



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2018 – 12:36 AM EST

PDB ID : 4B83
Title : Mus musculus Acetylcholinesterase in complex with N-(2-Diethylamino- ethyl)-3-methoxy-benzenesulfonamide
Authors : Andersson, C.D.; Forsgren, N.; Akfur, C.; Allgardsson, A.; Berg, L.; Qian, W.; Ekstrom, F.; Linusson, A.
Deposited on : 2012-08-24
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

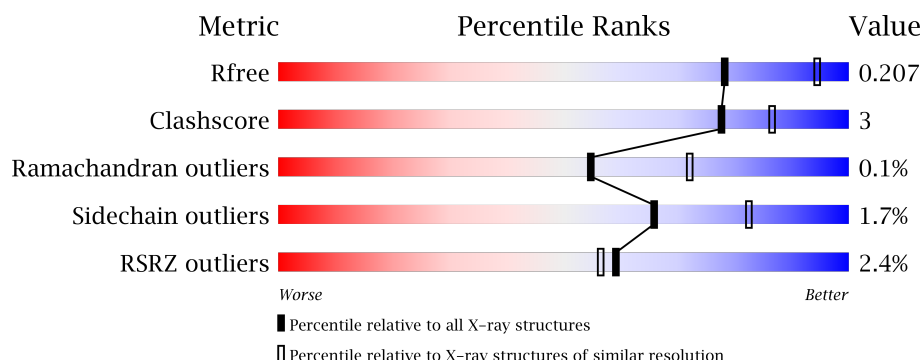
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	548	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	B	548	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </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
2	B3V	A	1543	-	-	-	X
3	EDO	A	1552	-	-	-	X
3	EDO	A	1555	-	-	-	X
3	EDO	B	1543	-	-	-	X
4	NAG	A	1546	-	-	-	X
4	NAG	B	1546	-	-	-	X
5	PEG	A	1548	-	-	-	X
5	PEG	B	1547	-	-	-	X
7	PE8	A	1556	-	-	-	X
8	PG4	B	1552	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8975 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

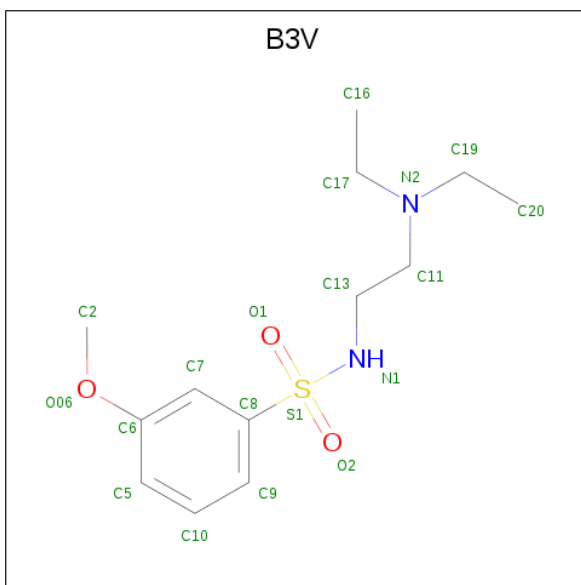
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	2	0
			4196	2693	728	761	14			
1	B	533	Total	C	N	O	S	0	4	0
			4177	2683	720	760	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLU	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is N-[2-(diethylamino)ethyl]-3-methoxy-benzenesulfonamide (three-letter code: B3V) (formula: C₁₃H₂₂N₂O₃S).



