



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:56 am GMT

PDB ID : 1F0J
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 4B2B
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Deposited on : 2000-05-16
Resolution : 1.77 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

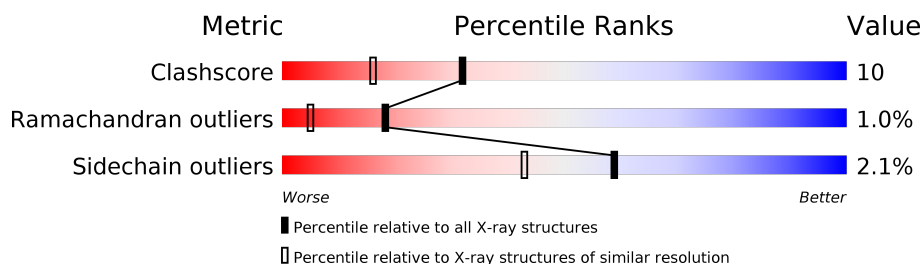
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6318 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 PHOSPHODIESTERASE 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2835	1787	482	545	21			
1	B	337	Total	C	N	O	S	0	0	0
			2719	1715	461	524	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	ALA	SER	ENGINEERED	UNP Q07343
A	489	ALA	SER	ENGINEERED	UNP Q07343
B	487	ALA	SER	ENGINEERED	UNP Q07343
B	489	ALA	SER	ENGINEERED	UNP Q07343

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	As 2	0	0
4	A	3	Total 3	As 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	415	Total 415	O 415	0	0
5	B	340	Total 340	O 340	0	0

Note EDS was not executed.

Chain A:

77% 15% 7%

Position 1: S162 (Lys), D419 (Asp), E423 (Glu), P430 (Pro), M431 (Met), C432 (Cys), D433 (Asp), K434 (Lys), H435 (His), T436 (Thr), I447 (Ile), D448 (Asp), Y449 (Tyr), I450 (Ile), V451 (Val), H452 (His), P453 (Pro), I469 (Ile), W479 (Trp), M483 (Met), I484 (Ile), Q485 (Gln), Q486 (Gln), A487 (Ala), Q488 (Gln), A489 (Ala), P490 (Pro), L491 (Leu), L492 (Leu), ASP (Asp), GLU (Glu), GLN (Gln), N496 (Asn), R497 (Arg), D498 (Asp), G501 (Gly), F506 (Phe), Q507 (Gln), F508 (Phe), GLU (Glu), LEU (Leu), THR (Thr), LEU (Leu), ASP (Asp), GLU (Glu), P396 (Pro), N395 (Asn), V383 (Val), D379 (Asp), Y377 (Tyr), N376 (Asn), D375 (Asp), L374 (Leu), L373 (Leu), T367 (Thr), E362 (Glu), V361 (Val), K358 (Lys), L357 (Leu), D356 (Asp), S348 (Ser), K336 (Lys), K328 (Lys), Q316 (Gln), K313 (Lys), E300 (Glu), M296 (Met), L295 (Leu), E263 (Glu), T260 (Thr), L237 (Leu), F181 (Phe), E171 (Glu), K168 (Lys), E161 (Glu), S154 (Ser), I163 (Ile), S162 (Lys).

Chain B:

