



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:20 AM UTC

PDB ID : 1B7A / pdb_00001b7a
Title : STRUCTURE OF THE PHOSPHATIDYLETHANOLAMINE-BINDING
PROTEIN FROM BOVINE BRAIN
Authors : Serre, L.; Vallee, B.; Bureau, N.; Schoentgen, F.; Zelwer, C.
Deposited on : 1999-01-21
Resolution : 2.25 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

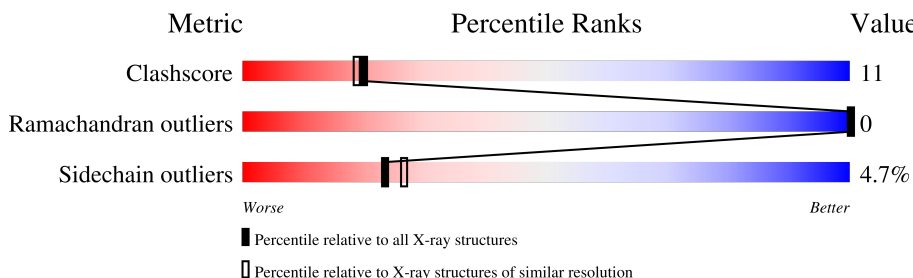
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	

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	OPE	A	1501[A]	-	X	-	-
2	OPE	A	1501[B]	-	X	-	-
2	OPE	B	2501[A]	-	-	X	-
2	OPE	B	2501[B]	-	X	-	-

2 Entry composition [i](#)

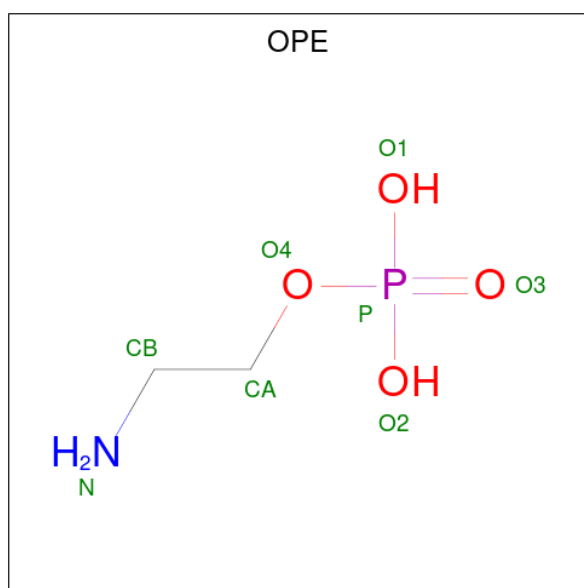
There are 3 unique types of molecules in this entry. The entry contains 3145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHATIDYLETHANOLAMINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	1	0
			1470	936	252	279	3			
1	B	186	Total	C	N	O	S	0	3	0
			1479	940	254	282	3			

- Molecule 2 is PHOSPHORIC ACID MONO-(2-AMINO-ETHYL) ESTER (CCD ID: OPE) (formula: $C_2H_8NO_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			16	4	2	8	2		
2	B	1	Total	C	N	O	P	0	1
			16	4	2	8	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total 93	O 93	0	0
3	B	71	Total 71	O 71	0	0

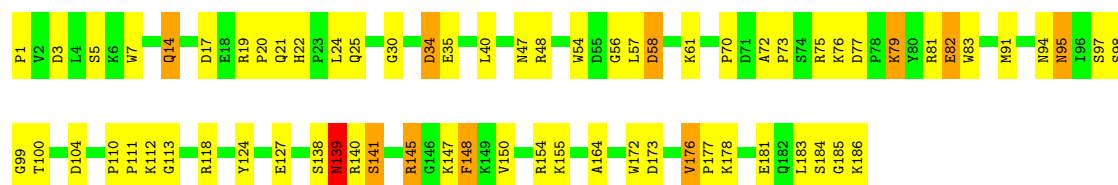
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

