



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:58 AM GMT

PDB ID : 4BC0
Title : Structure of mouse acetylcholinesterase inhibited by CBDP (12-h soak) : Cresyl-phosphoserine adduct
Authors : Carletti, E.; Colletier, J.-P.; Schopfer, L.M.; Santoni, G.; Masson, P.; Lockridge, O.; Nachon, F.; Weik, M.
Deposited on : 2012-09-30
Resolution : 3.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

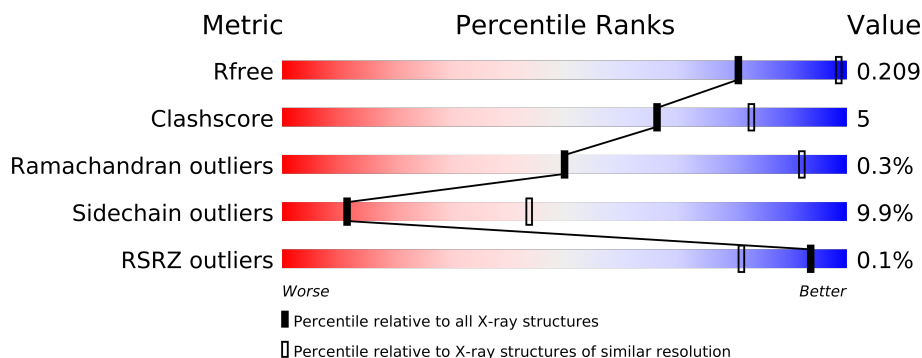
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.35 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}	66092	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	543	
1	B	543	
1	C	543	
1	D	543	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	701	-	X
3	NAG	B	701	-	X
3	NAG	C	701	-	X
3	NAG	D	701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	D	703	-	X
4	SO4	A	1547	-	X
5	CL	C	3002	-	X
5	CL	D	3000	-	X
5	CL	D	3002	-	X

2 Entry composition i

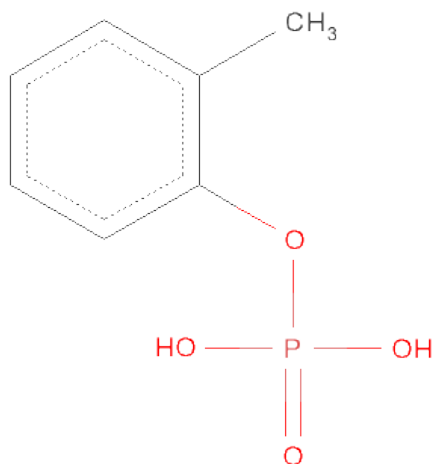
There are 6 unique types of molecules in this entry. The entry contains 17432 atoms, of which 0 are hydrogen and 0 are deuterium.

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	542	Total	C	N	O	S	0	0	0
			4215	2702	733	766	14			
1	B	539	Total	C	N	O	S	0	0	0
			4191	2689	727	761	14			
1	C	540	Total	C	N	O	S	0	0	0
			4200	2694	728	764	14			
1	D	540	Total	C	N	O	S	0	0	0
			4200	2694	728	764	14			

- Molecule 2 is (2-METHYLPHENYL) DIHYDROGEN PHOSPHATE (three-letter code: 4OJ) (formula: C₇H₉O₄P).



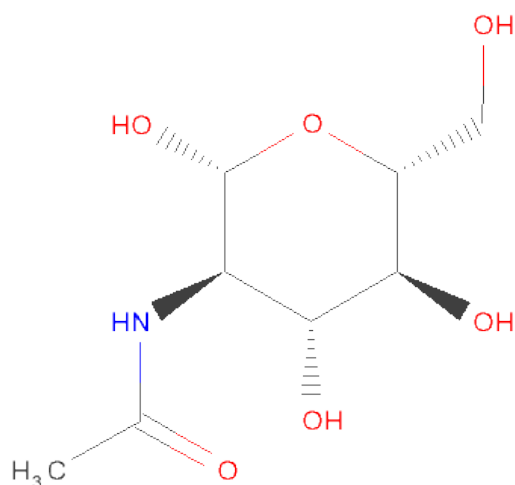
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	7	3	1		
2	B	1	Total	C	O	P	0	0
			11	7	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			11	7	3	1		
2	D	1	Total	C	O	P	0	0
			11	7	3	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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



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

- Molecule 6 is water.

