Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID	:	1DPM / pdb_00001dpm
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE ZINC-CONTAINING PHOSPHOTRIESTERASE WITH BOUND SUBSTRATE ANALOG DIETHYL 4-METHYLBENZYLPHOSPHONATE
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Deposited on	:	1996-02-13
Resolution	:	2.10 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:

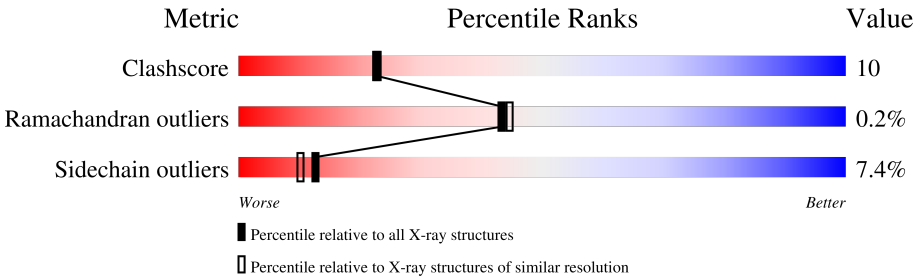
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	72% 23% 5%
1	B	329	74% 20% 5%

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
3	EBP	A	900	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5361 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.

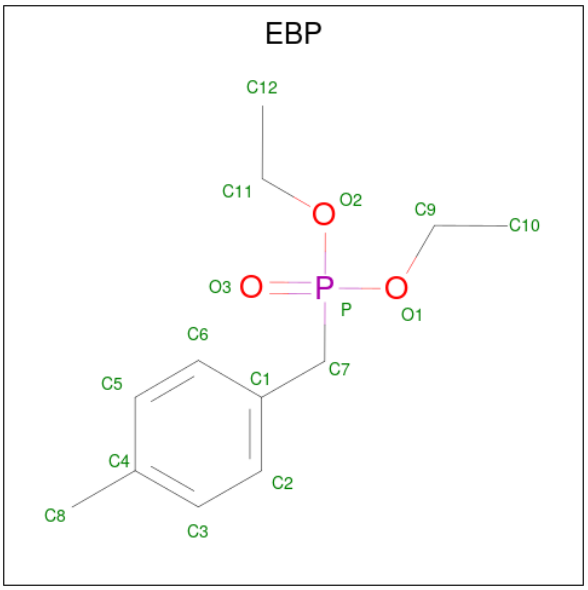
- Molecule 1 is a protein called PHOSPHOTRIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2515	1592	449	467	7			
1	B	329	Total	C	N	O	S	0	0	0
			2509	1589	446	467	7			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

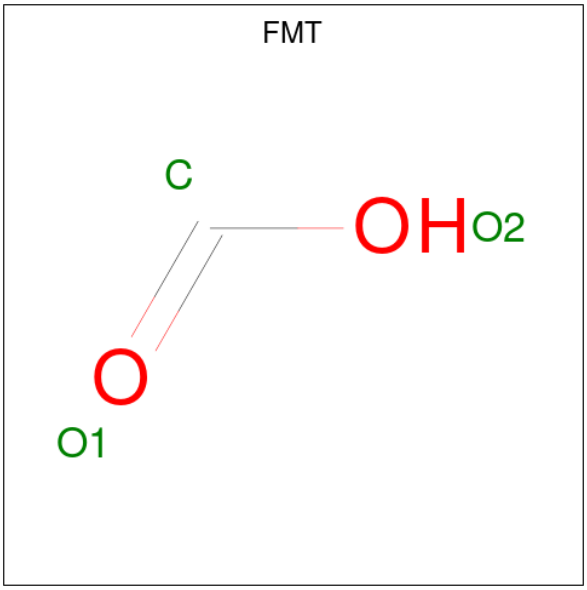
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is DIETHYL 4-METHYLBENZYLPHOSPHONATE (CCD ID: EBP) (formula: $C_{12}H_{19}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	12	3	1		
3	A	1	Total	C	O	P	0	0
			16	12	3	1		
3	B	1	Total	C	O	P	0	0
			16	12	3	1		
3	B	1	Total	C	O	P	0	0
			16	12	3	1		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	143	Total	O	0	0
			143	143		