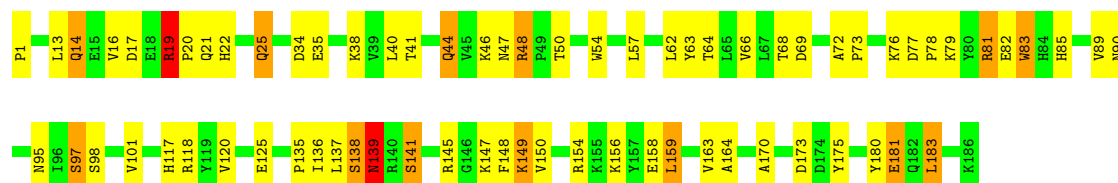
• Molecule 1: PHOSPHATIDYLETHANOLAMINE-BINDING PROTEIN

Chain A: 



• Molecule 1: PHOSPHATIDYLETHANOLAMINE-BINDING PROTEIN

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.20Å 77.16Å 107.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 2.25	Depositor
% Data completeness (in resolution range)	90.0 (12.50-2.25)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	4.90	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3145	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.94	0/1513	2.10	54/2056 (2.6%)
1	B	0.87	0/1521	2.01	53/2063 (2.6%)
All	All	0.90	0/3034	2.05	107/4119 (2.6%)