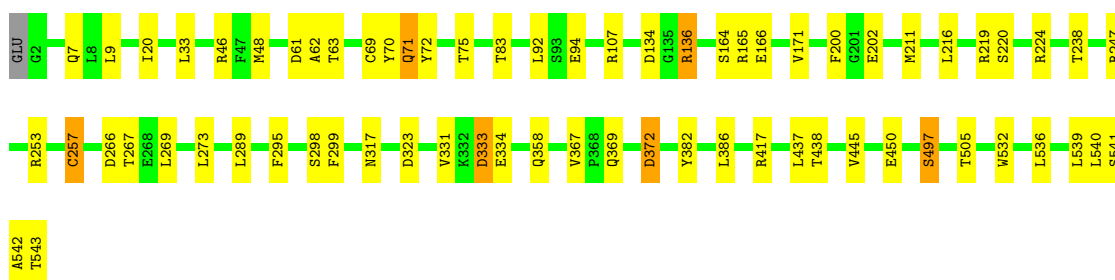
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	117	Total 117	O 117	0	0
6	B	82	Total 82	O 82	0	0
6	C	115	Total 115	O 115	0	0
6	D	97	Total 97	O 97	0	0

3 Residue-property plots

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.

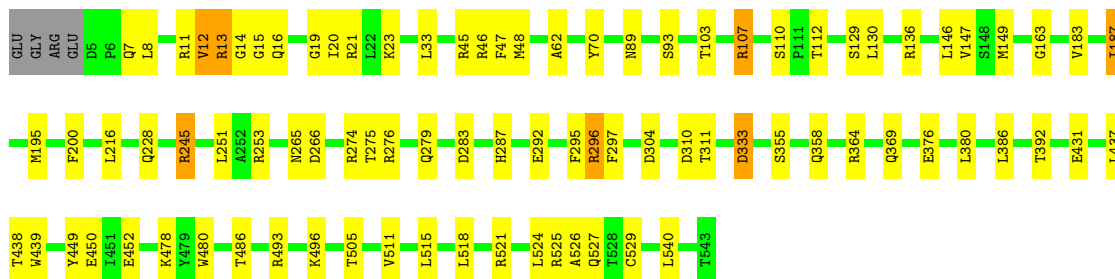
• Molecule 1: ACETYLCHOLINESTERASE

Chain A:



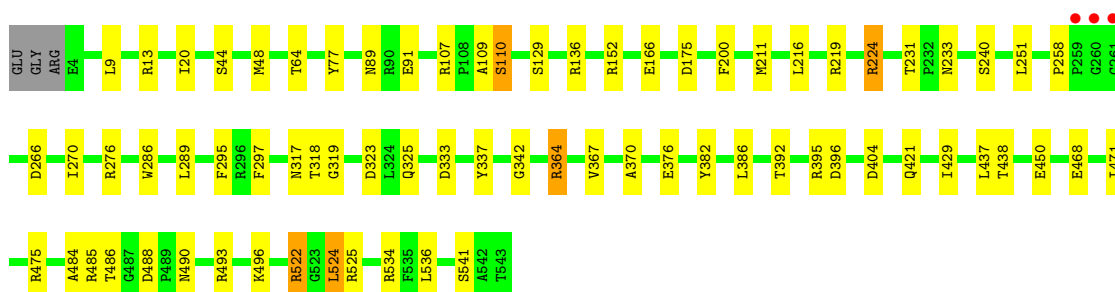
• Molecule 1: ACETYLCHOLINESTERASE

Chain B:



