



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:02 PM UTC

PDB ID : 3DRB / pdb_00003drb
Title : Crystal structure of Human Brain-type Creatine Kinase
Authors : Moon, J.H.; Bong, S.M.; Hwang, K.Y.; Chi, Y.M.
Deposited on : 2008-07-11
Resolution : 2.00 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

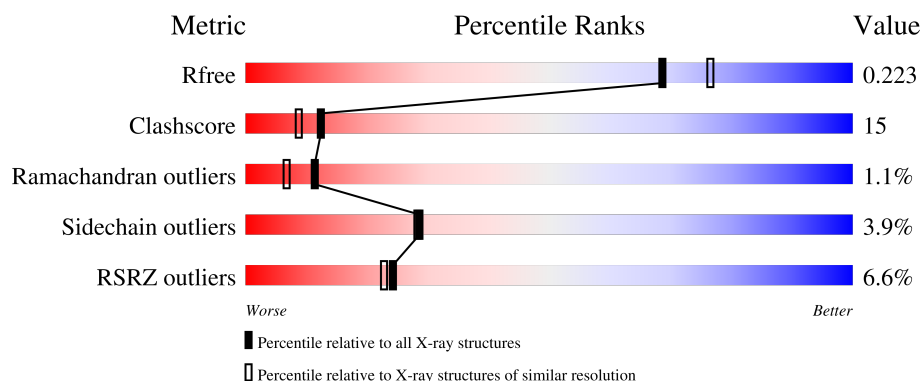
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	381	12% 74% 22% ..
1	B	381	63% 33% ..

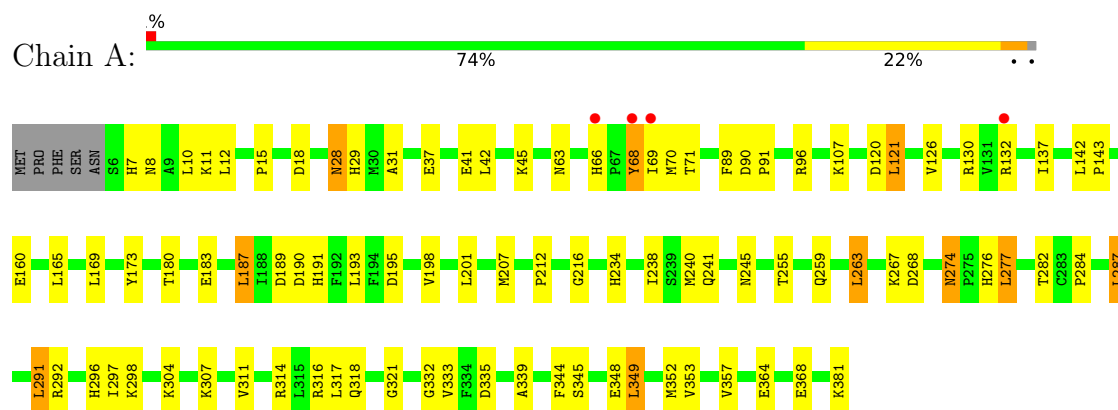
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total 299	O 299	0	0
4	B	233	Total 233	O 233	0	0