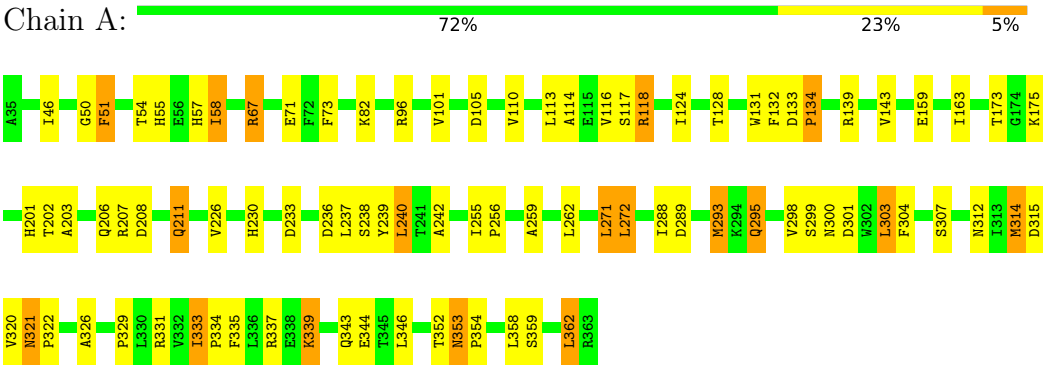
3 Residue-property plots (i)

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.

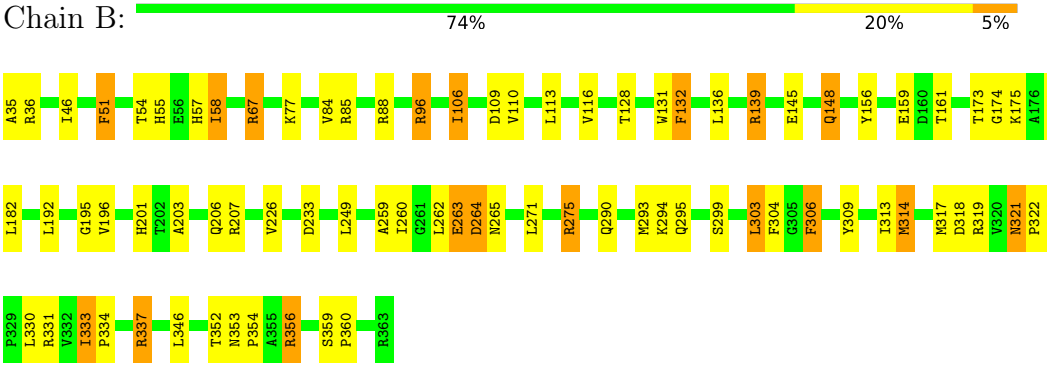
• Molecule 1: PHOSPHOTRIESTERASE

Chain A:



• Molecule 1: PHOSPHOTRIESTERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.60Å 91.40Å 69.40Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: EBP, FMT, ZN

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	1.39	5/2563 (0.2%)	1.58	30/3479 (0.9%)
1	B	1.35	5/2557 (0.2%)	1.60	28/3472 (0.8%)
All	All	1.37	10/5120 (0.2%)	1.59	58/6951 (0.8%)