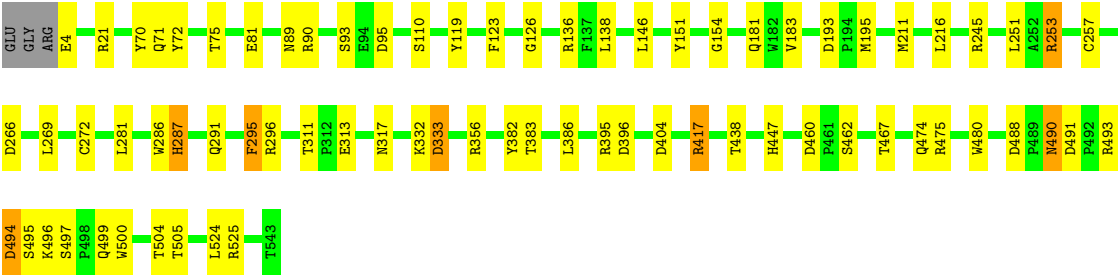
• Molecule 1: ACETYLCHOLINESTERASE

Chain C:



• Molecule 1: ACETYLCHOLINESTERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 174.04Å 225.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 3.35 48.61 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.62-3.35) 96.7 (48.61-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.162 , 0.208 0.163 , 0.209	Depositor DCC
R_{free} test set	2263 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 19.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 75488 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17432	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OJ, CL, SO4, NAG

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	0.46	0/4341	0.70	1/5931 (0.0%)
1	B	0.43	0/4317	0.67	0/5900
1	C	0.47	0/4326	0.71	1/5912 (0.0%)
1	D	0.44	0/4326	0.68	1/5912 (0.0%)
All	All	0.45	0/17310	0.69	3/23655 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	9

