



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 08:09 PM GMT

PDB ID : 4BC1
Title : Structure of mouse acetylcholinesterase inhibited by CBDP (30-min soak): crystal-saligenin-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 : 2.95 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>

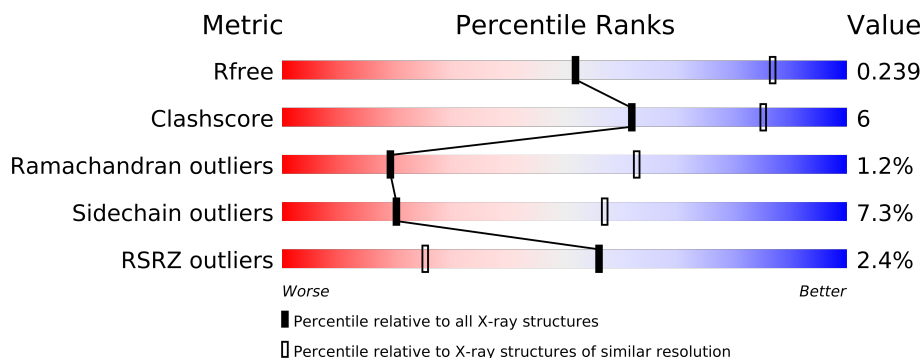
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.95 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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
2	TQV	C	600	-	X
3	NAG	A	701	-	X
3	NAG	D	701	-	X
3	NAG	D	703	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	CL	C	1544	-	X
5	SO4	A	1550	-	X
5	SO4	B	1546	-	X
5	SO4	C	1547	-	X
5	SO4	C	1548	-	X
5	SO4	C	1549	-	X
5	SO4	D	1546	-	X

2 Entry composition i

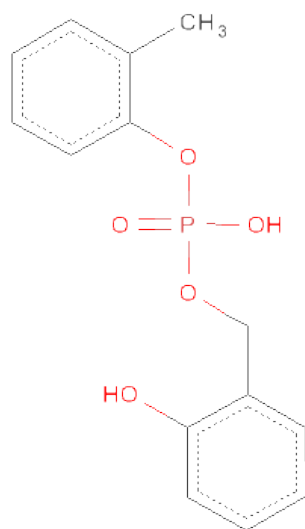
There are 6 unique types of molecules in this entry. The entry contains 17994 atoms, of which 0 are hydrogen and 0 are deuterium.

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	540	Total	C	N	O	S	0	3	0
			4224	2712	732	766	14			
1	B	539	Total	C	N	O	S	0	1	0
			4202	2698	728	762	14			
1	C	540	Total	C	N	O	S	0	4	0
			4230	2716	732	768	14			
1	D	540	Total	C	N	O	S	0	5	0
			4243	2723	741	765	14			

- Molecule 2 is O-CRESYL-SALIGENIN PHOSPHATE (three-letter code: TQV) (formula: C₁₄H₁₅O₅P).



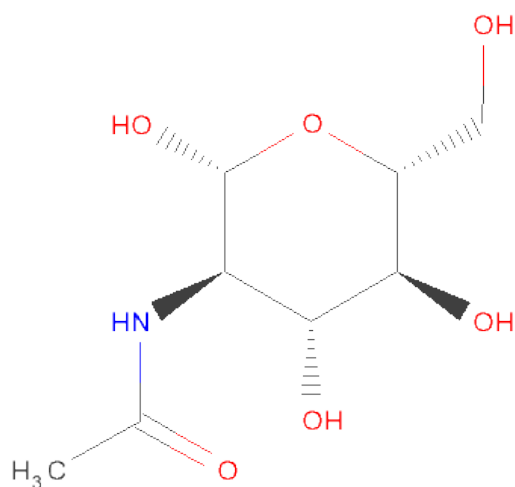
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			19	14	4	1		
2	B	1	Total	C	O	P	0	0
			19	14	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			19	14	4	1		
2	D	1	Total	C	O	P	0	0
			19	14	4	1		