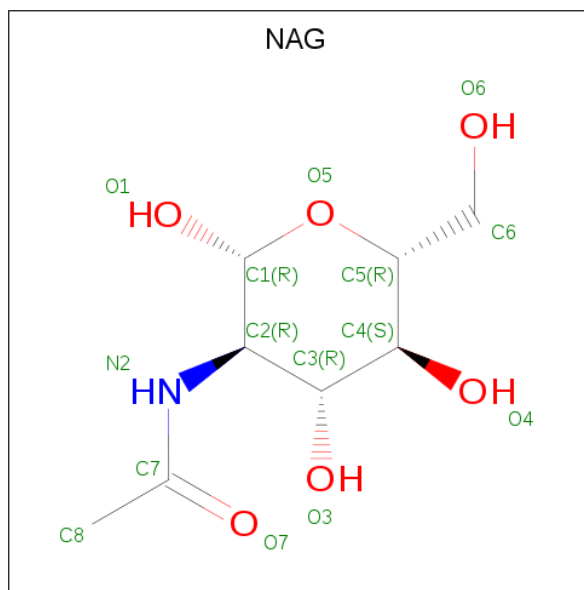
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



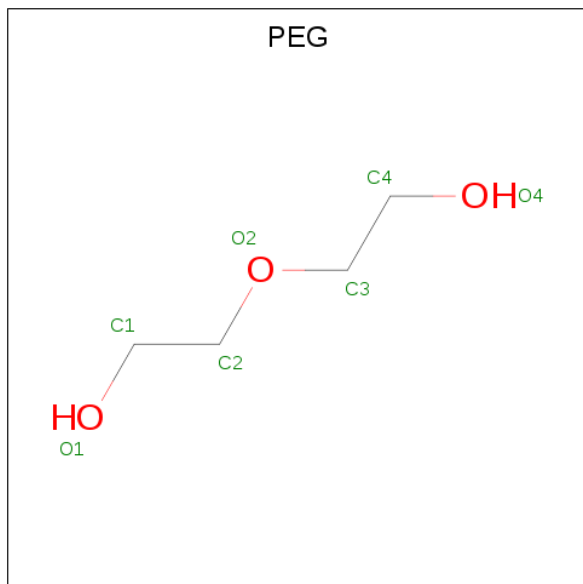
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



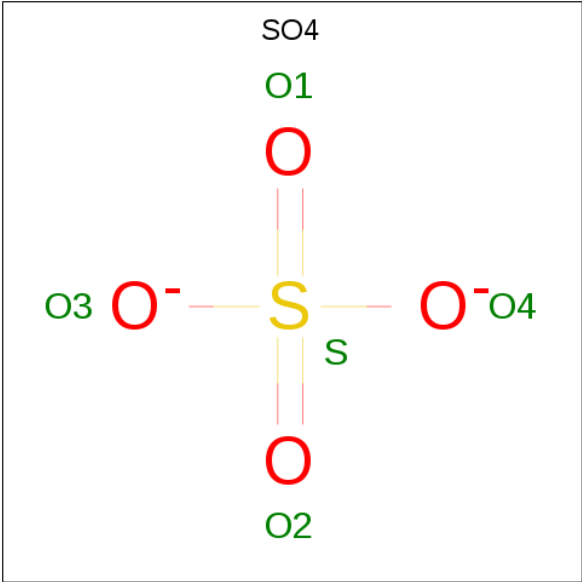
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



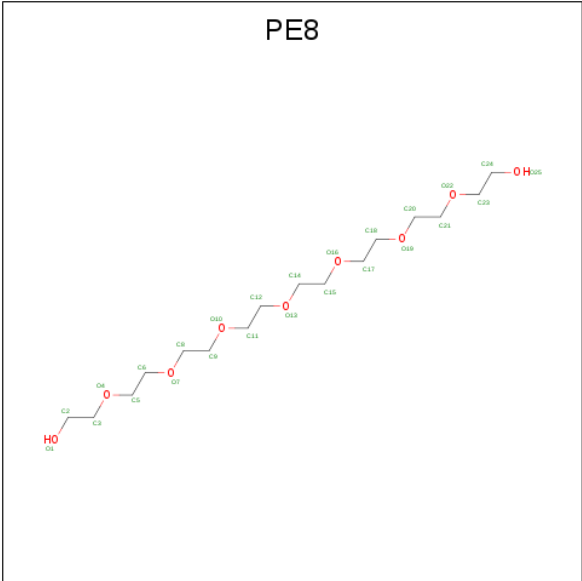
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