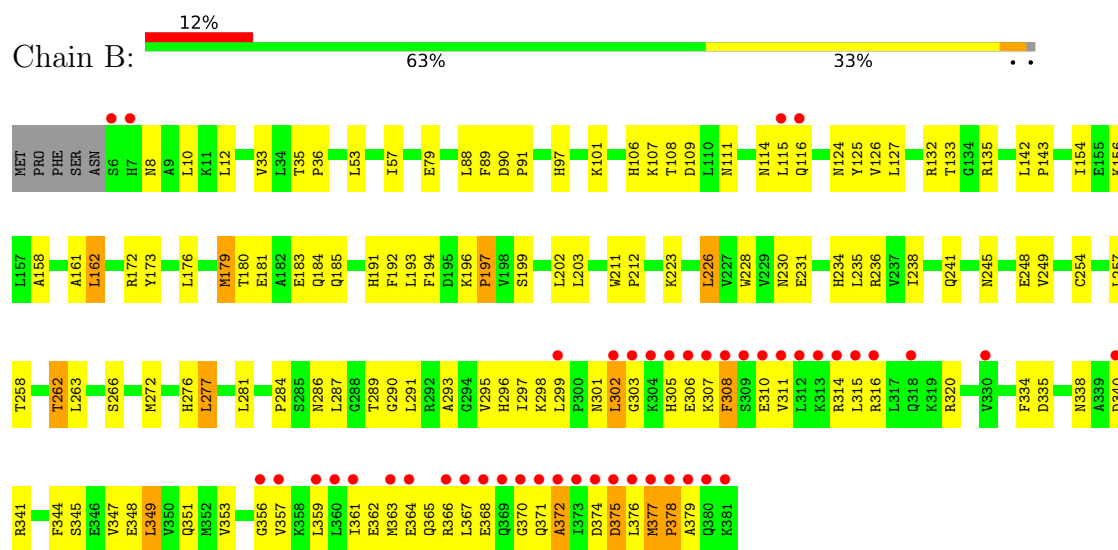
3 Residue-property plots

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: Creatine kinase B-type



• Molecule 1: Creatine kinase B-type



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.72Å 97.72Å 166.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.17 – 2.00 42.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.17-2.00) 99.5 (42.17-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.30 (at 1.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.196 , 0.227 0.192 , 0.223	Depositor DCC
R_{free} test set	3167 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6478	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: ADP, MG

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	0.36	0/3023	0.87	11/4087 (0.3%)
1	B	0.34	0/3023	0.88	8/4087 (0.2%)
All	All	0.35	0/6046	0.88	19/8174 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	N-CA-C	7.53	119.88	110.70
1	A	297	ILE	N-CA-C	6.77	118.55	108.46
1	B	143	PRO	N-CA-C	6.54	118.68	110.70
1	A	296	HIS	N-CA-C	-6.53	97.04	108.20
1	B	296	HIS	N-CA-C	-6.37	98.15	108.41
1	B	33	VAL	N-CA-C	6.14	116.87	111.90
1	A	63	ASN	CA-C-N	5.95	125.62	119.56
1	A	63	ASN	C-N-CA	5.95	125.62	119.56
1	A	291	LEU	N-CA-C	5.88	118.83	109.24
1	A	198	VAL	N-CA-C	-5.70	107.22	113.43
1	B	57	ILE	N-CA-C	5.49	119.11	112.80
1	A	120	ASP	N-CA-C	5.47	117.45	110.61
1	B	89	PHE	N-CA-C	5.41	117.18	111.28
1	B	230	ASN	N-CA-C	5.33	119.06	112.24
1	B	238	ILE	N-CA-C	5.31	116.38	108.46
1	A	282	THR	N-CA-C	5.14	116.57	111.07
1	A	89	PHE	N-CA-C	5.07	116.81	111.28
1	A	7	HIS	N-CA-C	-5.07	105.83	111.36
1	B	308	PHE	N-CA-C	-5.07	105.84	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2959	0	2894	70	2
1	B	2959	0	2894	116	0
2	B	1	0	0	0	0
3	B	27	0	12	3	0
4	A	299	0	0	10	0
4	B	233	0	0	10	0
All	All	6478	0	5800	181	2

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 15.