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	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	SER	CA-C-O	-12.97	103.22	119.31
1	A	48	ARG	NE-CZ-NH2	11.65	129.69	119.20
1	B	138	SER	CA-C-N	11.11	138.38	120.60
1	B	138	SER	C-N-CA	11.11	138.38	120.60
1	A	139	ASN	CB-CA-C	-11.03	87.05	110.32
1	A	148	PHE	CA-CB-CG	10.70	124.50	113.80
1	A	185	GLY	CA-C-N	10.61	140.80	121.70
1	A	185	GLY	C-N-CA	10.61	140.80	121.70
1	B	81	ARG	CD-NE-CZ	9.76	138.06	124.40
1	A	95	ASN	OD1-CG-ND2	-9.40	113.19	122.60
1	B	139	ASN	N-CA-CB	-8.89	95.21	110.32
1	A	76	LYS	CA-C-O	-8.83	111.06	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ASN	CB-CA-C	-8.76	91.84	110.32
1	B	77	ASP	CA-CB-CG	8.67	121.27	112.60
1	A	138	SER	CA-C-N	8.63	134.41	120.60
1	A	138	SER	C-N-CA	8.63	134.41	120.60
1	B	148	PHE	CA-CB-CG	8.60	122.40	113.80
1	A	40	LEU	CA-C-O	-8.54	111.94	121.51
1	B	181	GLU	N-CA-CB	8.32	122.36	110.12
1	B	97	SER	CA-C-O	-7.99	111.01	119.00
1	B	138	SER	CA-C-O	7.96	131.20	121.89
1	A	150	VAL	CA-C-O	-7.75	112.89	120.95
1	A	139	ASN	N-CA-CB	-7.50	97.56	110.32
1	A	140	ARG	CD-NE-CZ	7.37	134.71	124.40
1	B	139	ASN	N-CA-C	7.32	121.31	112.38
1	A	185	GLY	CA-C-O	7.26	131.47	121.46
1	A	97[A]	SER	CA-C-O	7.21	130.45	118.91
1	B	98	SER	N-CA-C	-7.01	101.79	110.41
1	A	104	ASP	CA-C-N	6.97	130.71	120.95
1	A	104	ASP	C-N-CA	6.97	130.71	120.95
1	A	95	ASN	CB-CG-OD1	6.94	134.69	120.80
1	A	186	LYS	N-CA-C	6.93	130.40	111.00
1	A	48	ARG	NH1-CZ-NH2	-6.88	110.36	119.30
1	B	76	LYS	CA-C-O	-6.73	113.76	120.82
1	B	136	ILE	CA-C-N	-6.69	113.23	122.93
1	B	136	ILE	C-N-CA	-6.69	113.23	122.93
1	A	113	GLY	CA-C-O	-6.68	111.96	119.04
1	A	184	SER	CA-CB-OG	-6.63	97.83	111.10
1	B	25	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	94	ASN	CA-C-O	6.48	127.60	119.95
1	B	50	THR	N-CA-C	-6.43	105.26	113.23
1	A	81	ARG	CD-NE-CZ	6.42	133.38	124.40
1	A	176	VAL	CA-C-O	6.38	123.56	118.71
1	A	155	LYS	CA-C-O	6.27	127.18	119.97
1	B	83	TRP	CA-C-O	-6.26	114.08	120.84
1	B	159	LEU	CA-C-O	-6.21	113.91	121.36
1	B	19	ARG	NH1-CZ-NH2	-6.19	111.25	119.30
1	A	99	GLY	O-C-N	6.19	128.76	122.88
1	A	24	LEU	O-C-N	-6.17	115.82	123.04
1	A	47	ASN	CA-C-O	6.15	129.00	121.56
1	B	149	LYS	CA-C-N	-6.05	112.17	120.46
1	B	149	LYS	C-N-CA	-6.05	112.17	120.46
1	B	98	SER	O-C-N	-6.04	115.28	122.65
1	B	101	VAL	CA-C-O	6.04	129.05	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASN	CB-CA-C	-5.90	101.07	111.05
1	B	101	VAL	O-C-N	-5.87	116.17	122.45
1	B	17	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	156	LYS	CA-C-O	-5.79	113.56	120.10