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

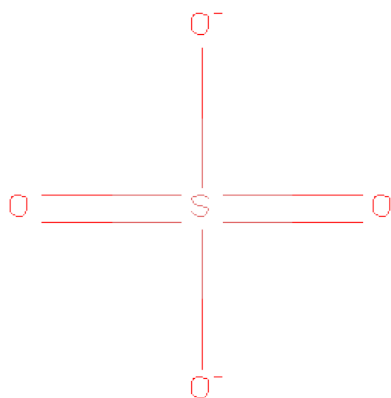


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- 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		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		
6	B	144	Total	O	0	0
			144	144		
6	C	258	Total	O	0	0
			258	258		
6	D	186	Total	O	0	0
			186	186		

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.

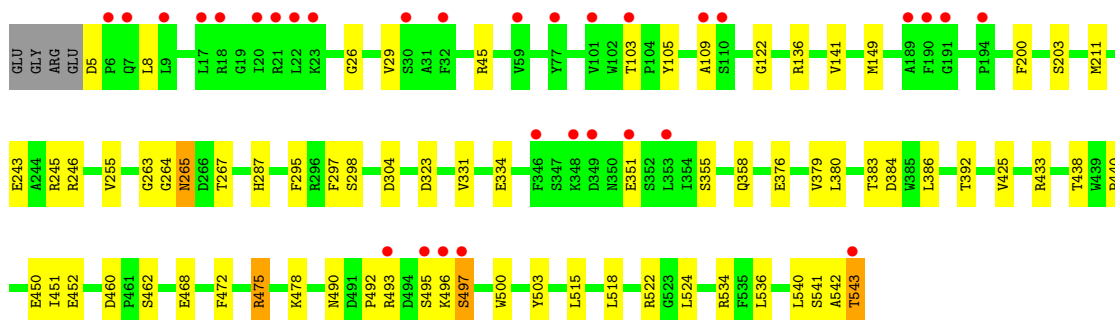
• Molecule 1: ACETYLCHOLINESTERASE

Chain A:



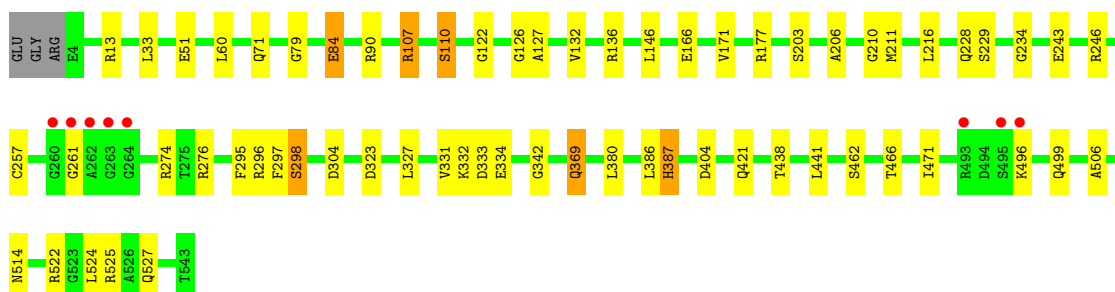
• Molecule 1: ACETYLCHOLINESTERASE

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	135.54Å 173.25Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.28-2.95) 99.7 (49.75-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.186 , 0.238 0.188 , 0.239	Depositor DCC
R_{free} test set	3343 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 111473 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17994	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: TQV, 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	0.50	1/4358 (0.0%)	0.67	0/5955
1	B	0.41	1/4329 (0.0%)	0.60	0/5916
1	C	0.49	1/4367 (0.0%)	0.66	0/5968
1	D	0.45	0/4382	0.64	0/5984
All	All	0.46	3/17436 (0.0%)	0.64	0/23823

