



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 5HCU / pdb_00005hcu
Title : Crystal structure of mouse acetylcholinesterase inhibited by DFP
Authors : Tran, T.H.; Tong, L.
Deposited on : 2016-01-04
Resolution : 2.42 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

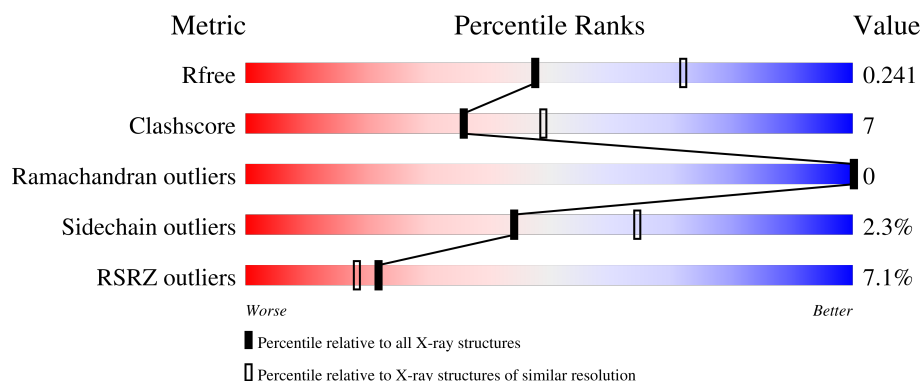
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	543	7% 87% 11% ..
1	B	543	7% 84% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8492 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	537	Total	C	N	O	P	S	0	0	0
			4207	2698	728	765	1	15			
1	B	530	Total	C	N	O	P	S	2	0	0
			4154	2668	718	753	1	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ASP	-	expression tag	UNP P21836
A	-1	PRO	-	expression tag	UNP P21836
A	0	MET	-	expression tag	UNP P21836
B	-2	ASP	-	expression tag	UNP P21836
B	-1	PRO	-	expression tag	UNP P21836
B	0	MET	-	expression tag	UNP P21836

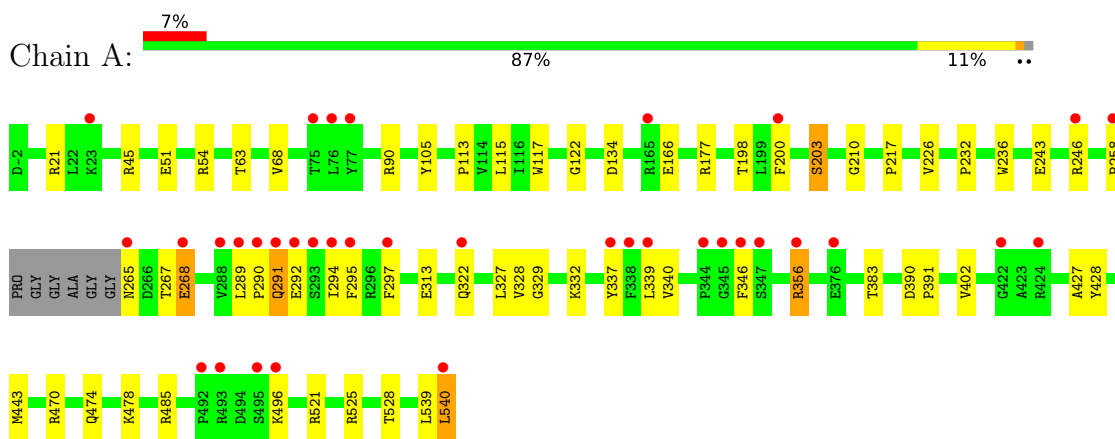
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	63	Total	O	0	0
			63	63		