1	A	58	ASP	CA-C-O	5.75	124.88	119.59
1	A	145	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	B	19	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	145	ARG	CA-C-N	5.71	129.85	121.05
1	B	145	ARG	C-N-CA	5.71	129.85	121.05
1	B	138	SER	O-C-N	-5.60	116.13	122.68
1	B	170	ALA	CA-C-O	-5.58	115.09	121.40
1	B	117	HIS	CA-CB-CG	5.58	119.38	113.80
1	A	17	ASP	N-CA-CB	5.53	119.97	111.46
1	A	173	ASP	CA-C-O	-5.47	115.50	121.14
1	B	78	PRO	CA-C-O	-5.46	117.27	121.31
1	A	139	ASN	N-CA-C	5.46	119.04	112.38
1	A	127	GLU	CA-C-O	5.45	125.64	119.27
1	A	82	GLU	CA-C-N	-5.44	115.76	122.84
1	A	82	GLU	C-N-CA	-5.44	115.76	122.84
1	A	75	ARG	NH1-CZ-NH2	5.43	126.35	119.30
1	A	47	ASN	O-C-N	-5.34	116.21	123.10
1	A	25	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	A	91	MET	CA-C-O	-5.30	114.43	120.58
1	A	79	LYS	CA-C-O	-5.28	114.13	120.10
1	A	81	ARG	O-C-N	-5.28	115.84	123.07
1	A	81	ARG	CA-C-N	5.26	131.16	121.70
1	A	81	ARG	C-N-CA	5.26	131.16	121.70
1	B	135	PRO	CB-CA-C	-5.24	104.53	111.23
1	B	158	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	148	PHE	O-C-N	5.22	129.11	123.10
1	B	85	HIS	CA-CB-CG	-5.22	108.58	113.80
1	B	47	ASN	OD1-CG-ND2	-5.20	117.41	122.60
1	B	44	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	100	THR	O-C-N	5.16	129.12	122.93
1	B	81	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	75	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	150	VAL	O-C-N	5.09	126.80	121.87
1	B	50	THR	N-CA-CB	5.08	118.36	110.44
1	B	118	ARG	O-C-N	-5.08	117.10	123.04
1	B	95	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	B	40	LEU	CA-C-O	-5.07	115.83	121.51
1	B	66	VAL	CA-C-N	-5.07	115.66	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	VAL	C-N-CA	-5.07	115.66	122.86
1	A	30	GLY	CA-C-O	5.07	125.43	119.45
1	B	76	LYS	CB-CA-C	-5.07	102.92	110.88
1	B	183	LEU	CA-C-N	5.07	131.46	121.58
1	B	183	LEU	C-N-CA	5.07	131.46	121.58
1	B	64	THR	CA-C-O	-5.05	115.19	120.80
1	B	68	THR	O-C-N	-5.03	117.05	123.24
1	B	19	ARG	CD-NE-CZ	5.02	131.43	124.40
1	A	34	ASP	CA-CB-CG	-5.02	107.58	112.60
1	A	35	GLU	O-C-N	-5.01	117.55	123.41
1	A	100	THR	CA-CB-OG1	-5.01	102.08	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ASN	Mainchain
1	B	13	LEU	Mainchain
1	B	139	ASN	Mainchain
1	B	83	TRP	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	1470	0	1435	26	0
1	B	1479	0	1436	32	0
2	A	16	0	4	5	0
2	B	16	0	4	7	0
3	A	93	0	0	0	0
3	B	71	0	0	5	0
All	All	3145	0	2879	67	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 11.