All (181) 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:137:ILE:H	1:A:234:HIS:HD2	1.16	0.93
1:B:367:LEU:HD12	1:B:368:GLU:N	1.84	0.92
1:B:293:ALA:H	1:B:338:ASN:HD21	1.18	0.86
1:A:37:GLU:O	1:A:41:GLU:HG3	1.77	0.83
1:A:42:LEU:HG	4:A:968:HOH:O	1.82	0.79
1:A:274:ASN:HD21	1:A:277:LEU:H	1.28	0.78
1:B:340:ASP:HB3	4:B:823:HOH:O	1.84	0.78
1:A:28:ASN:ND2	1:A:31:ALA:H	1.82	0.77
1:A:66:HIS:HB3	1:A:68:TYR:CE1	2.20	0.76
1:A:68:TYR:CE2	1:B:262:THR:HG23	2.21	0.75
1:A:45:LYS:HD2	4:A:968:HOH:O	1.87	0.74
1:B:363:MET:O	1:B:366:ARG:HG3	1.88	0.73
1:B:366:ARG:O	1:B:366:ARG:HD2	1.88	0.73
1:A:274:ASN:ND2	1:A:277:LEU:H	1.86	0.73
1:B:293:ALA:H	1:B:338:ASN:ND2	1.86	0.72
1:B:367:LEU:HD12	1:B:368:GLU:H	1.53	0.71
1:A:107:LYS:HE2	4:A:846:HOH:O	1.92	0.70
1:A:364:GLU:O	1:A:368:GLU:HG3	1.93	0.69
1:B:8:ASN:O	1:B:12:LEU:HD23	1.93	0.69
1:A:274:ASN:C	1:A:274:ASN:HD22	2.01	0.68
1:A:274:ASN:HD22	1:A:276:HIS:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HD23	1:B:356:GLY:HA2	1.76	0.68
1:A:29:HIS:CE1	1:A:70:MET:HE3	2.28	0.68
1:B:276:HIS:CD2	1:B:277:LEU:HD13	2.29	0.67
1:A:28:ASN:HA	1:A:70:MET:HG3	1.75	0.67
1:A:189:ASP:HB3	4:A:730:HOH:O	1.94	0.67
1:A:276:HIS:CD2	1:A:277:LEU:HD13	2.30	0.67
1:A:321:GLY:O	1:B:156:LYS:HE2	1.95	0.67
1:B:305:HIS:ND1	1:B:306:GLU:N	2.43	0.66
1:A:335:ASP:HB2	4:A:1060:HOH:O	1.93	0.66
1:B:125:TYR:HB3	1:B:297:ILE:HD11	1.77	0.66
1:B:302:LEU:HD23	1:B:364:GLU:HA	1.78	0.65
1:A:130:ARG:HH11	1:A:132:ARG:HD2	1.61	0.65
1:B:310:GLU:O	1:B:314:ARG:HG2	1.97	0.65
1:B:132:ARG:NE	3:B:400:ADP:O2B	2.30	0.64
1:B:254:CYS:O	1:B:258:THR:HG23	1.96	0.64
1:B:311:VAL:O	1:B:315:LEU:HD13	1.98	0.64
1:B:234:HIS:C	1:B:235:LEU:HD12	2.23	0.64
1:B:111:ASN:HD22	1:B:114:ASN:ND2	1.99	0.61
1:A:307:LYS:O	1:A:311:VAL:HG23	2.01	0.61
1:A:314:ARG:O	1:A:381:LYS:HG2	2.00	0.60
1:A:274:ASN:ND2	1:A:276:HIS:H	2.00	0.60
1:A:352:MET:HE3	1:A:381:LYS:HE2	1.82	0.59
1:A:284:PRO:HA	1:A:287:LEU:HD22	1.83	0.59
1:B:35:THR:HA	4:B:872:HOH:O	2.02	0.59
1:B:179:MET:HE3	1:B:184:GLN:HB2	1.85	0.59
1:B:361:ILE:O	1:B:364:GLU:HB3	2.01	0.59
1:B:199:SER:O	1:B:203:LEU:HD23	2.02	0.59
1:B:281:LEU:HD12	1:B:286:ASN:O	2.03	0.58
1:B:320:ARG:HB2	1:B:335:ASP:HB3	1.86	0.58
1:B:341:ARG:HH11	1:B:341:ARG:HG2	1.68	0.57
1:B:228:TRP:HB2	1:B:236:ARG:HB2	1.86	0.57
1:B:197:PRO:HD3	1:B:211:TRP:CE2	2.39	0.57
1:B:172:ARG:HG2	1:B:173:TYR:N	2.20	0.56
1:B:305:HIS:HD1	1:B:306:GLU:N	2.01	0.56
1:B:109:ASP:O	1:B:347:VAL:HG23	2.06	0.56
1:A:160:GLU:OE1	1:A:267:LYS:HE2	2.06	0.56
1:A:316:ARG:HB2	1:A:352:MET:HE1	1.88	0.55
1:B:127:LEU:HD12	1:B:127:LEU:N	2.21	0.55
1:B:366:ARG:HD2	1:B:366:ARG:C	2.31	0.55