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	497	SER	N-CA-C	-6.95	92.24	111.00
1	A	497	SER	N-CA-C	5.74	126.49	111.00
1	C	524	LEU	CA-CB-CG	5.50	127.96	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	CYS	Peptide
1	A	323	ASP	Peptide
1	A	497	SER	Peptide
1	A	541	SER	Peptide
1	B	496	LYS	Peptide
1	C	258	PRO	Peptide
1	C	342	GLY	Peptide
1	C	496	LYS	Peptide
1	D	257	CYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4215	0	0	20	0
1	B	4191	0	0	25	0
1	C	4200	0	0	18	0
1	D	4200	0	0	26	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	11	0	0	0	0
3	A	14	0	0	0	0
3	B	28	0	0	0	0
3	C	14	0	0	0	0
3	D	42	0	0	0	0
4	A	25	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	1	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
6	A	117	0	0	6	0
6	B	82	0	0	7	0
6	C	115	0	0	7	0
6	D	97	0	0	6	0
All	All	17432	0	0	87	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (87) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:286:TRP:NE1	6:C:2077:HOH:O	2.19	0.75
1:D:245:ARG:NE	6:D:2049:HOH:O	2.21	0.72
1:B:187:ILE:N	6:B:2032:HOH:O	2.24	0.69
1:A:334:GLU:OE1	6:A:2088:HOH:O	2.10	0.68
1:D:488:ASP:OD1	1:D:490:ASN:ND2	2.28	0.67
1:D:333:ASP:N	1:D:333:ASP:OD1	2.26	0.67
1:A:202:GLU:OE2	6:A:2060:HOH:O	2.13	0.67
1:D:138:LEU:N	6:D:2043:HOH:O	2.29	0.65
1:B:276:ARG:NH1	6:B:2047:HOH:O	2.30	0.64
1:A:46:ARG:NE	1:A:94:GLU:OE2	2.31	0.64
1:B:89:ASN:ND2	1:B:129:SER:O	2.33	0.61
1:A:331:VAL:N	1:A:334:GLU:OE2	2.34	0.60
1:D:460:ASP:OD1	1:D:462:SER:OG	2.20	0.60
1:C:485:ARG:NH2	6:C:2052:HOH:O	2.35	0.59
1:B:12:VAL:O	1:B:15:GLY:N	2.36	0.59
1:C:475:ARG:NH2	6:C:2107:HOH:O	2.34	0.59
1:B:265:ASN:O	6:B:2044:HOH:O	2.17	0.59
1:B:12:VAL:O	1:B:14:GLY:N	2.36	0.58
1:A:171:VAL:N	6:A:2049:HOH:O	2.35	0.58
1:D:295:PHE:O	1:D:296:ARG:NH1	2.37	0.57
1:B:304:ASP:N	1:B:304:ASP:OD1	2.37	0.57
1:B:46:ARG:O	1:B:274:ARG:NH1	2.37	0.57
1:D:395:ARG:NH1	1:D:396:ASP:OD1	2.38	0.57
1:A:372:ASP:N	1:A:372:ASP:OD1	2.38	0.57
1:C:364:ARG:NH2	1:C:370:ALA:O	2.37	0.56
1:B:431:GLU:OE2	1:B:521:ARG:NH2	2.38	0.56
1:B:333:ASP:OD1	1:B:333:ASP:N	2.37	0.56
1:A:219:ARG:NH1	6:A:2062:HOH:O	2.37	0.56
1:D:382:TYR:OH	1:D:404:ASP:OD2	2.25	0.54
1:D:245:ARG:NH2	1:D:266:ASP:OD2	2.41	0.54
1:A:69:CYS:O	1:A:71:GLN:NE2	2.40	0.54
1:B:245:ARG:NH2	1:B:266:ASP:OD1	2.41	0.54
1:D:89:ASN:O	1:D:90:ARG:NH1	2.41	0.53
1:B:296:ARG:NH1	1:B:369:GLN:OE1	2.42	0.53
1:B:279:GLN:NE2	1:B:283:ASP:OD1	2.42	0.53
1:C:337:TYR:N	6:C:2086:HOH:O	2.40	0.52
1:D:525:ARG:NH1	4:D:1544:SO4:O4	2.41	0.52
1:C:224:ARG:NH2	1:C:484:ALA:O	2.43	0.52
1:D:475:ARG:NH2	6:D:2093:HOH:O	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:522:ARG:NH1	6:C:2111:HOH:O	2.41	0.52
1:D:494:ASP:OD1	1:D:494:ASP:N	2.43	0.52
1:C:318:THR:OG1	1:C:319:GLY:N	2.43	0.51
1:B:33:LEU:N	1:B:62:ALA:O	2.43	0.51
1:A:72:TYR:N	6:A:2023:HOH:O	2.43	0.50
1:A:299:PHE:N	6:A:2078:HOH:O	2.46	0.49
1:A:450:GLU:OE1	1:A:450:GLU:N	2.46	0.49
1:C:89:ASN:ND2	1:C:129:SER:O	2.46	0.48
1:C:152:ARG:NH2	1:C:175:ASP:OD1	2.46	0.48
1:B:163:GLY:N	6:B:2028:HOH:O	2.45	0.48
1:D:317:ASN:OD1	1:D:417:ARG:NH1	2.46	0.48
1:C:219:ARG:NE	6:C:2065:HOH:O	2.46	0.48
1:A:33:LEU:N	1:A:62:ALA:O	2.46	0.48
1:B:310:ASP:OD1	1:B:311:THR:N	2.46	0.48
1:C:395:ARG:NH1	1:C:396:ASP:OD1	2.47	0.47
1:B:7:GLN:OE1	1:B:107:ARG:N	2.48	0.46
1:D:71:GLN:NE2	1:D:126:GLY:O	2.48	0.46
1:D:72:TYR:N	6:D:2026:HOH:O	2.49	0.46
1:A:382:TYR:OH	1:A:532:TRP:NE1	2.49	0.46
1:C:77:TYR:N	6:C:2027:HOH:O	2.48	0.45
1:A:333:ASP:OD1	1:A:445:VAL:N	2.49	0.45
1:C:109:ALA:O	1:C:110:SER:OG	2.34	0.45
1:A:289:LEU:O	1:D:253:ARG:NH1	2.49	0.45
1:D:447:HIS:N	6:D:2075:HOH:O	2.50	0.45
1:D:356:ARG:NH2	1:D:383:THR:OG1	2.50	0.45
1:B:47:PHE:N	6:B:2005:HOH:O	2.50	0.44
1:C:382:TYR:OH	1:C:404:ASP:OD2	2.36	0.44
1:B:253:ARG:NH1	1:C:289:LEU:O	2.51	0.44
1:D:119:TYR:O	1:D:151:TYR:OH	2.36	0.43
1:A:539:LEU:O	1:A:543:THR:N	2.52	0.42
1:B:452:GLU:N	6:B:2069:HOH:O	2.52	0.42
1:B:355:SER:N	1:B:358:GLN:OE1	2.52	0.42
1:D:490:ASN:OD1	1:D:500:TRP:N	2.53	0.42
1:B:8:LEU:O	1:B:19:GLY:N	2.53	0.41
1:A:134:ASP:OD2	1:A:136:ARG:NH1	2.53	0.41
1:B:364:ARG:NE	6:B:2061:HOH:O	2.53	0.41
1:D:193:ASP:OD1	1:D:195:MET:N	2.53	0.41
1:C:488:ASP:OD1	1:C:490:ASN:ND2	2.54	0.41
1:A:247:ARG:NH1	1:A:298:SER:O	2.54	0.41
1:A:266:ASP:O	1:A:269:LEU:N	2.54	0.41
1:B:228:GLN:NE2	1:B:450:GLU:OE2	2.53	0.41
1:D:504:THR:N	6:D:2094:HOH:O	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ASP:OD1	1:A:63:THR:OG1	2.39	0.41
1:B:439:TRP:NE1	1:B:449:TYR:OH	2.54	0.40
1:C:233:ASN:OD1	1:C:233:ASN:N	2.54	0.40
1:D:286:TRP:O	1:D:287:HIS:ND1	2.54	0.40
1:D:93:SER:OG	1:D:95:ASP:N	2.55	0.40
1:D:123:PHE:O	1:D:154:GLY:N	2.54	0.40