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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SER	CB-OG	6.05	1.50	1.42
1	C	203	SER	CB-OG	5.34	1.49	1.42
1	B	203	SER	CB-OG	5.07	1.48	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4224	0	0	28	0
1	B	4202	0	0	23	0
1	C	4230	0	0	24	0
1	D	4243	0	0	22	0
2	A	19	0	0	1	0
2	B	19	0	0	1	0
2	C	19	0	0	1	0
2	D	19	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	3	0	0	2	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	1	0
5	A	30	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	1	0
5	D	15	0	0	0	0
6	A	247	0	0	14	0
6	B	144	0	0	5	0
6	C	258	0	0	11	0
6	D	186	0	0	9	0
All	All	17994	0	0	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1544:CL:CL	6:A:2034:HOH:O	2.19	0.98
1:C:387[A]:HIS:ND1	6:C:2216:HOH:O	2.16	0.78
1:A:72:TYR:O	6:A:2052:HOH:O	2.02	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:508:GLN:NE2	6:A:2228:HOH:O	2.18	0.76
1:C:274:ARG:NH1	6:C:2041:HOH:O	2.17	0.76
1:C:387[A]:HIS:ND1	6:C:2215:HOH:O	2.19	0.75
1:D:39:GLU:OE2	6:D:2019:HOH:O	2.07	0.72
1:A:4:GLU:N	6:A:2001:HOH:O	2.23	0.71
1:D:497:SER:OG	6:D:2169:HOH:O	2.07	0.71
1:C:387[B]:HIS:ND1	6:C:2214:HOH:O	2.22	0.71
1:D:171:VAL:N	6:D:2081:HOH:O	2.23	0.70
1:D:155:THR:O	6:D:2080:HOH:O	2.09	0.70
1:C:122:GLY:N	2:C:600:TQV:O3P	2.24	0.70
1:A:165:ARG:NH2	4:A:1544:CL:CL	2.62	0.69
1:A:107:ARG:NH2	6:A:2010:HOH:O	2.28	0.65
1:A:4:GLU:OE1	1:A:18:ARG:NH1	2.28	0.64
1:B:379:VAL:O	1:B:383:THR:OG1	2.15	0.64
1:B:475:ARG:NH2	6:B:2131:HOH:O	2.30	0.64
1:A:120:GLY:N	6:A:2084:HOH:O	2.32	0.63
1:C:171:VAL:N	6:C:2115:HOH:O	2.32	0.62
1:B:534:ARG:NH1	6:B:2141:HOH:O	2.33	0.62
1:D:26:GLY:N	6:D:2013:HOH:O	2.31	0.61
1:B:122:GLY:N	2:B:600:TQV:O3P	2.33	0.61
1:A:46:ARG:O	1:A:274:ARG:NH1	2.34	0.60
1:D:119:TYR:O	1:D:151:TYR:OH	2.21	0.59
1:A:11:ARG:N	6:A:2011:HOH:O	2.35	0.59
1:A:122:GLY:N	2:A:600:TQV:O3P	2.36	0.59
1:B:452:GLU:N	6:B:2128:HOH:O	2.36	0.58
1:B:541:SER:O	1:B:543:THR:N	2.36	0.58
1:A:406:ASN:ND2	6:A:2159:HOH:O	2.36	0.58
1:C:71:GLN:NE2	1:C:126:GLY:O	2.37	0.58
1:B:5:ASP:OD2	1:B:105:TYR:OH	2.23	0.57
1:B:263:GLY:O	1:B:265:ASN:N	2.38	0.56
1:C:166:GLU:N	1:C:166:GLU:OE1	2.40	0.54
1:B:450:GLU:OE1	6:B:2061:HOH:O	2.18	0.54
1:C:296:ARG:NE	1:C:369[B]:GLN:OE1	2.41	0.54
1:B:384:ASP:N	6:B:2112:HOH:O	2.41	0.53
1:A:464:ASN:ND2	6:A:2210:HOH:O	2.42	0.53
1:D:333:ASP:N	1:D:333:ASP:OD1	2.40	0.53
1:B:243:GLU:OE2	1:B:246:ARG:NH2	2.42	0.52
1:D:417[B]:ARG:NH2	6:D:2143:HOH:O	2.42	0.52
1:C:90:ARG:NE	6:C:2056:HOH:O	2.43	0.52
1:C:527:GLN:N	5:C:1547:SO4:O3	2.44	0.51
1:B:323:ASP:N	1:B:323:ASP:OD1	2.43	0.51