1:B:315:LEU:HB3	4:B:842:HOH:O	2.06	0.55
1:B:158:ALA:O	1:B:162:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:MET:HE1	1:B:193:LEU:HD22	1.90	0.54
1:B:10:LEU:C	1:B:10:LEU:HD23	2.33	0.54
1:B:226:LEU:HD12	1:B:226:LEU:N	2.22	0.54
1:A:165:LEU:HB3	1:A:169:LEU:HB3	1.90	0.54
1:B:133:THR:HA	1:B:290:GLY:O	2.07	0.54
1:B:132:ARG:HD2	1:B:132:ARG:C	2.33	0.53
1:A:292:ARG:HH22	1:A:335:ASP:CG	2.16	0.53
1:A:241:GLN:HB2	4:A:691:HOH:O	2.07	0.53
1:A:274:ASN:ND2	1:A:274:ASN:C	2.67	0.53
1:A:318:GLN:HE21	1:A:339:ALA:HA	1.73	0.53
1:B:302:LEU:HD12	1:B:308:PHE:CD1	2.44	0.53
1:B:245:ASN:HD22	1:B:245:ASN:C	2.16	0.53
1:A:90:ASP:HB2	1:A:91:PRO:HD3	1.91	0.53
1:B:371:GLN:O	1:B:372:ALA:HB2	2.08	0.53
1:A:291:LEU:C	1:A:291:LEU:HD23	2.34	0.52
1:B:316:ARG:HD3	1:B:340:ASP:OD1	2.10	0.52
1:B:345:SER:OG	1:B:348:GLU:HG3	2.09	0.52
1:B:126:VAL:HG13	1:B:295:VAL:HB	1.91	0.52
1:B:179:MET:HE3	1:B:184:GLN:CB	2.40	0.52
1:B:90:ASP:HB2	1:B:91:PRO:HD3	1.92	0.52
1:B:179:MET:HE1	1:B:193:LEU:CD2	2.40	0.51
1:B:234:HIS:O	1:B:235:LEU:HD12	2.10	0.51
1:A:137:ILE:H	1:A:234:HIS:CD2	2.09	0.51
1:B:161:ALA:O	1:B:263:LEU:HD13	2.11	0.50
1:B:124:ASN:O	1:B:298:LYS:HD2	2.11	0.50
1:A:132:ARG:HG2	1:A:238:ILE:HG23	1.94	0.50
1:A:345:SER:OG	1:A:348:GLU:HG3	2.12	0.50
1:A:238:ILE:HD12	1:A:238:ILE:N	2.26	0.49
1:A:28:ASN:HD22	1:A:31:ALA:H	1.56	0.49
1:B:115:LEU:C	1:B:115:LEU:HD13	2.38	0.49
1:B:277:LEU:HD22	4:B:809:HOH:O	2.13	0.49
1:A:316:ARG:HD3	1:A:352:MET:HE1	1.94	0.49
1:B:303:GLY:HA3	1:B:334:PHE:CZ	2.48	0.49
1:A:71:THR:HG21	1:A:201:LEU:HD21	1.95	0.49
1:B:315:LEU:HD12	1:B:315:LEU:N	2.28	0.49
1:B:125:TYR:C	1:B:297:ILE:HD12	2.39	0.48
1:B:299:LEU:HB3	1:B:302:LEU:HB2	1.94	0.48
1:B:197:PRO:HA	1:B:202:LEU:HD23	1.96	0.48
1:A:259:GLN:NE2	4:A:1117:HOH:O	2.47	0.48
1:A:353:VAL:O	1:A:357:VAL:HG23	2.14	0.47
1:B:181:GLU:HB3	4:B:664:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HG3	4:A:821:HOH:O	2.12	0.47
1:B:301:ASN:ND2	1:B:364:GLU:OE2	2.47	0.47
1:A:69:ILE:HG23	1:A:69:ILE:O	2.15	0.47
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.80	0.46
1:B:301:ASN:CG	1:B:367:LEU:HD21	2.41	0.46
1:A:195:ASP:HB3	4:A:603:HOH:O	2.16	0.46
1:B:363:MET:O	1:B:366:ARG:CG	2.62	0.46
1:A:274:ASN:HD22	1:A:276:HIS:N	2.12	0.46
1:B:245:ASN:ND2	1:B:248:GLU:H	2.14	0.46
1:B:53:LEU:HD11	1:B:88:LEU:HD22	1.99	0.45
1:A:68:TYR:CD1	1:B:266:SER:HB3	2.51	0.45
1:A:240:MET:O	1:A:241:GLN:HB3	2.17	0.45
1:B:305:HIS:CD2	1:B:366:ARG:HE	2.35	0.45
1:A:180:THR:OG1	1:A:183:GLU:HG3	2.16	0.45
1:B:116:GLN:HG2	1:B:351:GLN:OE1	2.16	0.45
1:B:197:PRO:O	1:B:203:LEU:HD21	2.17	0.45
1:B:277:LEU:HG	1:B:287:LEU:HD13	1.98	0.45