There are no symmetry-related clashes.

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	540/543 (99%)	510 (94%)	29 (5%)	1 (0%)	56	94
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	30	80
1	C	538/543 (99%)	512 (95%)	25 (5%)	1 (0%)	56	94
1	D	538/543 (99%)	508 (94%)	30 (6%)	0	100	100
All	All	2153/2172 (99%)	2032 (94%)	115 (5%)	6 (0%)	50	92

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	ALA
1	B	13	ARG
1	B	12	VAL
1	B	526	ALA
1	C	110	SER
1	B	107	ARG

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	442/443 (100%)	404 (91%)	38 (9%)	15	54
1	B	440/443 (99%)	389 (88%)	51 (12%)	8	35
1	C	441/443 (100%)	395 (90%)	46 (10%)	10	41
1	D	441/443 (100%)	402 (91%)	39 (9%)	14	52
All	All	1764/1772 (100%)	1590 (90%)	174 (10%)	11	44

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	LEU
1	A	20	ILE
1	A	48	MET
1	A	70	TYR
1	A	71	GLN
1	A	75	THR
1	A	83	THR
1	A	92	LEU
1	A	107	ARG
1	A	136	ARG
1	A	164	SER
1	A	165	ARG
1	A	166	GLU
1	A	200	PHE
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	224	ARG
1	A	238	THR
1	A	253	ARG
1	A	257	CYS
1	A	267	THR
1	A	273	LEU
1	A	295	PHE
1	A	317	ASN
1	A	333	ASP
1	A	358	GLN
1	A	367	VAL
1	A	369	GLN