Position	69%	19%	11%
1	Q486	A487	P488
2	ALA	PRO	PRO
3	PRO	PRO	PRO
4	LEU	LEU	LEU
5	ASP	ASP	ASP
6	GLN	GLN	GLN
7	GLU	GLU	GLU
8	ASN	ASN	ASN
9	ARG	ARG	ARG
10	ASP	ASP	ASP
11	CYS	CYS	CYS
12	GLN	GLN	GLN
13	GLY	GLY	GLY
14	LEU	LEU	LEU
15	MET	MET	MET
16	GLU	GLU	GLU
17	LYS	LYS	LYS
18	PHE	PHE	PHE
19	GLN	GLN	GLN
20	PHE	PHE	PHE
21	GLU	GLU	GLU
22	LEU	LEU	LEU
23	THR	THR	THR
24	ASP	ASP	ASP
25	GLU	GLU	GLU
26	GLY	GLY	GLY
27	ASP	ASP	ASP
28	GLY	GLY	GLY
29	SER	SER	SER
30	GLY	GLY	GLY
31	GLY	GLY	GLY
32	PRO	PRO	PRO
33	GLU	GLU	GLU
34	LYS	LYS	LYS
35	GLY	GLY	GLY
36	GLY	GLY	GLY
37	GLY	GLY	GLY
38	GLY	GLY	GLY
39	HIS	HIS	HIS
40	SER	SER	SER
41	S152	S153	S159
42	T160	E161	E162
43	E163	E163	E163
44	T180	T180	T180
45	T196	M196	M196
46	T197	T197	T197
47	A198	A198	A198
48	T199	T199	T199
49	F200	F200	F200
50	Q201	Q201	Q201
51	D204	D204	D204
52	K207	K207	K207
53	T208	T208	T208
54	F209	F209	F209
55	T217	T217	T217
56	M220	M220	M220
57	L237	L237	L237
58	T260	T260	T260
59	L295	L295	L295
60	E300	E300	E300
61	L326	L326	L326
62	K328	K328	K328
63	K399	K399	K399
64	Q350	Q350	Q350
65	A351	A351	A351
66	Q352	Q352	Q352
67	T333	T333	T333
68	M337	M337	M337
69	L364	L364	L364
70	A355	A355	A355
71	D356	D356	D356
72	L357	L357	L357
73	K358	K358	K358
74	T359	T359	T359
75	M360	M360	M360
76	V361	V361	V361
77	E362	E362	E362
78	T363	T363	T363
79	K364	K364	K364
80	T372	T372	T372
81	L373	L373	L373
82	M376	M376	M376
83	T377	T377	T377
84	D379	D379	D379
85	R380	R380	R380
86	L381	L381	L381
87	K382	K382	K382
88	L393	L393	L393
89	S394	S394	S394
90	M395	M395	M395
91	P396	P396	P396
92	T397	T397	T397
93	W406	W406	W406
94	T410	T410	T410
95	M411	M411	M411
96	E412	E412	E412
97	F415	F415	F415
98	Q416	Q416	Q416
99	Q417	Q417	Q417
100	G418	G418	G418
101	D419	D419	D419
102	K420	K420	K420
103	E421	E421	E421
104	R422	R422	R422
105	E423	E423	E423
106	P430	P430	P430
107	M431	M431	M431
108	K434	K434	K434
109	H435	H435	H435
110	T436	T436	T436
111	V439	V439	V439
112	E440	E440	E440
113	K441	K441	K441
114	F446	F446	F446
115	I447	I447	I447
116	V451	V451	V451
117	P453	P453	P453
118	D460	D460	D460

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.54Å 159.58Å 109.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.77	Depositor
% Data completeness (in resolution range)	95.3 (18.00-1.77)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.204 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6318	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ZN, ARS, 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	0.33	0/2893	0.54	0/3919
1	B	0.30	0/2776	0.54	0/3766
All	All	0.32	0/5669	0.54	0/7685

There are no bond length outliers.

There are no bond angle outliers.