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	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ARG	CD-NE	12.07	1.63	1.46
1	A	353	ASN	N-CA	-7.44	1.41	1.46
1	B	333	ILE	CA-CB	6.36	1.57	1.54
1	A	134	PRO	CA-C	5.64	1.55	1.52
1	A	318	ASP	CG-OD1	5.55	1.35	1.25
1	B	109	ASP	C-O	-5.35	1.17	1.23
1	A	333	ILE	CA-CB	5.22	1.56	1.54
1	B	323	ASP	C-O	-5.19	1.17	1.24
1	B	318	ASP	CG-OD1	5.13	1.35	1.25
1	B	85	ARG	N-CA	-5.11	1.40	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	THR	N-CA-C	8.15	123.04	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	LEU	N-CA-C	8.07	122.39	112.23
1	B	106	ILE	N-CA-C	-7.65	105.25	112.83
1	B	174	GLY	N-CA-C	-7.58	102.14	112.52
1	A	320	VAL	CA-C-N	-7.38	115.78	122.28
1	A	320	VAL	C-N-CA	-7.38	115.78	122.28
1	A	331	ARG	N-CA-C	7.00	121.87	113.12
1	A	343	GLN	CA-C-N	6.95	129.90	120.38
1	A	343	GLN	C-N-CA	6.95	129.90	120.38
1	B	321	ASN	CA-C-N	6.89	126.59	119.56
1	B	321	ASN	C-N-CA	6.89	126.59	119.56
1	B	263	GLU	N-CA-CB	6.64	121.71	110.49
1	B	264	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	203	ALA	N-CA-C	-6.56	95.25	107.71
1	B	333	ILE	N-CA-CB	6.48	115.50	110.45
1	A	333	ILE	N-CA-CB	6.42	114.82	110.52
1	A	339	LYS	CA-C-N	-6.38	113.63	122.63
1	A	339	LYS	C-N-CA	-6.38	113.63	122.63
1	B	352	THR	N-CA-C	6.38	118.03	111.14
1	B	333	ILE	CA-C-O	6.35	122.95	118.69
1	B	159	GLU	CB-CA-C	-6.29	109.30	116.54
1	B	132	PHE	CA-C-N	-6.22	115.94	122.28
1	B	132	PHE	C-N-CA	-6.22	115.94	122.28
1	A	175	LYS	CB-CA-C	6.22	117.45	109.80
1	A	333	ILE	CA-C-O	6.21	123.43	118.71
1	B	275	ARG	N-CA-C	-6.19	100.48	110.32
1	B	306	PHE	N-CA-CB	-6.17	101.31	111.74
1	A	240	LEU	N-CA-C	6.15	118.52	111.02
1	B	304	PHE	CA-CB-CG	-6.13	107.67	113.80
1	A	293	MET	N-CA-C	6.05	117.95	111.36
1	B	54	THR	N-CA-C	6.04	120.49	113.18
1	B	264	ASP	N-CA-C	-5.99	106.06	113.19
1	A	321	ASN	CA-C-N	5.97	125.85	119.28
1	A	321	ASN	C-N-CA	5.97	125.85	119.28
1	B	128	THR	N-CA-CB	5.92	119.81	110.87
1	B	58	ILE	N-CA-C	-5.86	105.13	110.82
1	A	196	VAL	N-CA-CB	-5.86	103.95	109.99
1	A	159	GLU	CB-CA-C	-5.76	109.91	116.54
1	B	161	THR	N-CA-C	5.75	120.02	112.89
1	B	226	VAL	N-CA-C	5.72	116.11	108.11
1	B	174	GLY	CA-C-O	-5.45	116.86	122.25
1	A	295	GLN	CA-C-N	-5.45	115.12	122.91
1	A	295	GLN	C-N-CA	-5.45	115.12	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	THR	N-CA-CB	5.44	119.09	110.87
1	A	289	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	196	VAL	N-CA-CB	-5.41	104.44	110.23
1	A	288	ILE	N-CA-C	-5.39	105.24	110.42
1	A	352	THR	N-CA-C	5.39	116.96	111.14
1	A	128	THR	N-CA-C	-5.34	102.01	109.69
1	B	139	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	B	203	ALA	N-CA-C	-5.22	96.87	107.41
1	B	233	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	337	ARG	CA-C-N	5.16	127.72	120.28
1	B	337	ARG	C-N-CA	5.16	127.72	120.28
1	A	58	ILE	N-CA-C	-5.13	105.41	111.00
1	A	226	VAL	N-CA-C	5.05	115.98	108.46
1	A	300	ASN	CB-CA-C	-5.04	100.61	109.07
1	A	304	PHE	CA-CB-CG	-5.00	108.80	113.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	263	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2515	0	2542	56	0
1	B	2509	0	2531	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	32	0	38	8	0
3	B	32	0	38	10	0
4	A	3	0	0	1	0
4	B	3	0	0	1	0
5	A	120	0	0	3	0
5	B	143	0	0	6	0
All	All	5361	0	5149	107	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 10.