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Mol	Chain	Res	Type
1	A	372	ASP
1	A	386	LEU
1	A	417	ARG
1	A	437	LEU
1	A	438	THR
1	A	505	THR
1	A	536	LEU
1	A	540	LEU
1	B	11	ARG
1	B	13	ARG
1	B	16	GLN
1	B	20	ILE
1	B	21	ARG
1	B	23	LYS
1	B	45	ARG
1	B	48	MET
1	B	70	TYR
1	B	93	SER
1	B	103	THR
1	B	110	SER
1	B	112	THR
1	B	130	LEU
1	B	136	ARG
1	B	146	LEU
1	B	147	VAL
1	B	149	MET
1	B	183	VAL
1	B	187	ILE
1	B	195	MET
1	B	200	PHE
1	B	216	LEU
1	B	245	ARG
1	B	251	LEU
1	B	275	THR
1	B	287	HIS
1	B	292	GLU
1	B	295	PHE
1	B	296	ARG
1	B	297	PHE
1	B	333	ASP
1	B	376	GLU
1	B	380	LEU

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Mol	Chain	Res	Type
1	B	386	LEU
1	B	392	THR
1	B	437	LEU
1	B	438	THR
1	B	478	LYS
1	B	480	TRP
1	B	486	THR
1	B	493	ARG
1	B	505	THR
1	B	511	VAL
1	B	515	LEU
1	B	518	LEU
1	B	524	LEU
1	B	525	ARG
1	B	527	GLN
1	B	529	CYS
1	B	540	LEU
1	C	9	LEU
1	C	13	ARG
1	C	20	ILE
1	C	44	SER
1	C	48	MET
1	C	64	THR
1	C	91	GLU
1	C	107	ARG
1	C	136	ARG
1	C	166	GLU
1	C	200	PHE
1	C	211	MET
1	C	216	LEU
1	C	224	ARG
1	C	231	THR
1	C	240	SER
1	C	251	LEU
1	C	266	ASP
1	C	270	ILE
1	C	276	ARG
1	C	295	PHE
1	C	297	PHE
1	C	317	ASN
1	C	323	ASP
1	C	325	GLN

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Mol	Chain	Res	Type
1	C	333	ASP
1	C	364	ARG
1	C	367	VAL
1	C	376	GLU
1	C	386	LEU
1	C	392	THR
1	C	421	GLN
1	C	429	ILE
1	C	437	LEU
1	C	438	THR
1	C	450	GLU
1	C	468	GLU
1	C	471	ILE
1	C	486	THR
1	C	493	ARG
1	C	522	ARG
1	C	524	LEU
1	C	525	ARG
1	C	534	ARG
1	C	536	LEU
1	C	541	SER
1	D	4	GLU
1	D	21	ARG
1	D	70	TYR
1	D	75	THR
1	D	81	GLU
1	D	110	SER
1	D	136	ARG
1	D	146	LEU
1	D	181	GLN
1	D	183	VAL
1	D	211	MET
1	D	216	LEU
1	D	251	LEU
1	D	253	ARG
1	D	269	LEU
1	D	272	CYS
1	D	281	LEU
1	D	287	HIS
1	D	291	GLN
1	D	295	PHE
1	D	311	THR

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Mol	Chain	Res	Type
1	D	313	GLU
1	D	332	LYS
1	D	333	ASP
1	D	386	LEU
1	D	417	ARG
1	D	438	THR
1	D	467	THR
1	D	474	GLN
1	D	480	TRP
1	D	490	ASN
1	D	491	ASP
1	D	493	ARG
1	D	494	ASP
1	D	495	SER
1	D	496	LYS
1	D	499	GLN
1	D	505	THR
1	D	524	LEU