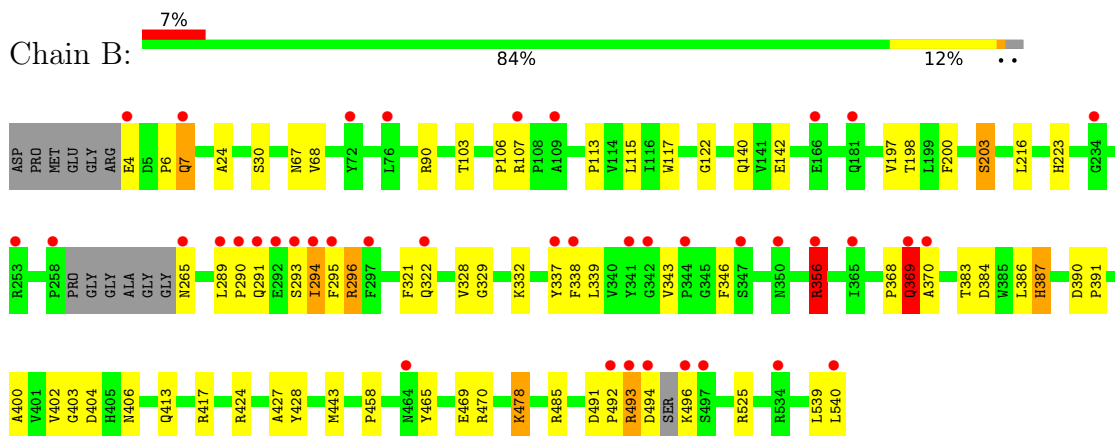
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	78.58Å 114.35Å 226.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.42 50.00 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.42) 88.4 (50.00-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.234 0.215 , 0.241	Depositor DCC
R_{free} test set	3969 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8492	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIS

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	0.75	2/4318 (0.0%)	0.83	5/5898 (0.1%)
1	B	0.75	2/4263 (0.0%)	0.98	20/5823 (0.3%)
All	All	0.75	4/8581 (0.0%)	0.91	25/11721 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	ARG	CZ-NH2	-13.12	1.16	1.33
1	A	290	PRO	N-CD	-8.42	1.35	1.47
1	B	356	ARG	CD-NE	-7.67	1.35	1.46
1	A	258	PRO	N-CD	-7.63	1.37	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	368	PRO	CA-C-N	-18.82	94.06	122.86
1	B	368	PRO	C-N-CA	-18.82	94.06	122.86
1	B	369	GLN	O-C-N	-16.84	100.64	122.20
1	B	6	PRO	CA-C-N	-10.41	106.12	122.67
1	B	6	PRO	C-N-CA	-10.41	106.12	122.67
1	B	493	ARG	CA-C-N	-7.55	108.11	121.70
1	B	493	ARG	C-N-CA	-7.55	108.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	A	267	THR	CA-C-N	6.26	129.49	120.79
1	A	267	THR	C-N-CA	6.26	129.49	120.79
1	A	268	GLU	O-C-N	6.23	128.75	122.08
1	B	469	GLU	CA-C-N	-5.99	111.12	121.66
1	B	469	GLU	C-N-CA	-5.99	111.12	121.66
1	B	321	PHE	CA-C-N	5.92	128.49	120.38
1	B	321	PHE	C-N-CA	5.92	128.49	120.38
1	B	294	ILE	CA-C-N	-5.91	114.23	122.74
1	B	294	ILE	C-N-CA	-5.91	114.23	122.74
1	B	356	ARG	NH1-CZ-NH2	5.74	126.76	119.30
1	A	289	LEU	CA-C-N	5.33	124.78	119.24
1	A	289	LEU	C-N-CA	5.33	124.78	119.24
1	B	289	LEU	CA-C-N	5.30	126.46	119.84
1	B	289	LEU	C-N-CA	5.30	126.46	119.84
1	B	107	ARG	CA-C-N	5.17	125.18	119.90
1	B	107	ARG	C-N-CA	5.17	125.18	119.90
1	B	293	SER	N-CA-C	5.06	116.61	108.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	GLN	Mainchain
1	B	7	GLN	Mainchain

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	4207	0	4098	62	1
1	B	4154	0	4047	58	1
2	A	68	0	0	4	0
2	B	63	0	0	5	0
All	All	8492	0	8145	120	1

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 7.