1:B:107:LYS:HD3	1:B:108:THR:H	1.82	0.44
1:B:361:ILE:O	1:B:365:GLN:HG3	2.17	0.44
1:B:375:ASP:OD1	1:B:376:LEU:N	2.46	0.44
1:B:377:MET:HB3	1:B:378:PRO:CD	2.48	0.44
1:A:304:LYS:HE3	4:B:805:HOH:O	2.16	0.44
1:B:377:MET:HB3	1:B:378:PRO:HD3	1.99	0.44
1:B:106:HIS:CE1	1:B:289:THR:HG23	2.52	0.44
1:B:125:TYR:O	1:B:297:ILE:HD12	2.18	0.44
1:B:301:ASN:OD1	1:B:302:LEU:N	2.50	0.44
1:B:353:VAL:O	1:B:357:VAL:HG23	2.17	0.44
1:A:255:THR:O	1:A:259:GLN:HG3	2.18	0.44
1:B:132:ARG:NH2	4:B:1131:HOH:O	2.50	0.43
1:B:97:HIS:C	4:B:896:HOH:O	2.62	0.43
1:B:341:ARG:HG2	1:B:341:ARG:NH1	2.32	0.43
1:A:121:LEU:HB3	1:A:126:VAL:HG21	2.01	0.43
1:B:97:HIS:HE1	1:B:284:PRO:O	2.01	0.43
1:A:187:LEU:HB3	1:A:193:LEU:HB2	2.00	0.43
1:A:173:TYR:OH	1:A:216:GLY:HA3	2.19	0.43
1:B:36:PRO:HD3	4:B:872:HOH:O	2.18	0.42
1:B:359:LEU:O	1:B:363:MET:SD	2.77	0.42
1:B:378:PRO:O	1:B:379:ALA:HB3	2.19	0.42
1:A:15:PRO:HD2	1:A:18:ASP:OD2	2.19	0.42
1:B:154:ILE:HD13	1:B:234:HIS:CD2	2.55	0.42
1:B:192:PHE:CE2	1:B:223:LYS:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:CB	1:A:349:LEU:HD13	2.50	0.42
1:B:316:ARG:NH1	4:B:823:HOH:O	2.51	0.42
1:B:366:ARG:HG3	1:B:366:ARG:NH1	2.35	0.42
1:B:376:LEU:C	1:B:376:LEU:HD23	2.45	0.42
1:B:79:GLU:HB2	1:B:272:MET:SD	2.59	0.42
1:A:207:MET:C	1:A:207:MET:SD	3.02	0.42
1:A:298:LYS:HG2	1:A:333:VAL:HG22	2.01	0.42
1:B:194:PHE:CG	1:B:231:GLU:HG3	2.55	0.41
1:B:377:MET:C	1:B:377:MET:SD	3.03	0.41
1:A:8:ASN:HD22	1:A:11:LYS:HE3	1.85	0.41
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.88	0.41
1:B:135:ARG:NH2	1:B:257:LEU:HD21	2.35	0.41
1:B:291:LEU:HD23	1:B:291:LEU:C	2.45	0.41
1:B:180:THR:OG1	1:B:183:GLU:HG3	2.21	0.41
1:B:377:MET:H	1:B:378:PRO:HD2	1.85	0.41
1:A:10:LEU:C	1:A:10:LEU:HD23	2.46	0.41
1:A:69:ILE:HG22	1:B:266:SER:HB2	2.02	0.41
1:A:69:ILE:HG21	1:B:266:SER:O	2.21	0.41
1:A:259:GLN:O	1:A:263:LEU:HD23	2.18	0.41
1:A:267:LYS:O	1:A:268:ASP:HB2	2.20	0.41
1:B:191:HIS:ND1	3:B:400:ADP:O2'	2.46	0.41
1:B:241:GLN:HG2	1:B:249:VAL:HG22	2.03	0.41
1:B:315:LEU:HD23	1:B:356:GLY:CA	2.46	0.41
1:B:344:PHE:HB2	1:B:349:LEU:HD13	2.02	0.41
1:B:185:GLN:OE1	1:B:196:LYS:HE3	2.21	0.41
1:B:245:ASN:C	1:B:245:ASN:ND2	2.78	0.41
1:B:366:ARG:HG3	1:B:366:ARG:HH11	1.85	0.41
1:A:28:ASN:HD22	1:A:28:ASN:C	2.28	0.41
1:A:130:ARG:NH1	1:A:132:ARG:HD2	2.32	0.41
1:B:191:HIS:HA	3:B:400:ADP:O2'	2.21	0.41
1:A:190:ASP:O	1:A:191:HIS:HB2	2.20	0.41
1:B:179:MET:HE3	1:B:184:GLN:CA	2.51	0.41
1:B:307:LYS:O	1:B:311:VAL:HG23	2.21	0.40
1:A:292:ARG:NH1	4:A:1118:HOH:O	2.45	0.40
1:B:315:LEU:N	1:B:315:LEU:CD1	2.85	0.40
1:B:298:LYS:O	1:B:299:LEU:HD23	2.22	0.40
1:B:108:THR:HG22	1:B:109:ASP:N	2.36	0.40