1:D:492:PRO:O	1:D:494:ASP:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:157:GLY:O	6:D:2081:HOH:O	2.20	0.51
1:B:355:SER:N	1:B:358:GLN:OE1	2.44	0.51
1:D:297[A]:PHE:CG	1:D:298:SER:N	2.79	0.50
1:A:289:LEU:O	1:D:253:ARG:NH1	2.45	0.50
1:D:435:SER:OG	1:D:469:GLU:OE1	2.29	0.50
1:C:51:GLU:N	6:C:2037:HOH:O	2.44	0.50
1:D:522[B]:ARG:NH2	6:D:2179:HOH:O	2.44	0.50
1:C:404:ASP:OD2	1:C:525:ARG:NH2	2.45	0.49
1:B:433:ARG:NH2	1:B:440:PRO:O	2.46	0.48
1:B:543:THR:O	1:B:543:THR:OG1	2.29	0.48
1:A:475:ARG:NH2	6:A:2220:HOH:O	2.47	0.48
1:C:274:ARG:NH2	6:C:2171:HOH:O	2.46	0.48
1:D:67:ASN:ND2	6:D:2041:HOH:O	2.46	0.47
1:A:356:ARG:NH2	1:A:383:THR:OG1	2.48	0.47
1:C:243:GLU:OE2	1:C:246:ARG:NH2	2.48	0.47
1:D:433:ARG:NH2	1:D:440:PRO:O	2.48	0.47
1:C:79:GLY:N	1:C:84:GLU:OE2	2.48	0.46
1:B:297[A]:PHE:CG	1:B:298:SER:N	2.82	0.46
1:C:331:VAL:N	1:C:334:GLU:OE2	2.49	0.46
1:C:107:ARG:NH2	6:C:2007:HOH:O	2.48	0.46
1:A:45:ARG:NH1	6:A:2034:HOH:O	2.48	0.46
1:D:112:THR:O	1:D:193:ASP:N	2.49	0.45
1:D:245:ARG:NH2	1:D:266:ASP:OD1	2.50	0.45
1:A:152:ARG:NH1	6:A:2035:HOH:O	2.50	0.45
1:B:460:ASP:OD2	1:B:462:SER:OG	2.35	0.44
1:D:46:ARG:NH2	1:D:94:GLU:OE2	2.50	0.44
1:C:297[A]:PHE:CG	1:C:298:SER:N	2.86	0.43
1:A:243:GLU:OE2	1:A:247:ARG:NE	2.51	0.43
1:C:304:ASP:OD1	1:C:304:ASP:N	2.50	0.43
1:D:74:ASP:OD2	1:D:341:TYR:OH	2.37	0.43
1:B:265:ASN:OD1	1:B:267:THR:OG1	2.36	0.43
1:A:433:ARG:NH2	1:A:439:TRP:O	2.51	0.43
1:A:282:VAL:O	1:A:284:HIS:N	2.52	0.43
1:A:107:ARG:NH1	1:A:189:ALA:O	2.52	0.43
1:C:234:GLY:O	6:C:2150:HOH:O	2.21	0.43
1:A:253:ARG:NH2	4:D:1991:CL:CL	2.89	0.43
1:B:425:VAL:O	1:B:503:TYR:N	2.52	0.42
1:D:452:GLU:OE2	1:D:465:TYR:OH	2.38	0.42
1:C:177:ARG:NH1	6:C:2124:HOH:O	2.52	0.42
1:D:425:VAL:O	1:D:503:TYR:N	2.53	0.41
1:C:332:LYS:NZ	1:C:333:ASP:OD2	2.54	0.41
1:B:304:ASP:N	1:B:304:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:GLY:N	6:A:2019:HOH:O	2.54	0.41
1:A:297[A]:PHE:CG	1:A:298:SER:N	2.88	0.41
1:A:170:ASN:OD1	1:A:302:VAL:N	2.54	0.41
1:A:246:ARG:NH1	6:A:2139:HOH:O	2.53	0.41
1:B:331:VAL:N	1:B:334:GLU:OE2	2.53	0.41
1:A:537:PRO:O	1:A:541:SER:OG	2.39	0.41
1:B:468:GLU:OE1	1:B:468:GLU:N	2.54	0.40
1:B:490:ASN:OD1	1:B:500:TRP:N	2.55	0.40
1:C:206:ALA:O	1:C:210:GLY:N	2.55	0.40
1:A:382:TYR:OH	1:A:404:ASP:OD2	2.40	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	541/543 (100%)	500 (92%)	35 (6%)	6 (1%)	21	66
1	B	538/543 (99%)	485 (90%)	45 (8%)	8 (2%)	15	56
1	C	542/543 (100%)	500 (92%)	36 (7%)	6 (1%)	21	66
1	D	543/543 (100%)	503 (93%)	34 (6%)	6 (1%)	21	66
All	All	2164/2172 (100%)	1988 (92%)	150 (7%)	26 (1%)	19	63