All (107) 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:314:MET:HE3	1:A:317:MET:HE2	1.44	0.97
1:A:314:MET:CE	1:A:317:MET:HE2	1.98	0.92
1:B:317:MET:SD	3:B:902:EBP:H82	2.15	0.86
1:A:317:MET:SD	3:A:900:EBP:H82	2.21	0.80
1:B:156:TYR:CG	3:B:903:EBP:H122	2.16	0.80
1:B:271:LEU:HD21	3:B:902:EBP:H5	1.70	0.73
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.72	0.70
1:B:156:TYR:CD2	3:B:903:EBP:H122	2.27	0.70
1:B:306:PHE:HE2	1:B:317:MET:HE1	1.57	0.68
1:B:293:MET:HG2	5:B:997:HOH:O	1.93	0.67
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.78	0.66
1:B:96:ARG:HD3	5:B:1032:HOH:O	1.96	0.63
1:A:46:ILE:HD12	1:A:359:SER:OG	1.98	0.63
1:A:271:LEU:CD2	3:A:900:EBP:H6	2.28	0.63
1:B:306:PHE:CE2	1:B:317:MET:HE1	2.35	0.62
1:B:313:ILE:HG13	1:B:317:MET:HE3	1.79	0.61
1:A:271:LEU:HD21	3:A:900:EBP:H6	1.82	0.61
1:B:156:TYR:CD1	3:B:903:EBP:H122	2.36	0.61
1:B:145:GLU:O	1:B:148:GLN:HB2	2.01	0.61
1:A:314:MET:HE3	1:A:317:MET:CE	2.26	0.60
1:A:312:ASN:O	1:A:315:ASP:HB2	2.01	0.60
1:B:57:HIS:O	1:B:303:LEU:HA	2.02	0.59
1:A:110:VAL:HG22	1:A:163:ILE:HD13	1.84	0.59
1:B:271:LEU:CD2	1:B:317:MET:HE2	2.32	0.59
1:B:294:LYS:O	1:B:356:ARG:NH2	2.36	0.57
1:B:271:LEU:HD21	3:B:902:EBP:C5	2.35	0.56
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.87	0.55
1:B:173:THR:O	1:B:173:THR:HG23	2.04	0.55
3:B:902:EBP:H72	5:B:924:HOH:O	2.07	0.54
1:A:57:HIS:O	1:A:303:LEU:HA	2.07	0.53
1:A:353:ASN:HB2	1:A:354:PRO:HD3	1.89	0.53
1:B:271:LEU:CD2	3:B:902:EBP:H5	2.40	0.52
1:B:206:GLN:O	1:B:207:ARG:HB2	2.09	0.52
1:B:275:ARG:HG3	5:B:1000:HOH:O	2.11	0.51
1:B:46:ILE:HD12	1:B:359:SER:OG	2.11	0.50
1:A:236:ASP:OD1	1:A:238:SER:OG	2.26	0.50
1:B:84:VAL:O	1:B:88:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:HIS:CE1	1:A:230:HIS:CE1	3.00	0.50
1:A:114:ALA:O	1:A:118:ARG:HG3	2.12	0.49
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.94	0.49
1:A:230:HIS:O	1:A:233:ASP:HB2	2.12	0.49
1:A:201:HIS:HB2	4:A:902:FMT:O1	2.13	0.49
1:A:131:TRP:CG	1:A:132:PHE:H	2.31	0.49
1:B:131:TRP:CG	1:B:132:PHE:H	2.31	0.49
1:A:51:PHE:C	1:A:51:PHE:CD1	2.92	0.48
1:A:50:GLY:HA3	1:A:96:ARG:HD3	1.94	0.48
1:B:317:MET:SD	3:B:902:EBP:C8	2.96	0.48
1:A:51:PHE:C	1:A:51:PHE:HD1	2.22	0.48
1:A:271:LEU:HD21	3:A:900:EBP:C6	2.43	0.48
1:B:136:LEU:CD2	1:B:139:ARG:NH2	2.77	0.48
1:B:35:ALA:N	5:B:936:HOH:O	2.47	0.47
1:B:51:PHE:CD1	1:B:51:PHE:C	2.92	0.47
1:B:51:PHE:C	1:B:51:PHE:HD1	2.21	0.47
1:B:353:ASN:N	1:B:354:PRO:CD	2.78	0.47
1:B:309:TYR:HD2	1:B:313:ILE:HG12	1.80	0.47
