG	A	535	14/15	0.86	0.25	-	62,68,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.