All (120) 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:265:ASN:CB	1:A:268:GLU:OE1	1.67	1.39
1:B:295:PHE:CE2	1:B:338:PHE:CD2	2.17	1.32
1:A:265:ASN:HB3	1:A:268:GLU:CD	1.65	1.20
1:A:485:ARG:NH1	2:A:601:HOH:O	1.80	1.11
1:A:115:LEU:HB3	1:A:200:PHE:HE2	0.99	1.10
1:B:295:PHE:CZ	1:B:338:PHE:CE2	2.40	1.10
1:A:115:LEU:HB3	1:A:200:PHE:CE2	1.88	1.09
1:A:291:GLN:NE2	1:A:292:GLU:H	1.50	1.08
1:A:356:ARG:NH2	1:A:383:THR:OG1	1.86	1.08
1:A:265:ASN:ND2	1:A:268:GLU:OE2	1.89	1.06
1:A:265:ASN:ND2	1:A:268:GLU:CD	2.22	0.98
1:A:243:GLU:OE2	1:A:246:ARG:NH1	1.98	0.96
1:B:295:PHE:HE2	1:B:338:PHE:CD2	1.82	0.93
1:A:265:ASN:HB3	1:A:268:GLU:OE1	0.74	0.91
1:A:265:ASN:HD22	1:A:268:GLU:CD	1.78	0.91
1:A:291:GLN:CD	1:A:292:GLU:H	1.78	0.91
1:B:295:PHE:CE2	1:B:338:PHE:CG	2.61	0.88
1:A:265:ASN:CB	1:A:268:GLU:CD	2.34	0.87
1:A:166:GLU:OE1	2:A:602:HOH:O	1.91	0.86
1:A:291:GLN:NE2	1:A:292:GLU:HB2	1.91	0.85
1:B:295:PHE:CZ	1:B:338:PHE:CD2	2.63	0.85
1:A:115:LEU:CB	1:A:200:PHE:HE2	1.88	0.83
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.12	0.82
1:A:291:GLN:NE2	1:A:292:GLU:N	2.30	0.79
1:A:117:TRP:HE3	1:A:200:PHE:CD1	2.01	0.79
1:A:265:ASN:CG	1:A:268:GLU:CD	2.51	0.79
1:B:424:ARG:NH2	2:B:602:HOH:O	2.14	0.78
1:B:142:GLU:OE1	1:B:478:LYS:HE2	1.87	0.74
1:A:115:LEU:HD22	1:A:200:PHE:CE2	2.23	0.73
1:A:115:LEU:HD22	1:A:200:PHE:CD2	2.25	0.72
1:B:494:ASP:OD2	1:B:496:LYS:HD3	1.90	0.71
1:B:7:GLN:OE1	1:B:106:PRO:CB	2.40	0.69
1:A:291:GLN:HE22	1:A:292:GLU:HB2	1.57	0.69
1:B:369:GLN:N	1:B:369:GLN:OE1	2.26	0.69
1:B:30:SER:HB2	1:B:103:THR:HG22	1.75	0.68
1:B:295:PHE:HZ	1:B:338:PHE:CE2	2.13	0.65
1:B:404:ASP:OD1	1:B:525:ARG:NH1	2.30	0.64
1:B:67:ASN:ND2	2:B:601:HOH:O	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLN:OE1	1:B:106:PRO:HB2	1.99	0.63
1:A:243:GLU:CD	1:A:246:ARG:HH11	2.06	0.63
1:B:197:VAL:H	1:B:223:HIS:CD2	2.16	0.63
1:A:117:TRP:CE3	1:A:200:PHE:CD1	2.85	0.63
1:A:236:TRP:CD1	1:A:295:PHE:CE1	2.88	0.62
1:B:197:VAL:H	1:B:223:HIS:HD2	1.47	0.62
1:B:356:ARG:NH2	1:B:383:THR:OG1	2.30	0.61
1:B:265:ASN:ND2	2:B:605:HOH:O	2.32	0.61
1:A:291:GLN:CD	1:A:292:GLU:N	2.57	0.60
1:B:295:PHE:CD2	1:B:338:PHE:CG	2.91	0.59
1:A:134:ASP:O	2:A:603:HOH:O	2.17	0.57
1:A:291:GLN:NE2	1:A:292:GLU:CB	2.65	0.57
1:A:539:LEU:C	1:A:540:LEU:HD12	2.30	0.57
1:A:117:TRP:HE3	1:A:200:PHE:CE1	2.22	0.56
1:B:294:ILE:O	1:B:295:PHE:HB2	2.08	0.53
1:B:400:ALA:HA	2:B:613:HOH:O	2.08	0.53
1:B:113:PRO:HG2	1:B:485:ARG:HG3	1.91	0.52
1:A:337:TYR:HA	1:A:443:MET:HE3	1.91	0.51
1:B:290:PRO:HB2	1:B:291:GLN:HG3	1.93	0.51
1:A:525:ARG:HG2	1:A:528:THR:HB	1.90	0.51
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.44	0.50
1:B:539:LEU:O	1:B:540:LEU:HD23	2.12	0.49
1:B:294:ILE:HD11	1:B:402:VAL:HG21	1.94	0.49
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.94	0.49