1:B:353:ASN:N	1:B:354:PRO:HD2	2.30	0.47
1:B:201:HIS:HB2	4:B:904:FMT:O2	2.15	0.46
1:A:67:ARG:CZ	1:B:67:ARG:HH12	2.28	0.46
1:B:259:ALA:O	1:B:262:LEU:HB2	2.16	0.46
1:B:321:ASN:HA	1:B:322:PRO:HD2	1.61	0.46
1:A:303:LEU:HD11	1:A:317:MET:HE1	1.97	0.46
1:A:333:ILE:HG23	1:A:346:LEU:HD13	1.98	0.46
1:B:179:PHE:O	1:B:182:LEU:HB2	2.16	0.46
1:B:106:ILE:HG22	1:B:106:ILE:O	2.16	0.46
1:A:71:GLU:H	1:A:71:GLU:CD	2.22	0.45
1:A:335:PHE:O	1:A:339:LYS:HG2	2.17	0.45
1:A:117:SER:HB2	1:A:124:ILE:HD12	1.99	0.44
1:A:110:VAL:HG22	1:A:163:ILE:CD1	2.46	0.44
1:A:133:ASP:N	1:A:134:PRO:CD	2.81	0.44
1:A:202:THR:HB	1:A:208:ASP:HB2	2.00	0.44
1:A:67:ARG:NH1	1:B:67:ARG:NH1	2.66	0.44
3:A:901:EBP:H6	3:A:901:EBP:H92	2.00	0.44
1:B:327:PHE:O	1:B:328:ILE:C	2.59	0.44
1:B:314:MET:HE2	1:B:317:MET:HB2	2.00	0.43
1:A:317:MET:SD	3:A:900:EBP:C8	3.02	0.43
1:A:322:PRO:HD2	5:A:1003:HOH:O	2.18	0.43
1:A:301:ASP:O	3:A:900:EBP:H3	2.19	0.43
1:B:195:GLY:O	1:B:360:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:HE21	1:A:295:GLN:HB3	1.68	0.43
1:A:329:PRO:HA	1:A:333:ILE:HG12	2.00	0.43
1:B:263:GLU:C	1:B:265:ASN:H	2.26	0.43
1:B:177:THR:HB	1:B:178:PRO:HD2	2.01	0.42
1:B:271:LEU:CD2	1:B:317:MET:CE	2.97	0.42
1:A:173:THR:O	1:A:173:THR:HG23	2.20	0.42
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.83	0.42
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.89	0.42
1:A:176:ALA:N	1:A:211:GLN:OE1	2.47	0.42
1:A:259:ALA:O	1:A:262:LEU:HB2	2.20	0.42
1:A:55:HIS:CE1	1:A:230:HIS:HE1	2.38	0.42
1:B:330:LEU:O	1:B:334:PRO:HG2	2.20	0.41
3:B:903:EBP:H71	3:B:903:EBP:H91	1.87	0.41
1:A:326:ALA:O	1:A:329:PRO:HD2	2.20	0.41
1:A:82:LYS:NZ	5:A:921:HOH:O	2.53	0.41
1:A:239:TYR:O	1:A:242:ALA:HB3	2.20	0.41
1:B:333:ILE:HG22	5:B:931:HOH:O	2.19	0.41
1:B:55:HIS:CD2	1:B:55:HIS:C	2.98	0.41
1:B:57:HIS:HB2	1:B:303:LEU:HB3	2.02	0.41
1:A:237:LEU:HD12	1:A:240:LEU:HD12	2.03	0.41
1:A:143:VAL:HG12	5:A:928:HOH:O	2.21	0.41
1:A:339:LYS:HD3	1:A:339:LYS:HA	1.89	0.41
1:A:195:GLY:HA3	1:A:362:LEU:HD13	2.03	0.41
1:A:317:MET:CE	3:A:900:EBP:H82	2.50	0.41
1:A:321:ASN:HA	1:A:322:PRO:HD2	1.80	0.41
1:A:105:ASP:OD2	1:A:131:TRP:HB3	2.21	0.41
1:A:73:PHE:CZ	1:A:307:SER:HB3	2.56	0.40
1:A:206:GLN:O	1:A:207:ARG:HB2	2.20	0.40
1:A:259:ALA:HB2	1:A:272:LEU:HB2	2.03	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	327/329 (99%)	313 (96%)	13 (4%)	1 (0%)	36 36
1	B	327/329 (99%)	318 (97%)	9 (3%)	0	100 100
All	All	654/658 (99%)	631 (96%)	22 (3%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	VAL