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 chains 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 ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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
4	SO4	A	1544	-	4,4,4	0.13	0	6,6,6	0.12	0
4	SO4	A	1545	-	4,4,4	0.17	0	6,6,6	0.21	0
4	SO4	A	1546	-	4,4,4	0.18	0	6,6,6	0.15	0
4	SO4	A	1547	-	4,4,4	0.10	0	6,6,6	0.27	0
4	SO4	A	1548	-	4,4,4	0.17	0	6,6,6	0.15	0
2	4OJ	A	600	1	9,11,12	0.82	0	11,14,17	0.99	1 (9%)
3	NAG	A	701	1	12,14,15	0.62	0	15,19,21	0.93	1 (6%)
4	SO4	B	1544	-	4,4,4	0.15	0	6,6,6	0.31	0
4	SO4	B	1545	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	B	1546	-	4,4,4	0.13	0	6,6,6	0.09	0
2	4OJ	B	600	1	9,11,12	0.73	0	11,14,17	1.13	1 (9%)
3	NAG	B	701	1	12,14,15	0.46	0	15,19,21	1.55	4 (26%)
3	NAG	B	702	1	12,14,15	0.59	0	15,19,21	1.39	2 (13%)
4	SO4	C	1546	-	4,4,4	0.17	0	6,6,6	0.40	0
4	SO4	C	1547	-	4,4,4	0.19	0	6,6,6	0.30	0
2	4OJ	C	600	1	9,11,12	0.68	0	11,14,17	1.03	1 (9%)
3	NAG	C	701	1	12,14,15	0.49	0	15,19,21	1.21	1 (6%)
4	SO4	D	1544	-	4,4,4	0.18	0	6,6,6	0.26	0
4	SO4	D	1545	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	D	1546	-	4,4,4	0.14	0	6,6,6	0.11	0
2	4OJ	D	600	1	9,11,12	1.02	1 (11%)	11,14,17	1.11	1 (9%)
3	NAG	D	701	1	12,14,15	0.58	0	15,19,21	1.43	1 (6%)
3	NAG	D	702	1	12,14,15	0.83	0	15,19,21	1.76	3 (20%)
3	NAG	D	703	1	12,14,15	0.49	0	15,19,21	1.00	1 (6%)

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
4	SO4	A	1544	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1545	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1546	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1547	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1548	-	-	0/0/0/0	0/0/0/0
2	4OJ	A	600	1	-	0/2/4/5	0/1/1/1
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	SO4	B	1544	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1545	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1546	-	-	0/0/0/0	0/0/0/0
2	4OJ	B	600	1	-	0/2/4/5	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
4	SO4	C	1546	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1547	-	-	0/0/0/0	0/0/0/0
2	4OJ	C	600	1	-	0/2/4/5	0/1/1/1
3	NAG	C	701	1	-	0/6/23/26	0/1/1/1
4	SO4	D	1544	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1545	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1546	-	-	0/0/0/0	0/0/0/0
2	4OJ	D	600	1	-	0/2/4/5	0/1/1/1
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	703	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	4OJ	P13-O1P	-2.62	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAG	O5-C5-C6	5.04	112.27	106.98
3	D	702	NAG	O5-C5-C6	4.21	111.40	106.98
3	D	702	NAG	C2-N2-C7	3.95	129.72	123.09
3	B	701	NAG	O5-C5-C6	3.22	110.36	106.98
3	D	703	NAG	O5-C5-C6	3.13	110.27	106.98
2	D	600	4OJ	O12-C5-C6	2.89	120.93	118.48
3	B	702	NAG	O5-C5-C6	2.82	109.94	106.98
3	B	702	NAG	O5-C5-C4	2.76	114.16	110.65
2	B	600	4OJ	O12-C5-C6	2.75	120.81	118.48
3	C	701	NAG	O5-C5-C6	2.65	109.76	106.98
2	C	600	4OJ	O12-C5-C6	2.62	120.70	118.48
3	A	701	NAG	O5-C5-C6	2.59	109.70	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	NAG	C4-C3-C2	-2.48	105.24	111.32
3	B	701	NAG	C2-N2-C7	2.47	127.24	123.09
3	B	701	NAG	O5-C5-C4	2.47	113.79	110.65
2	A	600	4OJ	O12-C5-C6	2.38	120.50	118.48
3	D	702	NAG	O7-C7-C8	-2.03	118.07	122.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	702	NAG	C1