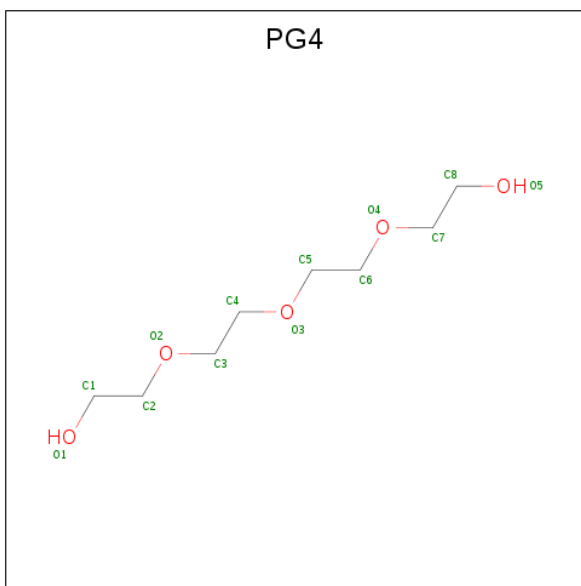
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

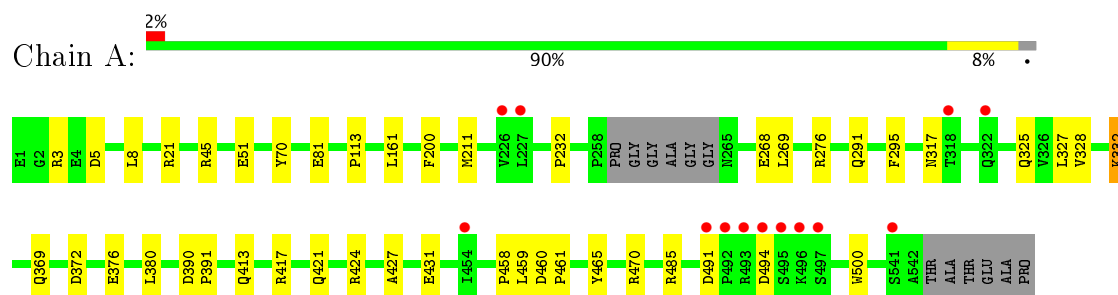
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	212	Total	O	0	0
			212	212		
9	B	162	Total	O	0	0
			162	162		

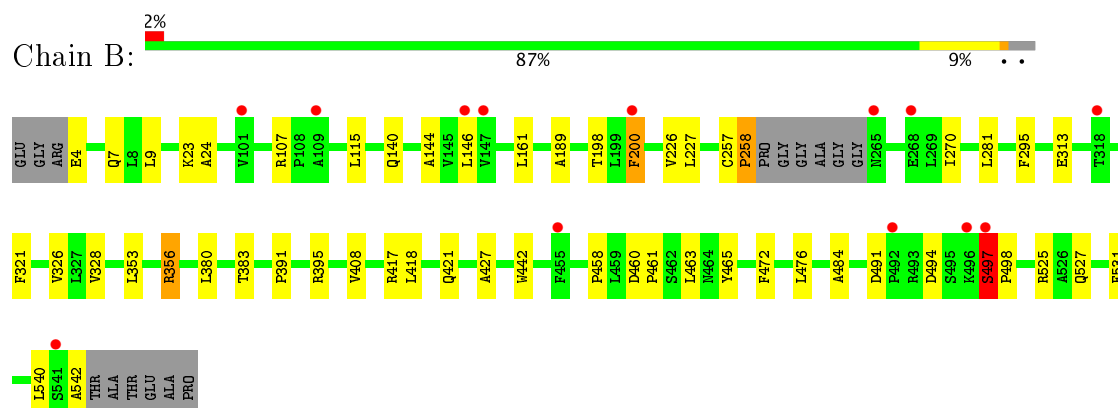
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.58Å 111.86Å 227.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 2.40 29.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.04-2.40) 100.0 (29.08-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.222 0.178 , 0.207	Depositor DCC
R_{free} test set	1585 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8975	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PE8, NAG, B3V, EDO, PG4, SO4, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/4326	0.53	0/5910
1	B	0.35	0/4313	0.53	1/5895 (0.0%)
All	All	0.37	0/8639	0.53	1/11805 (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	B	258	PRO	N-CA-CB	5.51	109.91	103.30

There are no chirality outliers.