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	GLY
1	B	495	SER
1	B	542	ALA
1	D	497	SER
1	A	283	ASP
1	C	496	LYS
1	D	260	GLY
1	A	257	CYS

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Mol	Chain	Res	Type
1	A	261	GLY
1	A	497	SER
1	C	127	ALA
1	A	262	ALA
1	B	109	ALA
1	B	492	PRO
1	B	497	SER
1	C	110	SER
1	C	342	GLY
1	D	25	PRO
1	D	261	GLY
1	B	26	GLY
1	C	261	GLY
1	C	506	ALA
1	A	523	GLY
1	D	342	GLY
1	B	255	VAL
1	D	498	PRO

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	444/443 (100%)	411 (93%)	33 (7%)	20	56
1	B	441/443 (100%)	408 (92%)	33 (8%)	19	56
1	C	445/443 (100%)	410 (92%)	35 (8%)	18	52
1	D	446/443 (101%)	416 (93%)	30 (7%)	23	62
All	All	1776/1772 (100%)	1645 (93%)	131 (7%)	20	56

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	VAL
1	A	23	LYS
1	A	70	TYR

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Mol	Chain	Res	Type
1	A	81	GLU
1	A	84	GLU
1	A	107	ARG
1	A	132	VAL
1	A	136	ARG
1	A	149	MET
1	A	159	LEU
1	A	164	SER
1	A	200	PHE
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	253	ARG
1	A	257	CYS
1	A	267	THR
1	A	295	PHE
1	A	313	GLU
1	A	317	ASN
1	A	325	GLN
1	A	326	VAL
1	A	328	VAL
1	A	376	GLU
1	A	386	LEU
1	A	417	ARG
1	A	437	LEU
1	A	441	LEU
1	A	497	SER
1	A	540	LEU
1	A	543	THR
1	B	8	LEU
1	B	29	VAL
1	B	45	ARG
1	B	103	THR
1	B	136	ARG
1	B	141	VAL
1	B	149	MET
1	B	200	PHE
1	B	211	MET
1	B	245	ARG
1	B	265	ASN
1	B	287	HIS
1	B	295	PHE

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Mol	Chain	Res	Type
1	B	351	GLU
1	B	376	GLU
1	B	380	LEU
1	B	386	LEU
1	B	392	THR
1	B	438	THR
1	B	451	ILE
1	B	472	PHE
1	B	475	ARG
1	B	478	LYS
1	B	493	ARG
1	B	496	LYS
1	B	497	SER
1	B	515	LEU
1	B	518	LEU
1	B	522	ARG
1	B	524	LEU
1	B	536	LEU
1	B	540	LEU
1	B	543	THR
1	C	13	ARG
1	C	33	LEU
1	C	60	LEU
1	C	84	GLU
1	C	107	ARG
1	C	110	SER
1	C	132	VAL
1	C	136	ARG
1	C	146	LEU
1	C	211	MET
1	C	216	LEU
1	C	228	GLN
1	C	229	SER
1	C	257	CYS
1	C	276	ARG
1	C	295	PHE
1	C	298	SER
1	C	323	ASP
1	C	327	LEU
1	C	369[A]	GLN
1	C	369[B]	GLN
1	C	380	LEU