1:A:236:TRP:CD2	1:A:295:PHE:HE1	2.31	0.49
1:B:337:TYR:HA	1:B:443:MET:HE3	1.95	0.48
1:A:236:TRP:CG	1:A:295:PHE:HE1	2.31	0.48
1:B:203:MIS:O2P	1:B:203:MIS:H32	2.13	0.48
1:A:21:ARG:HD2	1:A:105:TYR:CZ	2.49	0.48
1:B:295:PHE:HE2	1:B:338:PHE:HD2	1.53	0.48
1:B:492:PRO:C	1:B:493:ARG:HG2	2.40	0.47
1:A:122:GLY:N	1:A:203:MIS:O1P	2.41	0.47
1:A:356:ARG:NH2	1:A:383:THR:CG2	2.78	0.47
1:B:295:PHE:CZ	1:B:338:PHE:CZ	2.99	0.47
1:B:493:ARG:O	1:B:494:ASP:C	2.55	0.47
1:B:295:PHE:CD2	1:B:402:VAL:CG1	2.99	0.47
1:A:117:TRP:CE3	1:A:200:PHE:CE1	3.02	0.46
1:B:117:TRP:HE3	1:B:200:PHE:CD2	2.33	0.46
1:B:294:ILE:O	1:B:295:PHE:CB	2.62	0.46
1:B:478:LYS:HE3	1:B:478:LYS:HB2	1.65	0.46
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TRP:CE3	1:A:200:PHE:HD1	2.32	0.46
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.50	0.45
1:B:390:ASP:HA	1:B:391:PRO:HD3	1.79	0.45
1:A:236:TRP:CE2	1:A:295:PHE:HE1	2.34	0.45
1:B:117:TRP:HE3	1:B:200:PHE:CE2	2.34	0.45
1:B:369:GLN:O	1:B:370:ALA:C	2.59	0.45
1:A:265:ASN:CB	1:A:268:GLU:OE2	2.62	0.45
1:A:113:PRO:HG2	1:A:485:ARG:HG3	1.98	0.45
1:B:117:TRP:CE3	1:B:200:PHE:CE2	3.04	0.45
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.51	0.45
1:A:236:TRP:CG	1:A:295:PHE:CE1	3.05	0.45
1:B:122:GLY:N	1:B:203:MIS:O2P	2.46	0.45
1:B:384:ASP:OD2	1:B:387:HIS:HD2	2.00	0.44
1:A:236:TRP:CD1	1:A:295:PHE:HE1	2.34	0.44
1:A:200:PHE:HB3	1:A:226:VAL:HB	1.99	0.43
1:B:328:VAL:O	1:B:427:ALA:HA	2.18	0.43
1:B:403:GLY:HA3	2:B:613:HOH:O	2.17	0.43
1:B:294:ILE:HD13	1:B:343:VAL:CG2	2.49	0.43
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.42
1:A:356:ARG:NH2	1:A:383:THR:CB	2.79	0.42
1:A:470:ARG:O	1:A:474:GLN:HG3	2.20	0.42
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.55	0.42
1:B:68:VAL:HG23	1:B:90:ARG:HB2	2.02	0.42
1:B:115:LEU:HD23	1:B:198:THR:HB	2.01	0.42
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.50	0.42
1:A:226:VAL:HG22	1:A:327:LEU:HB3	2.02	0.42
1:A:294:ILE:HD11	1:A:402:VAL:HG21	2.01	0.42
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.54	0.42
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.54	0.42
1:B:30:SER:HB2	1:B:103:THR:CG2	2.49	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.41
1:A:115:LEU:HD23	1:A:198:THR:HB	2.03	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.81	0.41
1:B:494:ASP:OD1	1:B:496:LYS:HG3	2.20	0.41
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.01	0.41
1:B:386:LEU:HD23	1:B:386:LEU:HA	1.92	0.41
1:B:413:GLN:O	1:B:417:ARG:HG2	2.21	0.41
1:A:521:ARG:NH1	2:A:607:HOH:O	2.32	0.41
1:B:117:TRP:CE3	1:B:200:PHE:CD2	3.09	0.41
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.55	0.40
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:O	1:B:493:ARG:NH1[4_445]	1.85	0.35