All (2) 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:245:ASN:ND2	1:A:245:ASN:ND2[7_555]	1.99	0.21
1:A:41:GLU:OE2	1:A:41:GLU:OE2[8_554]	2.19	0.01

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	374/381 (98%)	365 (98%)	8 (2%)	1 (0%)	36	35
1	B	374/381 (98%)	348 (93%)	19 (5%)	7 (2%)	6	3
All	All	748/762 (98%)	713 (95%)	27 (4%)	8 (1%)	11	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	374	ASP
1	B	372	ALA
1	B	377	MET
1	B	378	PRO
1	B	375	ASP
1	A	332	GLY
1	B	370	GLY
1	B	197	PRO

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	322/327 (98%)	309 (96%)	13 (4%)	28	27
1	B	322/327 (98%)	310 (96%)	12 (4%)	30	30
All	All	644/654 (98%)	619 (96%)	25 (4%)	28	28

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	28	ASN
1	A	68	TYR
1	A	121	LEU
1	A	142	LEU
1	A	187	LEU
1	A	212	PRO
1	A	263	LEU
1	A	274	ASN
1	A	277	LEU
1	A	287	LEU
1	A	317	LEU
1	A	349	LEU
1	B	101	LYS
1	B	142	LEU
1	B	162	LEU
1	B	176	LEU
1	B	179	MET
1	B	212	PRO
1	B	226	LEU
1	B	262	THR
1	B	277	LEU
1	B	302	LEU
1	B	349	LEU
1	B	362	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	27	ASN
1	A	28	ASN
1	A	114	ASN
1	A	186	GLN

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Mol	Chain	Res	Type
1	A	222	ASN
1	A	230	ASN
1	A	234	HIS
1	A	274	ASN
1	A	286	ASN
1	A	296	HIS
1	A	318	GLN
1	A	365	GLN
1	A	371	GLN
1	B	27	ASN
1	B	29	HIS
1	B	58	GLN
1	B	97	HIS
1	B	111	ASN
1	B	114	ASN
1	B	124	ASN
1	B	145	HIS
1	B	184	GLN
1	B	185	GLN
1	B	222	ASN
1	B	245	ASN
1	B	286	ASN
1	B	338	ASN
1	B	371	GLN
1	B	380	GLN

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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	ADP	B	400	2	28,29,29	1.20	2 (7%)	43,45,45	3.45	19 (44%)

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	ADP	B	400	2	-	1/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	ADP	PA-O3A	3.64	1.63	1.59
3	B	400	ADP	C5-C4	2.13	1.42	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	ADP	O2B-PB-O1B	-8.46	77.87	110.83
3	B	400	ADP	O2B-PB-O3A	8.24	132.26	104.64
3	B	400	ADP	O3B-PB-O2B	-6.86	82.07	107.80
3	B	400	ADP	O3B-PB-O3A	-6.81	81.79	104.64
3	B	400	ADP	O3A-PB-O1B	-6.36	77.55	111.04
3	B	400	ADP	O5'-PA-O1A	-5.27	88.06	108.94
3	B	400	ADP	C5-C4-N3	-5.22	119.53	126.72
3	B	400	ADP	N3-C2-N1	-4.68	121.50	128.58
3	B	400	ADP	N3-C4-N9	4.44	134.72	127.17
3	B	400	ADP	O3B-PB-O1B	4.40	127.98	110.83
3	B	400	ADP	O2A-PA-O3A	4.36	119.06	107.27
3	B	400	ADP	O2A-PA-O5'	-4.33	87.93	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	ADP	C2-N3-C4	3.75	120.99	111.83
3	B	400	ADP	C5-N7-C8	3.70	109.27	103.45
3	B	400	ADP	C4-C5-N7	-2.96	107.19	110.58
3	B	400	ADP	O4'-C4'-C3'	2.85	110.82	105.15
3	B	400	ADP	C3'-C2'-C1'	2.39	105.98	101.46
3	B	400	ADP	N9-C8-N7	-2.37	110.57	113.94
3	B	400	ADP	C5'-C4'-C3'	-2.09	107.68	115.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