All (67) 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)
2:B:2501[B]:OPE:N	2:B:2501[B]:OPE:CB	1.69	1.56
2:A:1501[A]:OPE:N	2:A:1501[A]:OPE:CB	1.71	1.51
2:A:1501[B]:OPE:N	2:A:1501[B]:OPE:CB	1.69	1.50
2:B:2501[A]:OPE:N	2:B:2501[A]:OPE:CB	1.71	1.50
2:B:2501[A]:OPE:N	2:B:2501[A]:OPE:CA	2.07	1.18
2:A:1501[A]:OPE:N	2:A:1501[A]:OPE:CA	2.05	1.17
2:B:2501[B]:OPE:N	2:B:2501[B]:OPE:CA	2.10	1.12
2:A:1501[B]:OPE:N	2:A:1501[B]:OPE:CA	2.12	1.11
1:A:14:GLN:HE21	1:A:14:GLN:H	1.14	0.96
1:A:58:ASP:HB3	1:A:61:LYS:HD2	1.61	0.83
1:B:14:GLN:HE21	1:B:14:GLN:H	1.30	0.80
1:B:19:ARG:NH1	1:B:20:PRO:O	2.19	0.75
1:B:19:ARG:HH11	1:B:19:ARG:HG2	1.54	0.72
1:A:14:GLN:H	1:A:14:GLN:NE2	1.88	0.70
1:B:16:VAL:HG21	1:B:120:VAL:HG21	1.74	0.70
1:B:73:PRO:HA	2:B:2501[B]:OPE:CB	2.31	0.61
1:A:14:GLN:HE21	1:A:14:GLN:N	1.92	0.61
1:B:35:GLU:HG2	3:B:2569:HOH:O	2.02	0.58
1:A:54:TRP:CH2	1:A:57:LEU:HD13	2.39	0.57
1:B:141:SER:HA	1:B:183:LEU:O	2.06	0.55
1:A:124:TYR:CE2	1:A:154:ARG:HG2	2.41	0.55
1:A:3:ASP:OD1	1:A:5:SER:OG	2.25	0.55
1:B:25:GLN:HE21	1:B:25:GLN:HA	1.73	0.53
1:A:95:ASN:C	1:A:95:ASN:HD22	2.16	0.53
1:B:22:HIS:O	1:B:164:ALA:HA	2.07	0.53
2:B:2501[A]:OPE:N	2:B:2501[A]:OPE:O4	2.42	0.52
1:B:48:ARG:HG2	3:B:2536:HOH:O	2.09	0.52
1:A:58:ASP:CB	1:A:61:LYS:HD2	2.37	0.50
1:B:41:THR:OG1	1:B:44:GLN:HG3	2.11	0.50
1:B:34:ASP:OD1	1:B:38:LYS:HD2	2.12	0.49
1:A:82:GLU:HB2	1:A:148:PHE:O	2.12	0.48
1:A:141:SER:HA	1:A:183:LEU:O	2.12	0.48
1:B:1:PRO:HD2	3:B:2569:HOH:O	2.13	0.48
1:A:112:LYS:HB2	1:A:172:TRP:CD1	2.49	0.48
1:B:149:LYS:O	1:B:150:VAL:C	2.57	0.47
1:B:1:PRO:N	1:B:34:ASP:O	2.47	0.47
1:B:19:ARG:NH1	1:B:19:ARG:HG2	2.24	0.46
1:A:181:GLU:HG3	1:B:180:TYR:CE2	2.51	0.46
1:B:72:ALA:HA	1:B:73:PRO:HA	1.70	0.45
1:A:7:TRP:CE2	1:A:20:PRO:HD3	2.52	0.44
1:B:137:LEU:HB3	3:B:2556:HOH:O	2.17	0.44
1:A:72:ALA:HA	1:A:73:PRO:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PRO:HD3	1:B:79:LYS:HG2	1.98	0.44
1:A:56:GLY:O	1:A:57:LEU:C	2.60	0.43
1:B:154:ARG:HA	1:B:159:LEU:HD12	2.00	0.43
1:A:83:TRP:CH2	1:A:145:ARG:HG3	2.54	0.43
1:B:62:LEU:HB3	1:B:90:ASN:HA	2.00	0.43
1:A:5:SER:HA	1:A:19:ARG:NH2	2.34	0.43
1:B:63:TYR:CE1	1:B:125:GLU:HG3	2.53	0.43
1:A:176:VAL:HB	1:A:177:PRO:HD3	2.00	0.42
1:B:138:SER:HB2	3:B:2558:HOH:O	2.20	0.42
1:A:73:PRO:HD2	1:A:77:ASP:O	2.19	0.42
1:A:110:PRO:HA	1:A:111:PRO:HD3	1.87	0.42
1:A:124:TYR:CZ	1:A:154:ARG:HG2	2.55	0.42
2:A:1501[A]:OPE:CA	2:A:1501[A]:OPE:HN1	2.19	0.41
1:B:173:ASP:OD1	1:B:173:ASP:C	2.62	0.41
1:A:70:PRO:HD2	1:A:118:ARG:O	2.21	0.41
1:B:54:TRP:CH2	1:B:57:LEU:HD13	2.56	0.41
1:A:22:HIS:O	1:A:164:ALA:HA	2.21	0.41
1:A:73:PRO:HD2	1:A:79:LYS:HG2	2.03	0.41
1:B:89:VAL:O	1:B:90:ASN:HB2	2.21	0.41
1:B:81:ARG:HA	1:B:82:GLU:HA	1.72	0.41
1:B:69:ASP:OD2	2:B:2501[A]:OPE:O3	2.39	0.40
1:A:1:PRO:N	1:A:34:ASP:O	2.53	0.40
1:B:46:LYS:HB2	1:B:175:TYR:CZ	2.56	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	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	B	185/186 (100%)	176 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	369/372 (99%)	356 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	161/162 (99%)	155 (96%)	6 (4%)	30	37
1	B	161/162 (99%)	152 (94%)	9 (6%)	19	20
All	All	322/324 (99%)	307 (95%)	15 (5%)	23	26