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Mol	Chain	Res	Type
1	C	386	LEU
1	C	387[A]	HIS
1	C	387[B]	HIS
1	C	421	GLN
1	C	438	THR
1	C	441	LEU
1	C	462	SER
1	C	466	THR
1	C	471	ILE
1	C	499	GLN
1	C	514	ASN
1	C	522	ARG
1	C	524	LEU
1	D	9	LEU
1	D	11	ARG
1	D	13	ARG
1	D	23	LYS
1	D	103	THR
1	D	110	SER
1	D	132	VAL
1	D	140	GLN
1	D	211	MET
1	D	216	LEU
1	D	281	LEU
1	D	285	GLU
1	D	291	GLN
1	D	295	PHE
1	D	298	SER
1	D	318	THR
1	D	333	ASP
1	D	364	ARG
1	D	372	ASP
1	D	386	LEU
1	D	413	GLN
1	D	437	LEU
1	D	438	THR
1	D	441	LEU
1	D	459	LEU
1	D	467	THR
1	D	491	ASP
1	D	496	LYS
1	D	499	GLN

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Mol	Chain	Res	Type
1	D	536	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 37 ligands modelled in this entry, 11 are monoatomic - leaving 26 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	$\# Z > 2$
5	SO4	A	1545	-	4,4,4	0.09	0	6,6,6	0.23	0
5	SO4	A	1546	-	4,4,4	0.15	0	6,6,6	0.09	0
5	SO4	A	1547	-	4,4,4	0.25	0	6,6,6	0.22	0
5	SO4	A	1548	-	4,4,4	0.16	0	6,6,6	0.17	0
5	SO4	A	1549	-	4,4,4	0.19	0	6,6,6	0.38	0
5	SO4	A	1550	-	4,4,4	0.18	0	6,6,6	0.13	0
2	TQV	A	600	1	18,20,21	1.10	1 (5%)	23,26,29	1.05	1 (4%)
3	NAG	A	701	1	12,14,15	0.52	0	15,19,21	0.91	1 (6%)
5	SO4	B	1545	-	4,4,4	0.18	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1546	-	4,4,4	0.19	0	6,6,6	0.14	0
5	SO4	B	1547	-	4,4,4	0.19	0	6,6,6	0.12	0
2	TQV	B	600	1	18,20,21	1.07	1 (5%)	23,26,29	1.31	5 (21%)
3	NAG	B	701	1	12,14,15	0.63	0	15,19,21	1.62	3 (20%)
3	NAG	B	702	1	12,14,15	0.49	0	15,19,21	1.49	1 (6%)
5	SO4	C	1547	-	4,4,4	0.21	0	6,6,6	0.13	0
5	SO4	C	1548	-	4,4,4	0.24	0	6,6,6	0.37	0
5	SO4	C	1549	-	4,4,4	0.20	0	6,6,6	0.10	0
2	TQV	C	600	1	18,20,21	1.05	1 (5%)	23,26,29	1.44	2 (8%)
3	NAG	C	701	1	12,14,15	0.45	0	15,19,21	1.03	1 (6%)
5	SO4	D	1545	-	4,4,4	0.19	0	6,6,6	0.11	0
5	SO4	D	1546	-	4,4,4	0.16	0	6,6,6	0.25	0
5	SO4	D	1547	-	4,4,4	0.20	0	6,6,6	0.09	0
2	TQV	D	600	1	18,20,21	1.08	1 (5%)	23,26,29	1.31	4 (17%)
3	NAG	D	701	1	12,14,15	0.44	0	15,19,21	1.30	1 (6%)
3	NAG	D	702	1	12,14,15	0.55	0	15,19,21	1.39	3 (20%)
3	NAG	D	703	1	12,14,15	0.49	0	15,19,21	1.55	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