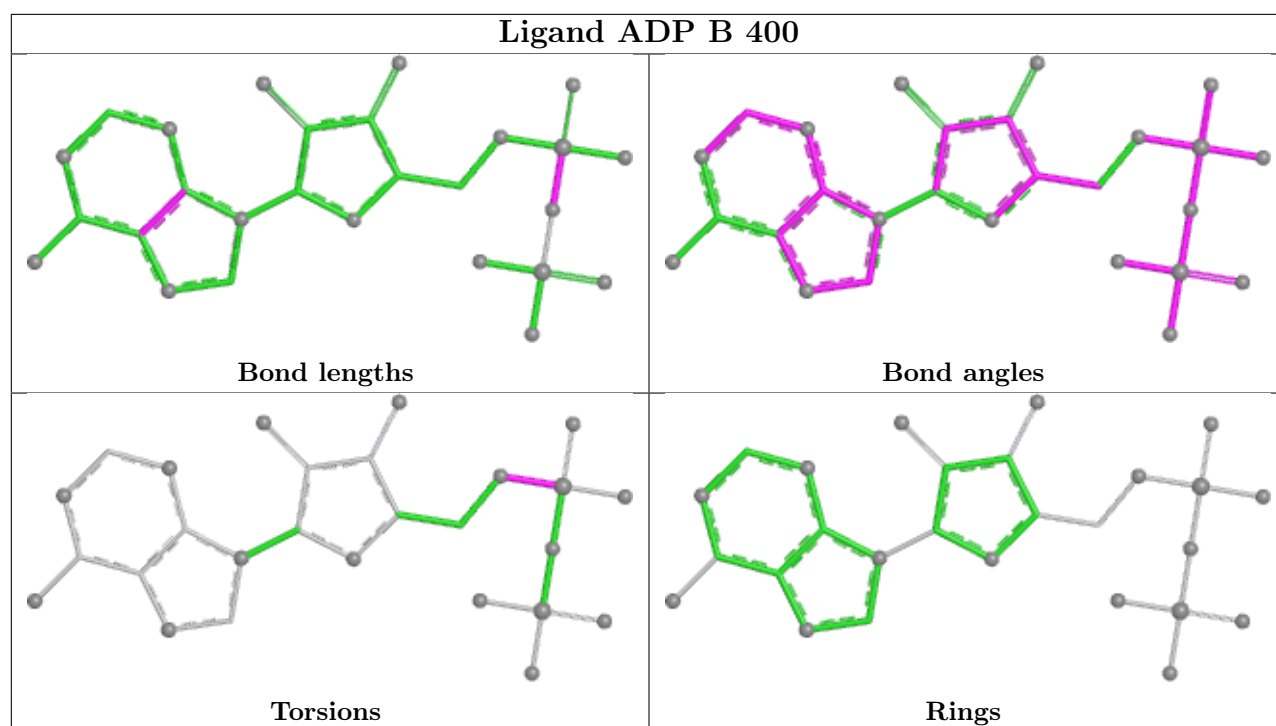
Mol	Chain	Res	Type	Atoms
3	B	400	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	376/381 (98%)	-0.23	4 (1%) 78 77	14, 23, 41, 65	0
1	B	376/381 (98%)	0.48	46 (12%) 8 7	15, 28, 74, 100	0
All	All	752/762 (98%)	0.13	50 (6%) 24 23	14, 25, 54, 100	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	ILE	7.7
1	B	376	LEU	7.6
1	B	372	ALA	6.6
1	B	381	LYS	6.6
1	B	377	MET	6.4
1	B	379	ALA	6.1
1	B	363	MET	6.1
1	A	68	TYR	5.8
1	B	359	LEU	5.5
1	B	380	GLN	5.1
1	B	378	PRO	4.9
1	B	367	LEU	4.6
1	A	69	ILE	4.3
1	B	368	GLU	4.3
1	B	308	PHE	3.7
1	B	371	GLN	3.6
1	B	299	LEU	3.6
1	B	366	ARG	3.6
1	B	370	GLY	3.6
1	B	302	LEU	3.5
1	B	369	GLN	3.5
1	B	315	LEU	3.4
1	B	305	HIS	3.2
1	B	356	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	375	ASP	3.0
1	B	304	LYS	3.0
1	B	374	ASP	3.0
1	B	307	LYS	2.9
1	A	66	HIS	2.9
1	B	311	VAL	2.9
1	B	364	GLU	2.8
1	B	314	ARG	2.6
1	B	357	VAL	2.6
1	B	303	GLY	2.6
1	B	310	GLU	2.5
1	B	340	ASP	2.5
1	B	115	LEU	2.3
1	B	330	VAL	2.3
1	B	313	LYS	2.3
1	B	309	SER	2.3
1	B	7	HIS	2.2
1	B	306	GLU	2.2
1	B	360	LEU	2.2
1	B	316	ARG	2.2
1	B	361	ILE	2.1
1	A	132	ARG	2.1
1	B	6	SER	2.0
1	B	116	GLN	2.0
1	B	312	LEU	2.0
1	B	318	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