There are no planarity outliers.

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	4196	0	4091	23	0
1	B	4177	0	4056	32	0
2	A	31	0	26	0	0
2	B	38	0	44	1	0
3	A	24	0	36	1	0
3	B	24	0	36	1	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	20	0	0
5	B	7	0	10	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	25	0	34	4	0
8	B	13	0	18	0	0
9	A	212	0	0	2	0
9	B	162	0	0	0	0
All	All	8975	0	8410	57	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 3.

All (57) 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:B:356:ARG:NH2	1:B:383:THR:OG1	2.24	0.70
7:A:1556:PE8:H241	1:B:527:GLN:HE21	1.57	0.69
1:A:45[A]:ARG:NH1	1:A:51:GLU:OE1	2.28	0.66
1:A:485:ARG:HD3	3:A:1552:EDO:H22	1.81	0.60
1:A:459:LEU:HD12	1:A:470:ARG:HG2	1.82	0.60
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.85	0.58
1:A:291:GLN:OE1	1:A:369[B]:GLN:NE2	2.38	0.57
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.87	0.57
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.88	0.54
1:B:497:SER:HB2	1:B:498:PRO:C	2.29	0.53
1:A:317:ASN:O	1:A:421:GLN:NE2	2.41	0.52
7:A:1556:PE8:H182	1:B:531:PHE:HD1	1.75	0.51
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.94	0.50
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.48	0.49
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.95	0.49
1:B:326:VAL:HG21	1:B:418:LEU:HD13	1.93	0.49
1:B:4:GLU:OE2	1:B:9:LEU:HD11	2.13	0.49
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.48	0.49
1:A:45[B]:ARG:HG3	9:A:2033:HOH:O	2.12	0.48
1:B:313[B]:GLU:HG2	1:B:313[B]:GLU:H	1.52	0.47
1:B:321:PHE:HD2	1:B:421:GLN:HB3	1.80	0.47
1:B:472:PHE:CZ	1:B:476:LEU:HD11	2.50	0.47
1:B:417:ARG:HD2	1:B:417:ARG:HA	1.72	0.46
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.97	0.46
1:A:81:GLU:HG3	9:A:2053:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LYS:HA	1:B:23:LYS:HD2	1.67	0.46
1:B:7:GLN:O	1:B:107:ARG:NH1	2.48	0.46
1:B:189:ALA:HB2	5:B:1547:PEG:H31	1.97	0.45
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.98	0.44
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.99	0.44
1:A:317:ASN:HA	1:A:417:ARG:HH11	1.82	0.44
1:A:376:GLU:O	1:A:380:LEU:HG	2.18	0.44
2:B:1549:B3V:H171	2:B:1549:B3V:H203	1.71	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.43
1:B:460:ASP:HA	1:B:461:PRO:HD3	1.85	0.43
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.80	0.43
1:B:144:ALA:HA	3:B:1543:EDO:H21	2.00	0.43
1:B:540:LEU:C	1:B:542:ALA:H	2.21	0.43
1:A:332:LYS:HG3	1:A:431:GLU:HG2	2.01	0.43
1:B:161:LEU:HD13	1:B:270:ILE:HD11	2.00	0.43
1:A:45[B]:ARG:HA	1:A:45[B]:ARG:HD2	1.83	0.42
1:B:257:CYS:HA	1:B:258:PRO:HA	1.71	0.42
1:B:328:VAL:O	1:B:427:ALA:HA	2.19	0.42
1:B:115:LEU:HD21	1:B:484:ALA:HB2	2.01	0.42
1:A:491:ASP:HB3	1:A:494:ASP:HB3	2.00	0.42
1:A:5:ASP:HB3	1:A:8:LEU:HD12	2.02	0.41
7:A:1556:PE8:H212	1:B:531:PHE:HB2	2.01	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.19	0.41
7:A:1556:PE8:H122	7:A:1556:PE8:H151	1.76	0.41
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.55	0.41
1:A:211:MET:HG3	1:A:232:PRO:HB3	2.02	0.41
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.91	0.41
1:A:276:ARG:HD3	1:A:276:ARG:HA	1.91	0.41
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.51	0.40
1:A:325:GLN:HG2	1:A:424:ARG:HH21	1.86	0.40
1:B:115:LEU:HD23	1:B:198:THR:HB	2.02	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	534/548 (97%)	514 (96%)	20 (4%)	0	100	100
1	B	533/548 (97%)	517 (97%)	15 (3%)	1 (0%)	51	67
All	All	1067/1096 (97%)	1031 (97%)	35 (3%)	1 (0%)	55	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER

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	442/446 (99%)	433 (98%)	9 (2%)	60	79
1	B	440/446 (99%)	434 (99%)	6 (1%)	71	86
All	All	882/892 (99%)	867 (98%)	15 (2%)	66	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	21	ARG
1	A	70	TYR
1	A	200	PHE
1	A	268	GLU
1	A	295	PHE
1	A	332	LYS
1	A	372	ASP
1	A	413	GLN
1	B	146	LEU
1	B	200	PHE
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	295	PHE
1	B	356	ARG
1	B	497	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 ligands 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	B3V	A	1543	-	19,19,19	1.78	3 (15%)	25,25,25	1.60	5 (20%)
3	EDO	A	1544	-	3,3,3	0.62	0	2,2,2	0.91	0
3	EDO	A	1545	-	3,3,3	0.61	0	2,2,2	1.01	0
4	NAG	A	1546	1	14,14,15	0.46	0	15,19,21	1.32	1 (6%)
5	PEG	A	1547	-	6,6,6	0.75	0	5,5,5	0.96	0
5	PEG	A	1548	-	6,6,6	0.66	0	5,5,5	1.04	0
4	NAG	A	1549	1	14,14,15	0.41	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	1550	-	3,3,3	0.61	0	2,2,2	0.86	0
3	EDO	A	1551	-	3,3,3	0.64	0	2,2,2	0.87	0
3	EDO	A	1552	-	3,3,3	0.68	0	2,2,2	0.80	0
2	B3V	A	1553	-	10,10,19	2.08	3 (30%)	14,14,25	1.64	3 (21%)
6	SO4	A	1554	-	4,4,4	0.16	0	6,6,6	0.23	0
3	EDO	A	1555	-	3,3,3	0.63	0	2,2,2	0.93	0
7	PE8	A	1556	-	24,24,24	0.79	0	23,23,23	0.78	0
3	EDO	B	1543	-	3,3,3	0.61	0	2,2,2	0.89	0
2	B3V	B	1544	-	19,19,19	1.97	2 (10%)	25,25,25	1.68	5 (20%)
3	EDO	B	1545	-	3,3,3	0.64	0	2,2,2	0.88	0
4	NAG	B	1546	1	14,14,15	0.43	0	15,19,21	1.30	1 (6%)
5	PEG	B	1547	-	6,6,6	0.77	0	5,5,5	0.93	0
3	EDO	B	1548	-	3,3,3	0.60	0	2,2,2	0.91	0
2	B3V	B	1549	-	19,19,19	1.78	2 (10%)	25,25,25	1.63	7 (28%)
6	SO4	B	1550	-	4,4,4	0.15	0	6,6,6	0.21	0
3	EDO	B	1551	-	3,3,3	0.65	0	2,2,2	0.88	0
8	PG4	B	1552	-	12,12,12	0.70	0	11,11,11	1.15	0
3	EDO	B	1553	-	3,3,3	0.65	0	2,2,2	0.88	0
3	EDO	B	2000	-	3,3,3	0.65	0	2,2,2	0.91	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
2	B3V	A	1543	-	-	0/19/19/19	0/1/1/1
3	EDO	A	1544	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1545	-	-	0/1/1/1	0/0/0/0
4	NAG	A	1546	1	-	0/6/23/26	0/1/1/1
5	PEG	A	1547	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1548	-	-	0/4/4/4	0/0/0/0
4	NAG	A	1549	1	-	0/6/23/26	0/1/1/1
3	EDO	A	1550	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1551	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1552	-	-	0/1/1/1	0/0/0/0
2	B3V	A	1553	-	-	0/6/6/19	0/1/1/1
6	SO4	A	1554	-	-	0/0/0/0	0/0/0/0
3	EDO	A	1555	-	-	0/1/1/1	0/0/0/0
7	PE8	A	1556	-	-	0/22/22/22	0/0/0/0
3	EDO	B	1543	-	-	0/1/1/1	0/0/0/0
2	B3V	B	1544	-	-	0/19/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1545	-	-	0/1/1/1	0/0/0/0
4	NAG	B	1546	1	-	0/6/23/26	0/1/1/1
5	PEG	B	1547	-	-	0/4/4/4	0/0/0/0
3	EDO	B	1548	-	-	0/1/1/1	0/0/0/0
2	B3V	B	1549	-	-	0/19/19/19	0/1/1/1
6	SO4	B	1550	-	-	0/0/0/0	0/0/0/0
3	EDO	B	1551	-	-	0/1/1/1	0/0/0/0
8	PG4	B	1552	-	-	0/10/10/10	0/0/0/0
3	EDO	B	1553	-	-	0/1/1/1	0/0/0/0
3	EDO	B	2000	-	-	0/1/1/1	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1549	B3V	C8-S1	-5.68	1.68	1.76
2	A	1543	B3V	C8-S1	-5.31	1.68	1.76
2	A	1553	B3V	C8-S1	-5.26	1.68	1.77
2	B	1544	B3V	C8-S1	-4.83	1.69	1.76
2	A	1543	B3V	C7-C8	2.08	1.43	1.39
2	A	1553	B3V	C7-C8	2.21	1.42	1.38
2	A	1553	B3V	S1-N1	2.60	1.66	1.60
2	B	1549	B3V	S1-N1	3.03	1.65	1.61
2	A	1543	B3V	S1-N1	3.45	1.66	1.61
2	B	1544	B3V	S1-N1	5.57	1.69	1.61