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	532/543 (98%)	516 (97%)	16 (3%)	0	100	100
1	B	523/543 (96%)	506 (97%)	17 (3%)	0	100	100
All	All	1055/1086 (97%)	1022 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	431 (98%)	11 (2%)	42	62
1	B	436/443 (98%)	427 (98%)	9 (2%)	47	67
All	All	878/886 (99%)	858 (98%)	20 (2%)	44	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	291	GLN
1	A	297	PHE
1	A	313	GLU
1	A	322	GLN
1	A	332	LYS
1	A	340	VAL
1	A	356	ARG
1	A	478	LYS
1	A	496	LYS
1	A	540	LEU
1	B	4	GLU
1	B	216	LEU
1	B	296	ARG
1	B	322	GLN
1	B	332	LYS
1	B	356	ARG
1	B	387	HIS
1	B	470	ARG
1	B	478	LYS

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

Mol	Chain	Res	Type
1	A	140	GLN
1	A	291	GLN
1	A	413	GLN
1	B	181	GLN
1	B	223	HIS
1	B	387	HIS
1	B	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	MIS	A	203	1	11,12,13	1.36	1 (9%)	11,16,18	1.67	3 (27%)
1	MIS	B	203	1	11,12,13	1.00	0	11,16,18	1.17	1 (9%)

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	MIS	A	203	1	-	9/11/13/15	-
1	MIS	B	203	1	-	9/11/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	MIS	P-O2P	2.74	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	MIS	O3P-P-O2P	-2.97	100.31	109.81
1	A	203	MIS	O1P-P-O3P	2.74	117.86	106.70
1	B	203	MIS	O3P-P-O2P	2.26	117.03	109.81
1	A	203	MIS	OG-P-O2P	-2.16	100.38	108.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	MIS	N-CA-CB-OG
1	A	203	MIS	C-CA-CB-OG
1	A	203	MIS	CB-OG-P-O1P
1	A	203	MIS	CB-OG-P-O2P
1	A	203	MIS	CB-OG-P-O3P
1	A	203	MIS	C1-O3P-P-OG