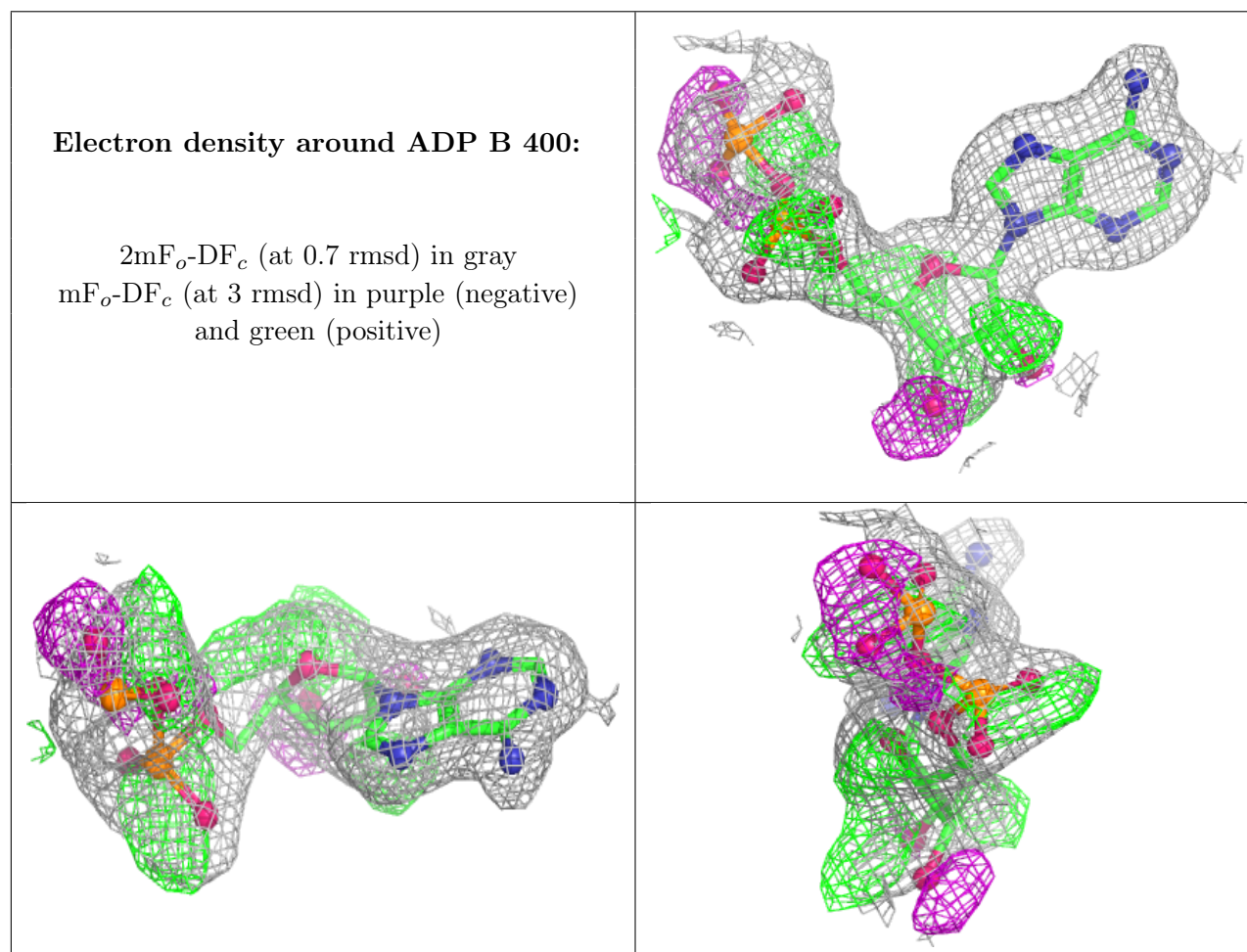
There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	ADP	B	400	27/27	0.83	0.16	29,37,50,54	0
2	MG	B	500	1/1	0.84	0.13	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.