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	21	GLN
1	A	139	ASN
1	A	141	SER
1	A	147	LYS
1	A	178	LYS
1	B	14	GLN
1	B	19	ARG
1	B	21	GLN
1	B	48	ARG
1	B	139	ASN
1	B	141	SER
1	B	147	LYS
1	B	163	VAL
1	B	181	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	25	GLN
1	A	95	ASN
1	A	139	ASN
1	B	14	GLN
1	B	25	GLN
1	B	95	ASN
1	B	139	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	OPE	B	2501[B]	-	7,7,7	4.64	4 (57%)	9,9,9	4.60	3 (33%)
2	OPE	A	1501[A]	-	7,7,7	4.69	4 (57%)	9,9,9	3.17	6 (66%)
2	OPE	A	1501[B]	-	7,7,7	4.61	3 (42%)	9,9,9	5.36	2 (22%)
2	OPE	B	2501[A]	-	7,7,7	4.61	3 (42%)	9,9,9	3.00	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OPE	B	2501[B]	-	-	4/5/5/5	-
2	OPE	A	1501[A]	-	-	1/5/5/5	-
2	OPE	A	1501[B]	-	-	4/5/5/5	-
2	OPE	B	2501[A]	-	-	0/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501[B]	OPE	CB-CA	-10.24	1.07	1.49
2	B	2501[B]	OPE	CB-CA	-10.12	1.07	1.49
2	A	1501[A]	OPE	CB-CA	-9.94	1.08	1.49
2	B	2501[A]	OPE	CB-CA	-9.82	1.08	1.49
2	B	2501[A]	OPE	P-O3	5.81	1.68	1.50
2	B	2501[B]	OPE	P-O3	5.68	1.68	1.50
2	A	1501[A]	OPE	P-O3	5.64	1.68	1.50
2	A	1501[B]	OPE	P-O3	5.46	1.67	1.50
2	B	2501[A]	OPE	CB-N	3.26	1.71	1.46
2	A	1501[A]	OPE	CB-N	3.26	1.71	1.46
2	A	1501[B]	OPE	CB-N	3.06	1.69	1.46
2	B	2501[B]	OPE	CB-N	3.01	1.69	1.46
2	A	1501[A]	OPE	P-O1	-2.41	1.45	1.54
2	B	2501[B]	OPE	P-O2	-2.06	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501[B]	OPE	P-O4-CA	13.19	154.08	118.21
2	B	2501[B]	OPE	P-O4-CA	12.50	152.20	118.21
2	A	1501[B]	OPE	O4-CA-CB	8.81	141.43	109.17
2	A	1501[A]	OPE	O4-CA-CB	6.37	132.49	109.17
2	B	2501[A]	OPE	P-O4-CA	6.20	135.08	118.21
2	B	2501[A]	OPE	O4-CA-CB	5.37	128.84	109.17
2	B	2501[B]	OPE	O4-CA-CB	5.20	128.18	109.17
2	A	1501[A]	OPE	P-O4-CA	5.09	132.05	118.21
2	A	1501[A]	OPE	O2-P-O4	-2.72	99.58	106.67
2	A	1501[A]	OPE	CA-CB-N	-2.56	91.57	114.11
2	B	2501[A]	OPE	CA-CB-N	-2.42	92.79	114.11
2	A	1501[A]	OPE	O1-P-O4	2.25	112.53	106.67
2	A	1501[A]	OPE	O2-P-O1	2.16	115.92	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2501[B]	OPE	CA-CB-N	-2.03	96.22	114.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501[A]	OPE	CA-O4-P-O3
2	A	1501[B]	OPE	CB-CA-O4-P
2	A	1501[B]	OPE	CA-O4-P-O1
2	A	1501[B]	OPE	CA-O4-P-O2
2	B	2501[B]	OPE	O4-CA-CB-N
2	B	2501[B]	OPE	CA-O4-P-O1
2	B	2501[B]	OPE	CA-O4-P-O2
2	B	2501[B]	OPE	CA-O4-P-O3
2	A	1501[B]	OPE	CA-O4-P-O3

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2501[B]	OPE	3	0
2	A	1501[A]	OPE	3	0
2	A	1501[B]	OPE	2	0
2	B	2501[A]	OPE	4	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.