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	2835	0	2750	46	1
1	B	2719	0	2643	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	415	0	0	10	0
5	B	340	0	0	7	0
All	All	6318	0	5393	107	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 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:B:356:ASP:HB3	1:B:382:GLN:NE2	1.84	0.93
1:B:356:ASP:HB3	1:B:382:GLN:HE21	1.35	0.91
1:B:300:GLU:HG2	5:B:1548:HOH:O	1.80	0.80
1:A:295:LEU:HG	5:A:1349:HOH:O	1.86	0.74
1:B:376:ASN:HD22	1:B:376:ASN:H	1.33	0.74
1:A:487:ALA:HB1	1:A:488:PRO:CD	2.19	0.72
1:B:397:THR:HB	1:B:469:ILE:HG23	1.72	0.71
1:A:397:THR:HB	1:A:469:ILE:HG23	1.72	0.71
1:A:496:ASN:ND2	1:A:497:ARG:H	1.88	0.70
1:B:159:ASN:HD21	1:B:162:ASN:HD22	1.39	0.70
1:A:154:SER:HB2	5:A:1615:HOH:O	1.92	0.69
1:B:159:ASN:HD21	1:B:162:ASN:ND2	1.91	0.68
1:A:435:HIS:O	1:A:436:THR:HG23	1.96	0.65
1:B:419:ASP:O	1:B:423:GLU:HG3	1.96	0.65
1:A:487:ALA:HB1	1:A:488:PRO:HD2	1.80	0.64
1:A:300:GLU:HG2	5:A:1611:HOH:O	1.96	0.64
1:B:295:LEU:O	1:B:295:LEU:HD23	1.98	0.64
1:A:496:ASN:HB3	1:A:501:GLY:HA3	1.80	0.63
1:A:419:ASP:O	1:A:423:GLU:HG3	1.99	0.63
1:A:485:PRO:O	1:A:487:ALA:N	2.32	0.63
1:B:376:ASN:HD22	1:B:376:ASN:N	1.96	0.63
1:A:296:MET:HE3	5:A:1437:HOH:O	2.01	0.61
1:A:152:SER:HB3	5:A:1615:HOH:O	2.00	0.60
1:A:412:GLU:O	1:A:416:GLN:HG3	2.02	0.59
1:B:485:PRO:O	1:B:487:ALA:N	2.36	0.59
1:B:412:GLU:O	1:B:416:GLN:HG3	2.02	0.59
1:B:376:ASN:ND2	1:B:376:ASN:H	1.99	0.59
1:A:395:ASN:HB2	1:A:396:PRO:HD3	1.85	0.58
1:B:160:THR:O	1:B:163:GLU:HB2	2.04	0.58
1:B:152:SER:HB3	1:B:217:ILE:CD1	2.33	0.58
1:A:181:PHE:CD1	1:A:237:LEU:HD21	2.40	0.57
1:A:484:ILE:O	1:A:485:PRO:C	2.43	0.56
1:B:395:ASN:HB2	1:B:396:PRO:HD3	1.87	0.56
1:B:430:PRO:O	1:B:431:MET:HB2	2.06	0.56
1:B:159:ASN:O	1:B:161:GLU:N	2.39	0.55
1:A:367:THR:HG22	1:A:373:LEU:HD21	1.89	0.53
1:B:260:THR:HG23	5:B:1370:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:HE3	5:A:1277:HOH:O	2.09	0.53
1:A:376:ASN:ND2	1:A:379:ASP:OD2	2.43	0.52
1:B:204:ASP:OD1	1:B:207:LYS:HD2	2.09	0.52
1:B:197:TYR:CE2	1:B:201:GLN:OE1	2.63	0.51
1:A:376:ASN:HD21	1:A:379:ASP:CG	2.14	0.51
1:B:328:LYS:O	1:B:332:GLN:HG3	2.10	0.51
1:B:152:SER:HB3	1:B:217:ILE:HD12	1.90	0.51
1:A:313:LYS:NZ	1:A:316:GLN:HE22	2.09	0.51
1:A:168:LYS:O	1:A:171:GLU:HG3	2.11	0.50
1:B:152:SER:N	5:B:1551:HOH:O	2.45	0.50
1:B:295:LEU:C	1:B:295:LEU:HD23	2.32	0.50
1:A:430:PRO:O	1:A:431:MET:HB2	2.12	0.49
1:B:195:ILE:O	1:B:199:ILE:HG13	2.12	0.49
1:B:373:LEU:HD23	5:B:1414:HOH:O	2.11	0.49
1:A:336:LYS:HE3	1:A:377:TYR:CZ	2.48	0.49
1:B:417:GLN:O	1:B:421:GLU:HG3	2.12	0.48
1:A:447:ILE:HA	1:A:451:VAL:HB	1.95	0.48
1:B:431:MET:HE1	5:B:1486:HOH:O	2.14	0.48
1:B:452:HIS:HB3	1:B:453:PRO:HD3	1.94	0.48
1:B:486:GLN:NE2	1:B:487:ALA:H	2.12	0.48
1:A:348:SER:HA	1:A:497:ARG:HG2	1.96	0.48
1:B:467:GLN:HG2	5:B:1324:HOH:O	2.14	0.47
1:B:376:ASN:ND2	1:B:379:ASP:OD2	2.38	0.47
1:B:485:PRO:O	1:B:486:GLN:C	2.52	0.47
1:B:393:LEU:HD22	1:B:446:PHE:HZ	1.79	0.47