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1549	B3V	O2-S1-N1	-3.53	101.34	107.03
2	B	1544	B3V	C9-C8-C7	-3.41	116.34	120.61
2	A	1543	B3V	C9-C8-C7	-3.20	116.60	120.61
2	B	1549	B3V	C13-C11-N2	-2.87	106.42	112.83
2	B	1549	B3V	C9-C8-C7	-2.81	117.09	120.61
2	B	1544	B3V	C13-C11-N2	-2.52	107.20	112.83
2	A	1553	B3V	C9-C8-C7	-2.18	117.31	120.43
2	B	1549	B3V	O1-S1-N1	2.04	110.32	107.03
2	A	1543	B3V	C11-C13-N1	2.05	113.73	110.03
2	A	1543	B3V	C5-C6-C7	2.15	123.45	120.53
2	A	1543	B3V	C9-C8-S1	2.17	122.16	119.77
2	B	1549	B3V	C5-C6-C7	2.19	123.50	120.53
2	B	1549	B3V	C9-C8-S1	2.22	122.22	119.77
2	A	1553	B3V	C5-C6-C7	2.31	123.38	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1544	B3V	C5-C6-C7	2.37	123.74	120.53
2	B	1544	B3V	C9-C8-S1	2.71	122.76	119.77
4	A	1549	NAG	C1-O5-C5	2.73	115.93	112.17
2	A	1553	B3V	C10-C9-C8	3.89	123.05	118.96
2	B	1549	B3V	C10-C9-C8	4.19	123.37	118.96
2	A	1543	B3V	C10-C9-C8	4.33	123.52	118.96
4	B	1546	NAG	C1-O5-C5	4.44	118.28	112.17
2	B	1544	B3V	C10-C9-C8	4.48	123.68	118.96
4	A	1546	NAG	C1-O5-C5	4.65	118.57	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1552	EDO	1	0
7	A	1556	PE8	4	0
3	B	1543	EDO	1	0
5	B	1547	PEG	1	0
2	B	1549	B3V	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, 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	536/548 (97%)	-0.32	13 (2%) 59 56	30, 43, 71, 115	0
1	B	533/548 (97%)	-0.20	13 (2%) 59 56	34, 49, 73, 111	0
All	All	1069/1096 (97%)	-0.26	26 (2%) 59 56	30, 46, 72, 115	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LYS	6.1
1	B	497	SER	5.4
1	A	495	SER	4.7
1	A	494	ASP	4.4
1	A	493	ARG	4.0
1	A	497	SER	3.5
1	A	492	PRO	3.4
1	B	318	THR	3.1
1	B	109	ALA	3.0