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Mol	Chain	Res	Type	Atoms
1	A	203	MIS	C1-O3P-P-O1P
1	A	203	MIS	C3-C1-O3P-P
1	B	203	MIS	N-CA-CB-OG
1	B	203	MIS	C-CA-CB-OG
1	B	203	MIS	CB-OG-P-O2P
1	B	203	MIS	CB-OG-P-O3P
1	B	203	MIS	C1-O3P-P-OG
1	B	203	MIS	C3-C1-O3P-P
1	A	203	MIS	C1-O3P-P-O2P
1	B	203	MIS	CB-OG-P-O1P
1	B	203	MIS	C1-O3P-P-O1P
1	B	203	MIS	C1-O3P-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	MIS	1	0
1	B	203	MIS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	536/543 (98%)	0.31	36 (6%) 24 20	39, 54, 88, 140	1 (0%)
1	B	529/543 (97%)	0.47	40 (7%) 20 16	41, 59, 91, 132	2 (0%)
All	All	1065/1086 (98%)	0.39	76 (7%) 22 18	39, 56, 90, 140	3 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	LEU	8.1
1	A	290	PRO	6.6
1	A	540	LEU	6.5
1	B	295	PHE	6.0
1	B	294	ILE	5.8
1	A	258	PRO	5.8
1	A	294	ILE	5.5
1	B	258	PRO	5.5
1	B	496	LYS	5.1
1	B	289	LEU	4.9
1	B	342	GLY	4.9
1	A	496	LYS	4.8
1	A	289	LEU	4.8
1	A	295	PHE	4.7
1	A	337	TYR	4.6
1	B	356	ARG	4.4
1	B	494	ASP	4.4
1	B	291	GLN	4.2
1	B	493	ARG	4.1
1	A	291	GLN	4.0
1	A	297	PHE	3.9
1	A	346	PHE	3.9
1	A	338	PHE	3.8
1	B	492	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	SER	3.8
1	A	268	GLU	3.8
1	A	200	PHE	3.7
1	B	337	TYR	3.5
1	B	4	GLU	3.5
1	B	497	SER	3.5
1	A	492	PRO	3.4
1	B	290	PRO	3.3
1	A	288	VAL	3.2
1	B	293	SER	3.1
1	B	350	ASN	3.1
1	A	339	LEU	3.0
1	B	7	GLN	3.0
1	A	292	GLU	3.0
1	B	369	GLN	2.9
1	B	297	PHE	2.9
1	A	344	PRO	2.8
1	B	181	GLN	2.7
1	B	347	SER	2.7
1	A	376	GLU	2.7
1	B	341	TYR	2.7
1	B	464	ASN	2.6
1	A	493	ARG	2.6
1	B	166	GLU	2.6
1	A	422	GLY	2.6
1	A	347	SER	2.6
1	A	495	SER	2.6
1	A	265	ASN	2.5
1	A	165	ARG	2.5
1	A	75	THR	2.5
1	B	322	GLN	2.4
1	A	424	ARG	2.4
1	A	77	TYR	2.4
1	B	292	GLU	2.4
1	A	76	LEU	2.3
1	B	107	ARG	2.3
1	B	234	GLY	2.3
1	B	534	ARG	2.3
1	B	338	PHE	2.2
1	B	370	ALA	2.2
1	B	253	ARG	2.2
1	B	76	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	344	PRO	2.2
1	A	23	LYS	2.1
1	B	265	ASN	2.1
1	B	72	TYR	2.1
1	B	109	ALA	2.1
1	A	322	GLN	2.1
1	A	246	ARG	2.1
1	A	356	ARG	2.1
1	B	365	ILE	2.1
1	A	345	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
1	MIS	A	203	13/14	0.85	0.21	43,56,117,132	0
1	MIS	B	203	13/14	0.85	0.20	53,65,117,118	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.