1:B:354:LEU:HG	1:B:358:LYS:HE3	1.96	0.46
1:B:161:GLU:H	1:B:161:GLU:HG3	1.47	0.46
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.98	0.46
1:A:433:ASP:HB3	1:A:436:THR:OG1	2.16	0.46
1:B:327:THR:OG1	1:B:330:GLN:HG3	2.14	0.46
1:B:440:GLU:HG2	1:B:441:LYS:N	2.30	0.46
1:A:358:LYS:O	1:A:362:GLU:HG3	2.15	0.46
1:B:358:LYS:O	1:B:362:GLU:HG3	2.16	0.46
1:A:168:LYS:HE2	1:A:168:LYS:HB3	1.65	0.45
1:B:439:VAL:HG13	1:B:440:GLU:N	2.32	0.45
1:A:496:ASN:ND2	1:A:497:ARG:N	2.60	0.45
1:B:159:ASN:ND2	1:B:162:ASN:ND2	2.61	0.44
1:B:486:GLN:O	1:B:487:ALA:HB3	2.17	0.44
1:B:357:LEU:O	1:B:360:MET:HB3	2.17	0.44
1:A:260:THR:OG1	1:A:263:GLU:HG3	2.18	0.44
1:A:398:LYS:HD2	5:A:1601:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:HA	5:A:1336:HOH:O	2.18	0.44
1:A:357:LEU:O	1:A:361:VAL:HG23	2.17	0.44
1:A:181:PHE:CE1	1:A:237:LEU:HD21	2.52	0.44
1:B:160:THR:OG1	1:B:161:GLU:N	2.50	0.44
1:A:328:LYS:NZ	5:A:1610:HOH:O	2.36	0.43
1:B:415:PHE:CE2	1:B:434:LYS:HG2	2.53	0.43
1:B:440:GLU:HG2	1:B:441:LYS:H	1.82	0.43
1:A:449:TYR:CD2	1:A:506:PHE:HB3	2.54	0.43
1:B:364:LYS:HD2	1:B:372:LEU:HD21	2.00	0.43
1:A:435:HIS:O	1:A:436:THR:CG2	2.67	0.43
1:B:333:THR:O	1:B:337:MET:HG3	2.17	0.43
1:A:496:ASN:CG	1:A:497:ARG:H	2.22	0.42
1:A:152:SER:CA	5:A:1336:HOH:O	2.66	0.42
1:A:336:LYS:HE3	1:A:377:TYR:OH	2.20	0.42
1:A:374:LEU:HD11	1:A:383:VAL:HG21	2.01	0.42
1:B:196:MET:HG3	1:B:220:MET:CE	2.49	0.42
1:B:180:ILE:HG23	1:B:237:LEU:HD11	2.01	0.42
1:B:357:LEU:O	1:B:361:VAL:HG23	2.20	0.42
1:B:377:TYR:HA	1:B:380:ARG:HE	1.84	0.42
1:B:460:ASP:HA	5:B:1540:HOH:O	2.19	0.42
1:B:486:GLN:HB2	1:B:486:GLN:HE21	1.62	0.41
1:B:204:ASP:OD2	1:B:207:LYS:HD2	2.20	0.41
1:A:479:TRP:O	1:A:483:MET:HG2	2.21	0.41
1:B:416:GLN:O	1:B:420:LYS:HG3	2.21	0.41
1:B:447:ILE:HA	1:B:451:VAL:HB	2.02	0.41
1:A:313:LYS:HZ2	1:A:316:GLN:HE22	1.69	0.41
1:B:377:TYR:CA	1:B:380:ARG:HH21	2.34	0.41
1:B:209:PHE:CD1	1:B:326:LEU:HD22	2.56	0.40
1:B:406:TRP:O	1:B:410:ILE:HG13	2.21	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:154:SER:OG	1:A:154:SER:OG[4_566]	2.16	0.04

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	347/377 (92%)	330 (95%)	14 (4%)	3 (1%)	20	6
1	B	335/377 (89%)	322 (96%)	9 (3%)	4 (1%)	15	4
All	All	682/754 (90%)	652 (96%)	23 (3%)	7 (1%)	18	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLN
1	A	488	PRO
1	B	160	THR
1	B	486	GLN
1	A	436	THR
1	B	153	ILE
1	B	487	ALA

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	317/340 (93%)	311 (98%)	6 (2%)	62	48
1	B	305/340 (90%)	298 (98%)	7 (2%)	56	38
All	All	622/680 (92%)	609 (98%)	13 (2%)	59	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	SER
1	A	161	GLU
1	A	356	ASP
1	A	486	GLN
1	A	496	ASN
1	A	498	ASP
1	B	159	ASN
1	B	161	GLU
1	B	376	ASN
1	B	436	THR
1	B	464	PRO
1	B	467	GLN
1	B	486	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	332	GLN
1	A	382	GLN
1	A	496	ASN
1	B	162	ASN
1	B	201	GLN
1	B	376	ASN
1	B	382	GLN
1	B	435	HIS
1	B	463	GLN
1	B	486	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.