There are no torsion outliers.

There are no ring outliers.

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	542/543 (99%)	-0.19	0	100 100	16, 35, 75, 135	2 (0%)
1	B	539/543 (99%)	-0.10	0	100 100	24, 61, 106, 152	0
1	C	540/543 (99%)	-0.23	3 (0%)	86 53	13, 30, 71, 145	1 (0%)
1	D	540/543 (99%)	-0.18	0	100 100	20, 43, 87, 128	1 (0%)
All	All	2161/2172 (99%)	-0.18	3 (0%)	93 81	13, 41, 94, 152	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	GLY	3.2
1	C	259	PRO	2.6
1	C	261	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	701	14/15	0.51	9.27	102,104,105,106	14
3	NAG	D	701	14/15	0.25	6.90	91,100,105,108	0
5	CL	D	3000	1/1	0.39	6.40	61,61,61,61	0
3	NAG	B	701	14/15	0.22	5.99	85,91,95,97	0
5	CL	D	3002	1/1	0.37	4.20	66,66,66,66	0
3	NAG	D	703	14/15	0.41	3.05	115,127,131,133	0
5	CL	C	3002	1/1	0.34	2.62	57,57,57,57	0
3	NAG	A	701	14/15	0.37	2.44	102,113,115,115	0
4	SO4	A	1547	5/5	0.36	2.32	100,101,102,102	0
4	SO4	C	1547	5/5	0.33	1.87	100,104,105,106	0
5	CL	C	3000	1/1	0.19	1.65	44,44,44,44	0
4	SO4	B	1544	5/5	0.19	1.49	79,84,85,85	0
3	NAG	B	702	14/15	0.40	1.48	61,97,104,106	0
2	4OJ	D	600	11/12	0.31	1.18	32,61,73,73	0
2	4OJ	C	600	11/12	0.23	0.62	23,55,61,61	0
4	SO4	B	1545	5/5	0.16	0.53	127,127,128,129	0
4	SO4	B	1546	5/5	0.34	0.51	126,127,127,128	0
4	SO4	D	1545	5/5	0.36	0.46	118,120,120,121	0
3	NAG	D	702	14/15	0.36	0.38	84,92,95,96	0
2	4OJ	B	600	11/12	0.22	0.25	35,78,84,86	0
2	4OJ	A	600	11/12	0.21	0.21	35,75,83,84	0
4	SO4	D	1546	5/5	0.15	-0.60	119,120,120,121	0
4	SO4	A	1546	5/5	0.22	-0.77	112,112,112,114	0
4	SO4	A	1544	5/5	0.12	-0.86	82,83,84,84	0
4	SO4	A	1548	5/5	0.22	-0.87	120,121,122,123	0
4	SO4	C	1546	5/5	0.11	-0.92	63,65,66,69	0
5	CL	C	1545	1/1	0.13	-1.17	51,51,51,51	0
4	SO4	A	1545	5/5	0.14	-1.55	113,113,115,117	0
5	CL	C	1544	1/1	0.16	-1.59	42,42,42,42	0
4	SO4	D	1544	5/5	0.12	-2.70	63,64,65,69	0
5	CL	D	3001	1/1	0.17	-7.27	54,54,54,54	0
5	CL	C	3001	1/1	0.11	-	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.