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	264/264 (100%)	248 (94%)	16 (6%)	17 15
1	B	263/264 (100%)	240 (91%)	23 (9%)	9 7
All	All	527/528 (100%)	488 (93%)	39 (7%)	13 10

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	58	ILE
1	A	67	ARG
1	A	113	LEU
1	A	116	VAL
1	A	139	ARG
1	A	211	GLN
1	A	271	LEU
1	A	293	MET
1	A	298	VAL
1	A	299	SER
1	A	303	LEU
1	A	314	MET
1	A	337	ARG
1	A	344	GLU

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Mol	Chain	Res	Type
1	A	362	LEU
1	B	36	ARG
1	B	51	PHE
1	B	58	ILE
1	B	67	ARG
1	B	77	LYS
1	B	96	ARG
1	B	110	VAL
1	B	113	LEU
1	B	116	VAL
1	B	148	GLN
1	B	175	LYS
1	B	249	LEU
1	B	260	ILE
1	B	264	ASP
1	B	290	GLN
1	B	295	GLN
1	B	299	SER
1	B	303	LEU
1	B	314	MET
1	B	319	ARG
1	B	331	ARG
1	B	337	ARG
1	B	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	295	GLN
1	B	155	GLN
1	B	290	GLN
1	B	295	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	FMT	B	904	1,2	2,2,2	0.52	0	1,1,1	0.30	0
4	FMT	A	902	1,2	2,2,2	0.06	0	1,1,1	0.25	0
3	EBP	A	901	-	16,16,16	3.37	3 (18%)	21,21,21	0.93	1 (4%)
3	EBP	A	900	-	16,16,16	3.30	3 (18%)	21,21,21	1.30	1 (4%)
3	EBP	B	902	-	16,16,16	3.30	3 (18%)	21,21,21	1.65	1 (4%)
3	EBP	B	903	-	16,16,16	3.52	4 (25%)	21,21,21	1.32	1 (4%)

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
3	EBP	A	900	-	-	0/13/13/13	0/1/1/1
3	EBP	B	903	-	-	2/13/13/13	0/1/1/1
3	EBP	B	902	-	-	2/13/13/13	0/1/1/1
3	EBP	A	901	-	-	3/13/13/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	EBP	P-C7	-12.70	1.60	1.79
3	A	901	EBP	P-C7	-12.23	1.61	1.79
3	A	900	EBP	P-C7	-11.92	1.61	1.79
3	B	902	EBP	P-C7	-11.41	1.62	1.79
3	B	902	EBP	C6-C5	4.00	1.45	1.38
3	B	902	EBP	C3-C2	3.80	1.45	1.38
3	A	901	EBP	C3-C2	3.80	1.45	1.38
3	B	903	EBP	C3-C2	3.62	1.44	1.38
3	A	901	EBP	C6-C5	3.27	1.44	1.38
3	A	900	EBP	C3-C2	3.06	1.43	1.38
3	A	900	EBP	C6-C5	2.99	1.43	1.38
3	B	903	EBP	C6-C5	2.79	1.43	1.38
3	B	903	EBP	C2-C1	2.48	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	EBP	P-C7-C1	6.92	130.40	113.76
3	A	900	EBP	P-C7-C1	4.52	124.62	113.76
3	B	903	EBP	P-C7-C1	4.50	124.58	113.76
3	A	901	EBP	C2-C3-C4	-3.08	117.82	121.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	EBP	C9-O1-P-C7
3	B	902	EBP	C9-O1-P-O2
3	B	902	EBP	C9-O1-P-O3
3	B	903	EBP	C9-O1-P-C7
3	A	901	EBP	C9-O1-P-O3
3	B	903	EBP	C9-O1-P-O3
3	A	901	EBP	C1-C7-P-O2

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	904	FMT	1	0
4	A	902	FMT	1	0
3	A	901	EBP	1	0
3	A	900	EBP	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	EBP	6	0
3	B	903	EBP	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.