1	A	541	SER	2.7
1	B	268	GLU	2.7
1	B	146	LEU	2.6
1	A	491	ASP	2.5
1	A	322	GLN	2.5
1	B	200	PHE	2.4
1	B	147	VAL	2.4
1	A	226	VAL	2.2
1	B	541	SER	2.2
1	A	454	ILE	2.2
1	A	318	THR	2.1
1	B	265	ASN	2.1
1	B	496	LYS	2.1
1	B	101	VAL	2.1
1	B	492	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	455	PHE	2.1
1	A	227	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	NAG	A	1546	14/15	0.76	0.39	8.55	63,72,73,74	0
4	NAG	B	1546	14/15	0.64	0.47	7.52	69,75,78,79	0
7	PE8	A	1556	25/25	0.89	0.24	6.68	52,68,90,90	0
3	EDO	A	1552	4/4	0.74	0.23	6.16	72,72,77,77	0
3	EDO	A	1555	4/4	0.83	0.17	3.83	77,77,78,79	0
2	B3V	A	1543	19/19	0.94	0.23	3.30	51,70,77,77	0
8	PG4	B	1552	13/13	0.82	0.19	2.64	64,85,87,87	0
3	EDO	B	1543	4/4	0.85	0.17	2.13	68,68,68,69	0
5	PEG	A	1548	7/7	0.89	0.19	2.07	70,71,93,93	0
5	PEG	B	1547	7/7	0.85	0.31	2.06	70,70,83,83	0
2	B3V	B	1544	19/19	0.92	0.19	1.98	47,68,88,88	0
3	EDO	B	1548	4/4	0.93	0.15	1.28	66,66,66,66	0
5	PEG	A	1547	7/7	0.89	0.15	1.12	58,59,78,79	0
2	B3V	B	1549	19/19	0.94	0.22	0.61	53,81,99,100	19
6	SO4	A	1554	5/5	0.93	0.18	0.50	85,86,86,86	0
3	EDO	A	1550	4/4	0.91	0.16	0.48	66,67,67,68	0
2	B3V	A	1553	12/19	0.85	0.20	0.09	60,60,95,96	12
3	EDO	B	1551	4/4	0.80	0.11	-0.74	75,75,76,76	0
6	SO4	B	1550	5/5	0.96	0.14	-0.92	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	1549	14/15	0.82	0.40	-	78,85,87,87	0
3	EDO	B	1553	4/4	0.91	0.13	-	61,61,91,91	0
3	EDO	B	2000	4/4	0.77	0.21	-	88,89,90,90	0
3	EDO	A	1545	4/4	0.84	0.20	-	77,78,78,78	0
3	EDO	A	1551	4/4	0.81	0.23	-	81,81,85,85	0
3	EDO	B	1545	4/4	0.84	0.20	-	88,88,91,91	0
3	EDO	A	1544	4/4	0.66	0.28	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.