5	SO4	A	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1547	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1548	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1549	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1550	-	-	0/0/0/0	0/0/0/0
2	TQV	A	600	1	-	0/7/9/11	0/2/2/2
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	SO4	B	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1547	-	-	0/0/0/0	0/0/0/0
2	TQV	B	600	1	-	0/7/9/11	0/2/2/2
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
5	SO4	C	1547	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1548	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1549	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TQV	C	600	1	-	0/7/9/11	0/2/2/2
3	NAG	C	701	1	-	0/6/23/26	0/1/1/1
5	SO4	D	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1547	-	-	0/0/0/0	0/0/0/0
2	TQV	D	600	1	-	0/7/9/11	0/2/2/2
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1	-	1/6/23/26	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TQV	C8-C9	-4.19	1.39	1.51
2	D	600	TQV	C8-C9	-4.18	1.39	1.51
2	B	600	TQV	C8-C9	-4.06	1.39	1.51
2	C	600	TQV	C8-C9	-3.91	1.40	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	NAG	O5-C5-C6	5.49	112.74	106.98
2	C	600	TQV	O1P-C8-C9	4.52	118.04	109.26
3	B	702	NAG	O5-C5-C4	4.18	115.96	110.65
3	D	701	NAG	O5-C5-C4	3.47	115.05	110.65
3	D	702	NAG	O5-C5-C4	3.34	114.89	110.65
3	B	701	NAG	C2-N2-C7	3.33	128.68	123.09
3	B	701	NAG	C3-C2-N2	2.97	116.28	111.76
3	B	701	NAG	O5-C5-C6	2.89	110.02	106.98
3	A	701	NAG	O5-C5-C6	2.80	109.92	106.98
3	D	702	NAG	O5-C5-C6	2.76	109.88	106.98
3	C	701	NAG	O5-C5-C6	2.75	109.86	106.98
2	A	600	TQV	P-O2P-C1	2.58	136.22	122.12
2	B	600	TQV	P-O2P-C1	2.55	136.04	122.12
2	D	600	TQV	C10-C9-C14	2.43	121.09	118.16
2	B	600	TQV	O2P-C1-C6	-2.40	116.45	118.48
2	D	600	TQV	O2P-C1-C6	-2.29	116.54	118.48
2	B	600	TQV	O1P-C8-C9	2.20	113.53	109.26
2	B	600	TQV	O2P-C1-C2	2.16	124.24	120.35
2	D	600	TQV	C7-C6-C1	-2.12	117.55	121.01
2	C	600	TQV	P-O2P-C1	2.10	133.61	122.12
2	B	600	TQV	C10-C9-C14	2.05	120.63	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	TQV	O1P-C8-C9	2.04	113.22	109.26
3	D	702	NAG	C3-C4-C5	2.03	113.82	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	NAG	C1-C2-C3-C4-C5-O5

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	540/543 (99%)	-0.32	9 (1%) 67 31	14, 33, 69, 138	0
1	B	539/543 (99%)	0.01	31 (5%) 22 12	26, 61, 107, 165	0
1	C	540/543 (99%)	-0.46	8 (1%) 70 32	14, 32, 72, 133	0
1	D	540/543 (99%)	-0.34	4 (0%) 84 44	21, 43, 79, 146	0
All	All	2159/2172 (99%)	-0.28	52 (2%) 56 25	14, 41, 94, 165	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	PRO	4.6
1	B	497	SER	4.5
1	B	543	THR	4.4
1	B	30	SER	4.2
1	D	493	ARG	4.2
1	B	21	ARG	4.0
1	C	493	ARG	4.0
1	B	59	VAL	3.8
1	B	32	PHE	3.7
1	A	497	SER	3.7
1	A	263	GLY	3.7
1	A	264	GLY	3.6
1	B	9	LEU	3.4
1	C	263	GLY	3.4
1	B	493	ARG	3.4
1	C	264	GLY	3.3
1	B	190	PHE	3.2
1	A	260	GLY	3.2
1	C	495	SER	3.0
1	C	261	GLY	3.0
1	D	21	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	495	SER	3.0
1	B	77	TYR	3.0
1	A	493	ARG	2.9
1	B	17	LEU	2.8
1	B	101	VAL	2.8
1	B	495	SER	2.8
1	B	189	ALA	2.7
1	B	351	GLU	2.7
1	B	6	PRO	2.7
1	B	109	ALA	2.7
1	B	349	ASP	2.7
1	B	346	PHE	2.6
1	B	496	LYS	2.6
1	B	353	LEU	2.6
1	C	496	LYS	2.5
1	C	262	ALA	2.5
1	B	7	GLN	2.5
1	A	262	ALA	2.5
1	A	543	THR	2.4
1	B	23	LYS	2.4
1	B	20	ILE	2.4
1	B	18	ARG	2.3
1	B	22	LEU	2.3
1	B	110	SER	2.3
1	D	495	SER	2.2
1	B	194	PRO	2.2
1	B	191	GLY	2.2
1	B	348	LYS	2.2
1	D	543	THR	2.2
1	B	103	THR	2.0
1	C	260	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(Å ²)	Q<0.9
4	CL	C	1544	1/1	0.14	17.67	55,55,55,55	0
3	NAG	D	703	14/15	0.33	13.86	109,127,137,141	0
5	SO4	A	1550	5/5	0.47	7.69	122,123,127,131	0
3	NAG	D	701	14/15	0.23	3.94	77,101,115,121	0
5	SO4	B	1546	5/5	0.29	3.34	166,166,167,169	0
5	SO4	D	1546	5/5	0.34	3.08	116,119,120,123	0
3	NAG	A	701	14/15	0.36	2.87	96,119,122,123	0
5	SO4	C	1548	5/5	0.18	2.80	54,56,62,66	0
5	SO4	C	1547	5/5	0.15	2.39	75,82,83,87	0
2	TQV	C	600	19/20	0.21	2.37	22,49,83,83	8
5	SO4	C	1549	5/5	0.26	2.34	113,116,118,119	0
3	NAG	D	702	14/15	0.32	1.89	60,102,109,110	0
3	NAG	C	701	14/15	0.36	1.89	120,126,134,134	0
2	TQV	A	600	19/20	0.22	1.89	27,44,57,59	8
5	SO4	D	1547	5/5	0.38	1.85	138,139,141,144	0
3	NAG	B	702	14/15	0.47	1.80	68,106,117,120	0
5	SO4	A	1548	5/5	0.22	1.70	92,93,96,100	0
2	TQV	D	600	19/20	0.22	1.58	34,46,116,118	8
2	TQV	B	600	19/20	0.23	1.58	42,60,97,97	8
5	SO4	B	1547	5/5	0.16	1.14	119,122,123,128	0
5	SO4	D	1545	5/5	0.17	0.93	68,69,72,79	0
3	NAG	B	701	14/15	0.17	0.84	98,103,107,110	0
5	SO4	A	1545	5/5	0.13	0.13	70,73,74,75	0
5	SO4	A	1549	5/5	0.22	0.06	106,116,120,121	0
5	SO4	A	1547	5/5	0.14	-0.19	59,60,71,72	0
4	CL	D	1544	1/1	0.20	-0.43	84,84,84,84	0
4	CL	C	1546	1/1	0.14	-1.10	72,72,72,72	0
4	CL	C	1990	1/1	0.10	-1.44	50,50,50,50	0
4	CL	D	1991	1/1	0.10	-1.47	82,82,82,82	0
5	SO4	B	1545	5/5	0.13	-1.48	75,90,92,97	0
5	SO4	A	1546	5/5	0.10	-1.53	110,110,112,115	0
4	CL	B	1544	1/1	0.18	-1.84	66,66,66,66	0
4	CL	C	1545	1/1	0.06	-2.67	35,35,35,35	0
4	CL	A	1990	1/1	0.07	-3.06	59,59,59,59	0
4	CL	A	1544	1/1	0.06	-4.44	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	A	1991	1/1	0.13	-14.29	66,66,66,66	0
4	CL	D	1990	1/1	0.11	-	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.